國 立 交 通 大 學

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碩 士 論 文

Simple digraph analogue of Brualdi-Hoffman-conjecture

簡 單 有 向 圖 的 布 勞 帝 - 賀 夫 曼 推 測

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摘要

在一有向圖中，若有向邊 ba 不屬於此圖之邊集合，則我們稱有向邊 ab 為單向。令 e 為一正整數，則存在唯一的正整數 s 及整數 t，使得 $e = s(s-1)+t$ 且 $0 \leq t \leq 2s-1$。本篇論文中，我們證明了當 e 滿足 $2s-7 \leq t \leq 2s-3$ 時且 t 不等於 0,1，在所有邊數為 e 的簡單有向圖中，擁有最大譜半徑的圖排除孤立點後即為 D。此圖 D 是由 s 個點的有向完全圖加上一個新的頂點 x 和新的 t 條邊，使頂點 x 與此完全圖中的 $\left\lfloor \frac{t}{2} \right\rfloor$ 個頂點相連且至多一個邊為單向所形成。

關鍵字: 譜半徑, 鄰接矩陣

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abstract

An arc ab is single-direction if ba is not an arc in a digraph. Let e be a positive integer. Then there is a unique pair (s, t) of integers such that $e = s(s-1) + t$, where s is positive and $0 \leq t \leq 2s-1$. For $2s-7 \leq t \leq 2s-3$ and $t \neq 0, 1$, we prove that the maximum spectral radius of a simple digraph D with e arcs and without isolated vertices is when D is obtained from complete digraph $\overleftrightarrow{K_s}$ by adding a new vertex x and t arcs, connecting x and $\lfloor \frac{t}{2} \rfloor$ vertices in $\overleftrightarrow{K_s}$ with at most one arc being single-direction.

Keywords: spectral radius, adjacency matrix

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Contents

1 Introduction

The digraphs in this thesis are simple without loops and without isolated vertices. Given a digraph D, the spectral radius of D is the spectral radius of its adjacency matrix, denoted by $\rho(D)$. Let e be a positive integer and let $\mathscr{D}(e)$ be the set of all simple digraphs with e arcs. The function $\rho(e)$ is defined to be the largest spectral radius of a digraph in $\mathscr{D}(e)$, that is

$$\rho(e) = \max\{\rho(D) \mid D \in \mathscr{D}(e)\}. \tag{1}$$

It is immediate from the above definitions that $\rho(0) = 0$, $\rho(1) = 0$, $\rho(2) = 1$ and $\rho(3) = 1$. Moreover, there are three non-isomorphic diagraphs with 3 arcs and spectral radius 1: (1) Adding a new vertex to a clique of order 2 and a single-direction arc from a vertex in the clique to the new vertex; (2) Adding a new vertex to a clique of order 2 and a single-direction arc from the new vertex to a vertex in the clique; (3) A directed cycle of order 3. Indeed their adjacency matrices (after suitable reordering of the vertices) are

$$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

Brualdi-Hoffman conjectured that the maximum spectral radius of a simple undirected graph with e edges is attained by adding a new vertex if necessary which is adjacent to the corresponding number of vertices of a complete graph and possibly adding some isolated vertices [2]. This conjecture was proved by Rowlinson in [6]. The following is the simple digraphs analogue of Brualdi-Hoffman-conjecture.

Conjecture 1.1. For integer $e \neq 3$, the maximum spectral radius of a simple digraph D with e arcs is when D is obtained from a clique by adding a new vertex if necessary and the corresponding number of arcs between the new vertex and some vertices in the clique with at most one arc being single-direction.

For a positive integer e, there is a unique pair (s, t) such that $e = s(s-1)+t$, where s is positive and $0 \le t \le 2s-1$. In 2015, Jin and Zhang [5] proved Conjecture 1.1 for the cases $t = 0, 1, 2s-2, 2s-1$ and $s > 4t^4+4$. In this paper, we prove Conjecture 1.1 for $2s-7 \le t \le 2s-3$ and $t \ne 0, 1$. Hence Conjecture 1.1 is solved for $e \le 21$ and remains open for $\sqrt[4]{\frac{s-4}{4}} \le t \le 2s-8$.

This thesis is organized as follows. In Section 2, we introduce notations used in this thesis and recall some basic concepts. In Section 3, we give a theorem that will be used in following sections. Section 4 gives some upper bounds of the spectral radius of the digraphs which we are concerned and we investigate properties of these bounds in Section 5. Section 6 talks about how we find $\rho(e)$ and characterize the extremal digraphs. To complementize, we also give a lower bound of the spectral radius of a digraph in Section 7.

2 Notation and Preliminaries

Let $[n] = \{1, 2, \dots, n\}$. Let D be a digraph with the vertex set $V(D) = [n]$ and the arc set $E(D) = \{ij \mid i \ne j \text{ and } i, j \in V(D)\}$. The *dual graph* D^t of D is the digraph with the vertex set $V(D)$ and arc set $E(D^t) = \{ji \mid ij \in E(D)\}$. The *adjacency matrix* $A(D) = (a_{ij})$ of D is defined by

$$a_{ij} = \begin{cases} 1, & \text{if } ij \in E(D); \\ 0, & \text{otherwise.} \end{cases}$$

The *spectral radius* of a square matrix A is defined by

$$\rho(A) = \max\{|\lambda| \mid \lambda \text{ is an eigenvalue of } A\}.$$

Recall that the spectral radius of a digraph D is the spectral radius of its adjacency matrix $A(D)$, denoted by $\rho(D)$. Note that the spectral radius $\rho(D)$ is independent of the ordering of the vertex set of D, and $\rho(D^t) = \rho(D)$. For a vertex $i \in V(D)$, the *out-degree*

d_i of i is defined to be the size of the set $\{j \mid ij \in E(D)\}$. A *clique* of order k in D is a subgraph that contains $k(k-1)$ arcs.

2.1 The set $\mathscr{D}^{**}(e)$

Let $\mathscr{D}^{**}(e)$ denote the set of all simple strongly connected digraphs with e arcs whose vertex set $[n]$ can be arranged such that

(i) If $ij \in E(D)$ then $i\ell \in E(D)$ for $\ell \leq j$ and $\ell \neq i$; and

(ii) $N^+(i) \setminus \{j\} \supseteq N^+(j) \setminus \{i\}$ for $1 \leq i < j \leq n$, where $N^+(i) = \{k \mid ik \in E(D)\}$.

As before let $e = s(s-1)+t$ and $0 \leq t \leq 2s-1$. Jin and Zhang [5, Proposition 2.5] showed that if $t \neq 1$ and $\rho(D) = \rho(e)$, then $D \in \mathscr{D}^{**}(e)$. Let $D \in \mathscr{D}^{**}(e)$ and the vertex set $V(D) = [n]$ be arranged to satisfy (i)-(ii) above. Since D is strongly connected, the out-degrees of 1 and n satisfy $d_1 = n-1$ and $d_n \geq 1$. Let k be the maximum integer such that the subgraph of D induced on $[k]$ is a clique. Then $d_i \geq k-1$ for $i \leq k$. Moreover, either $k = n$ or at least one of D and D^t whose vertex $k+1$ has out-degree $d_{k+1} \leq k-1$. The spectral radius $\rho(D)$ of the diagraph D satisfying $d_i \geq k-1$ for $i \leq k$ and

$$E(D) \cap ([n]-[k]) \times ([n]-[\ell]) = \emptyset, \tag{2}$$

where $\ell \leq k$ will be studied in Theorem 3.4.

3 The upper bound $\phi(k, \ell, e_1, e_2)$

For integers $1 \leq \ell \leq k < n$ and nonnegative integers d'_i with $i \in [k]$, the spectral radius of the following $n \times n$ matrix $C = (C_{ij})_{n\times n}$

$$C_{ij} = \begin{cases} 0, & \text{if } i = j \text{ or } (i,j) \in ([n]-[k]) \times ([n]-[\ell]); \\ d'_i - (n-1-k), & \text{if } 1 \leq i \leq k, j = n; \\ 1, & \text{otherwise.} \end{cases} \tag{3}$$

will serve as an upper bound of spectral radius in the main theorem of this section.

Remark 3.1. If $\ell < k$ then the matrix C in (3) has eigenvalue -1 with multiplicity $k-2$, eigenvalue 0 with multiplicity $n-k-1$ and the remaining three eigenvalues are the eigenvalues of the following matrix

$$\begin{pmatrix} \ell-1 & k-\ell & 1 \\ \ell & k-\ell-1 & 0 \\ \sum_{i=1}^{\ell} d_i' & \sum_{i=\ell+1}^{k} d_i' & 0 \end{pmatrix}, \tag{4}$$

whose characteristic polynomial is

$$f(\lambda) = \lambda^3 - (k-2)\lambda^2 - (e_1 + k - 1)\lambda - \ell e_2 + e_1(k-\ell-1), \tag{5}$$

where

$$e_1 = \sum_{i=1}^{\ell} d_i', \quad e_2 = \sum_{i=\ell+1}^{k} d_i'. \tag{6}$$

For the case $\ell = k$, the matrix C in (3) has eigenvalue -1 with multiplicity $k-1$, eigenvalue 0 with multiplicity $n-k-1zp$ and the remaining two eigenvalues are the eigenvalues of the following matrix

$$\begin{pmatrix} k-1 & 1 \\ \sum_{i=1}^{k} d_i' & 0 \end{pmatrix}, \tag{7}$$

whose characteristic polynomial is

$$f(\lambda) = \lambda^2 - (k-1)\lambda - e_1. \tag{8}$$

Since the matrices in (4) and (7) are nonnegative with an eigenvalue at least $k-1$, $\rho(C)$ is still the largest real eigenvalue of C and $\rho(C) = \rho(C+I) - 1$, despite that C is not necessarily nonnegative in general, where I is the $n \times n$ identity matrix.

Definition 3.2. Let $\phi(k, \ell, e_1, e_2)$ denote the spectral radius of the matrix C in (3), where $1 \leq \ell \leq k$ and $e_1, e_2 \geq 0$ are defined in (6).

Hence $\phi(k, \ell, e_1, e_2)$ is the maximum real root of the cubic polynomial in (5) if $\ell < k$, and $\phi(k, k, e_1, 0)$ is the maximum real root of the quadratic polynomial in (8).

Definition 3.3. For real matrices $M = (M_{ij})$ and $M' = (M'_{ij})$, we write $M \leq M'$ if $M_{ij} \leq M'_{ij}$ for all i, j.

Theorem 3.4. *Let D be a strongly connected digraph of order n such that there exists $1 \leq \ell \leq k < n$ with $E(D) \cap ([n] - [k]) \times ([n] - [\ell]) = \emptyset$. Let $A = A(D)$ and $C = (C_{ij})$ be as in (3) with*

$$d'_i := |\{j \in [n] - [k] \mid ij \in E(D)\}| \qquad (i \in [k])$$

Then $\rho(A) \leq \rho(C) = \phi(k, \ell, e_1, e_2)$. Moreover, $\rho(A) = \rho(C)$ if and only if $A_{ts} = C_{ts}$ for $1 \leq t \leq n$ and $1 \leq s \leq k$.

Proof. Let $Q = (Q_{ij})$ be the $n \times n$ matrix with

$$Q_{ij} = \begin{cases} 1, & \text{if } i = j \in [n] \text{ or } (i, j) \in ([n-1] - [k]) \times \{n\}; \\ 0, & \text{otherwise.} \end{cases}$$

Then the inverse of Q has entries

$$Q^{-1}_{ij} = \begin{cases} 1, & \text{if } i = j \in [n]; \\ -1, & \text{if } (i, j) \in ([n-1] - [k]) \times \{n\}; \\ 0, & \text{otherwise.} \end{cases}$$

Note that AQ (resp. CQ) has the same columns as A (resp. C) except that the last column of AQ (resp. CQ) is $(d'_1, d'_2, \ldots, d'_k, 0, \ldots, 0)^T$, which is the sum of the last $n - k$ columns of A (resp. C). Hence

$$AQ \leq CQ. \tag{9}$$

Note that $Q^{-1}(C + I)Q$ has the same first k rows and the same last row as $(C + I)Q$ has. The remaining $n - 1 - k$ rows of $Q^{-1}(C + I)Q$ are obtained by subtracting the last row from the corresponding row of $(C + I)Q$. Hence $Q^{-1}(C + I)Q$ is nonnegative. Then there exists a nonnegative and nonzero column vector $u = (u_1, u_2, \ldots, u_n)^T$ such that $Q^{-1}(C + I)Qu = \rho(C + I)u$, which implies $CQu = (\rho(C + I) - 1)Qu = \rho(C)u$. By (9) and since u is nonnegative,

$$AQu \leq CQu = \rho(C)Qu. \tag{10}$$

Since A is irreducible, there exists a positive row vector $v^T \neq 0$ such that $v^T A = \rho(A)v^T$. Multiplying v^T to the left of all terms in (10), we have

$$\rho(A)v^T Qu = v^T AQu \leq v^T CQu = \rho(C)v^T Qu. \tag{11}$$

Since Qu is nonnegative and v^T is positive, the term $v^T Qu$ is a positive. Delete $v^T Qu$ in both sides of (11) to obtain $\rho(A) \leq \rho(C)$ and finish the proof of the first part.

Suppose $\rho(A) = \rho(C)$. Then $v^T AQu = v^T CQu$ in (11). Since v^T is positive, $AQu = CQu$. Solving u from $Q^{-1}(C + I)Qu = \rho(C + I)u$, we find $u_i = 0$ for $i \in [n - 1] - [k]$ directly and $u_j > 0$ for $j \in [k] \cup \{n\}$ since $d'_1 > 0$. Hence $A_{ts} = (AQ)_{ts} = (CQ)_{ts} = C_{ts}$ for $(t, s) \in [n] \times [k]$.

Conversely, if $A_{ts} = C_{ts}$ for for $(t, s) \in [n] \times [k]$, then $AQu = CQu$, and inequality in (11) is equality, which implies $\rho(A) = \rho(C)$ as in the first part. $\square$

4 A partition of $\mathscr{D}^{**}(e)$

Let $e = s(s - 1) + t$ and $0 \leq t \leq 2s - 1$. We want to determine $\rho(e)$. By Jin and Zhang's result [5], for the case $t \neq 1$, it suffices to consider the digraphs in the set $\mathscr{D}^{**}(e)$. For $D \in \mathscr{D}^{**}(e)$, let $k = k(D)$ denote the largest integer c such that the subgraph of D induced on $[c]$ is a clique. Recall that $d_i = d_i(D)$ is the out-degree of node i in D. Note that $k = k(D) = k(D^t)$, and either $d_{k+1} \leq d_k$ or $d_{k+1} = d_k + 1 = k$ from the definition of k. Let $d_i^t := d_i(D^t)$, and we will use the notation

$$e_r = \sum_{i=k+1}^{n} d_i^t \ \text{ and } \ e_d = \sum_{i=k+1}^{n} d_i,$$

where n is the number of vertices of D. We assume $t \neq 0, 1$ and partition $\mathscr{D}^{**}(e)$ into six families:

$$\begin{aligned}
\mathscr{D}_1 &= \{D \in \mathscr{D}^{**}(e) \mid d_{k+1} \leq d_k \leq k-1, e_r < k-1 \text{ and } e_d < k-1\};\\
\mathscr{D}_2 &= \{D \in \mathscr{D}^{**}(e) \mid d_{k+1} \leq d_k \leq k-1, \text{ and } e_r \geq k-1 \text{ or } e_d \geq k-1\};\\
\mathscr{D}_3 &= \{D \in \mathscr{D}^{**}(e) \mid d_{k+1} = d_k + 1 = k, \text{ and } e_d \leq e_r\};\\
\mathscr{D}_4 &= \{D \in \mathscr{D}^{**}(e) \mid d_{k+1} = d_k + 1 = k, \text{ and } e_d > e_r\};\\
\mathscr{D}_5 &= \{D \in \mathscr{D}^{**}(e) \mid d^t_{k+1} = d^t_k + 1 = k, \text{ and } e_r \leq e_d\};\\
\mathscr{D}_6 &= \{D \in \mathscr{D}^{**}(e) \mid d^t_{k+1} = d^t_k + 1 = k, \text{ and } e_r > e_d\}.
\end{aligned}$$

The adjacency matrix of $D \in \mathscr{D}_i$ for $i \in [6]$ will be:

$$A(D) = \left(\begin{array}{c|c}
\begin{matrix} 0 & 1 & \cdots & 1 \\ 1 & 0 & & 1 \\ \vdots & & \ddots & \vdots \\ 1 & 1 & \cdots & 0 \end{matrix} & A_{12} \\
\hline
A_{21} & \begin{matrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{matrix}
\end{array}\right),$$

where there are e_r and e_d 1's in A_{12} and A_{21}, respectively.

Note that the condition $d_{k+1} \leq d_k \leq k-1$ is equivalent to $a_{k,k+1} = a_{k+1,k} = 0$, where $a_{p,q}$ is the entry of the adjacency matrix of D. Hence for $i \in [2]$, $D \in \mathscr{D}_i$ implies $D^t \in \mathscr{D}_i$. The condition $d_{k+1} = d_k + 1 = k$ and $e_d \leq e_r$ (resp. $e_d > e_r$) is equivalent to $d^t_{k+1} = d^t_k + 1 = k$ and $e_r \leq e_d$ (resp. $e_r > e_d$). Hence for $i \in \{3, 4\}$, $D \in \mathscr{D}_i$ if and only if $D^t \in \mathscr{D}_{i+2}$. For each family $\mathscr{D}_i$ and $D \in \mathscr{D}_i$, we apply Theorem 3.4 to get a suitable matrix C (in (3)) with $\rho(D) \leq \rho(C)$.

Lemma 4.1. *(i) Assume $D \in \mathscr{D}_1$. Then $k = s$. Moreover, if $V(D) = [s+1]$, then*

$\rho(D) = \phi(s, \ell, e_1, 0)$, *where*

$$\ell = \max(e_d, e_r), \quad e_1 = \min(e_d, e_r).$$

(ii) Assume $D \in \mathscr{D}_2$*. Then* $\rho(D) \leq \phi(k, k-1, e_1, 0)$*, where*

$$e_1 = \min(e_d, e_r).$$

Moreover, if $d_j = k-1$ *and* $e_1 = e_r$ *(or* $d_j^t = k-1$ *and* $e_1 = e_d$*) for any* $j \in [n] - [k]$*, then* $\rho(D) = \phi(k, k-1, e_1, 0)$*.*

(iii) Assume $D \in \mathscr{D}_3$ *(resp.* $D \in \mathscr{D}_5$*). Then* $\rho(D) \leq \phi(k, k-1, e_1, e_2)$*, where*

$$e_2 = d_k^t - k + 1, e_1 = -e_2 + e_d \quad (\text{resp. } e_2 = d_k - k + 1, e_1 = -e_2 + e_r).$$

(iv) Assume $D \in \mathscr{D}_4$ *(resp.* $D \in \mathscr{D}_6$*). Then* $\rho(D) \leq \phi(k, k, e_1, 0)$*, where*

$$e_1 = e_r \qquad (\text{resp. } e_1 = e_d).$$

Moreover, if $d_j = k$ *and* $e_1 = e_r$ *(or* $d_j^t = k$ *and* $e_1 = e_d$*) for any* $j \in [n] - [k]$*, then* $\rho(D) = \phi(k, k, e_1, 0)$*.*

Proof. We will use the property $\rho(D) = \rho(D^t)$ and apply Theorem 3.4 to the diagram D if $e_r \leq e_d$, and to the diagraph D^t otherwise. We define the matrix C in (3) by setting $k = k(D) = k(D^t)$ and ℓ in case (i) as claimed, $\ell = k-1$ in cases (ii)-(iii), and $\ell = k$ in case (iv). The last parameter d_i' is either $d_i - k + 1$ or $d_i^t - k + 1$ according to which D or D^t is applied. The lemma follows from Theorem 3.4 by the above setting. □

5 The shape of $\phi(k, \ell, e_1, e_2)$

Let $e = s(s-1) + t$ be a positive integer, where $0 \leq t \leq 2s - 1$ and $s \geq 1$. We want to determine the maximum value of $\phi(k, \ell, e_1, e_2)$ subject to $k(k-1) + \ell + e_1 + e_2 \leq e$ and $e_1 + e_2 \leq \left\lfloor \frac{e - k(k-1)}{2} \right\rfloor$. Hopefully this value is $\rho(e)$ and is when $k = s$, $e_2 = 0$ and $e_1 + \ell = t$. In this section we will investigate some properties of ϕ for each $\mathscr{D}_i$, where $i \in [6]$.

Lemma 5.1. *Assume $t \geq s-1$. Then*

$$\max\left\{\phi(k,k-1,e_1,0) \mid k\in[s], 0\leq e_1\leq \left\lfloor \frac{e-k(k-1)}{2}\right\rfloor\right\} = \phi\left(s,s-1,\left\lfloor\frac{t}{2}\right\rfloor,0\right).$$

Proof. From Definition 3.2, $\phi(k,k-1,e_1,0)$ is the maximum root of the function $f(\lambda)=\lambda^3-(k-2)\lambda^2-(e_1+k-1)\lambda$, which appears in (5) with $\ell=k-1$ and $e_2=0$. By the assumption, $e_1\leq\left\lfloor\frac{e-k(k-1)}{2}\right\rfloor$, and with equality and when $k=s$, we have $e_1=\left\lfloor\frac{t}{2}\right\rfloor$. Hence,

$$\begin{aligned}
\phi(k,k-1,e_1,0) =&\frac{(k-2)+\sqrt{(k-2)^2+4(e_1+k-1)}}{2}\\
=&\frac{(k-2)+\sqrt{k^2+4e_1}}{2}\\
\leq&\frac{(k-2)+\sqrt{k^2+4\left\lfloor\frac{e-k(k-1)}{2}\right\rfloor}}{2}\\
\leq&\frac{(s-2)+\sqrt{s^2+4\left\lfloor\frac{t}{2}\right\rfloor}}{2}\\
=&\phi\left(s,s-1,\left\lfloor\frac{t}{2}\right\rfloor,0\right),
\end{aligned}$$

where the second inequality follows from the increasing of its previous term as a function of k when $k\leq 1+\sqrt{e+\frac{1}{2}}$ and $k=s$ is in this range. □

Lemma 5.2. *Suppose $k\leq s-1\leq t, e_1+e_2\leq\frac{e-k(k-1)}{2}$ and $e_2\geq 1$. Then*

$$\phi(k,k-1,e_1,e_2)<\phi\left(k,k-1,\left\lfloor\frac{e-k(k-1)}{2}\right\rfloor,0\right).$$

Moreover,

$$max\{\phi(k,k-1,e_1,e_2)\}<\phi\left(s,s-1,\left\lfloor\frac{t}{2}\right\rfloor,0\right).$$

Proof. Let

$$\begin{aligned}
f(\lambda):=&\lambda^3-(k-2)\lambda^2-\left(\left\lfloor\frac{e-k(k-1)}{2}\right\rfloor+k-1\right)\lambda;\\
g(\lambda):=&\lambda^3-(k-2)\lambda^2-(e_1+k-1)\lambda-(k-1)e_2,
\end{aligned}$$

where

$$k \geq 1, e_1 + e_2 = \left\lfloor \frac{e - k(k-1)}{2} \right\rfloor \text{ and } e_2 \geq 1.$$

Consider the following function

$$f(\lambda) - g(\lambda) = \left(e_1 - \left\lfloor \frac{e - k(k-1)}{2} \right\rfloor \right) \lambda + (k-1)e_2 = e_2(k - 1 - \lambda),$$

which has a root $\alpha := k - 1$. And $f(\lambda)$ has the maximum real root:

$$\begin{aligned} \beta &:= \frac{(k-2) + \sqrt{(k-2)^2 + 4\left(\left\lfloor \frac{e-k(k-1)}{2} \right\rfloor + k - 1 \right)}}{2} \\ &= \frac{(k-2) + \sqrt{k^2 + 4\left\lfloor \frac{e-k(k-1)}{2} \right\rfloor}}{2} \\ &> \frac{(k-2) + k}{2} = k - 1 = \alpha, \end{aligned}$$

so $-g(\beta) = f(\beta) - g(\beta) < 0$ and $g(\beta) > 0$.

Since $f(\lambda) - g(\lambda)$ is linear and $g(\beta) > 0$, the maximum real root of $f(\lambda)$ is larger than $g(\lambda)$. On the other hand, the maximum real root of a cubic equation is increasing when the linear term and the constant term decrease, so $\phi(k, k-1, e_1, e_2)$ for $e_1 + e_2 \leq \frac{e-k(k-1)}{2}$ and $e_2 \geq 1$ has the maximum when $e_1 + e_2 = \left\lfloor \frac{e-k(k-1)}{2} \right\rfloor$. Recall that $\phi(k, k-1, e_1, e_2)$ for $e_1 + e_2 = \left\lfloor \frac{e-k(k-1)}{2} \right\rfloor$ is the maximum real root of $g(\lambda) = 0$, and $\phi\left(k, k-1, \left\lfloor \frac{e-k(k-1)}{2} \right\rfloor, 0\right)$ is the maximum real root of $f(\lambda) = 0$, we complete the proof of the first part. The second part immediately follows from the result of first part and Lemma 5.1

□

Lemma 5.3. *Suppose $t \geq s$. Then*

$$\max\left\{ \phi(k, k, e_1, 0) \mid k \in [s], 0 \leq e_1 \leq \left\lfloor \frac{e - k(k-1)}{2} \right\rfloor \right\} = \phi\left(s, s, \left\lfloor \frac{t}{2} \right\rfloor, 0 \right).$$

Proof. From Definition 3.2, $\phi(k, k, e_1, 0)$ is the maximum real root of the function $f(\lambda) = \lambda^2 - (k-1)\lambda - e_1$, which appears in (8). By the assumption, $e_1 \leq \left\lfloor \frac{e-k(k-1)}{2} \right\rfloor$, and with equality and when $k = s-1$, we have $e_1 = \left\lfloor \frac{t+2s-2}{2} \right\rfloor$. Hence

$$\begin{aligned}
\phi(k,k,e_1,0) =& \frac{(k-1)+\sqrt{(k-1)^2+4e_1}}{2} \\
\leq& \frac{(k-1)+\sqrt{(k-1)^2+4\left\lfloor \frac{e-k(k-1)}{2} \right\rfloor}}{2} \\
\leq& \frac{(s-2)+\sqrt{(s-2)^2+4\left\lfloor \frac{e-(s-1)(s-2)}{2} \right\rfloor}}{2} \\
=& \frac{(s-2)+\sqrt{(s-2)^2+4\left\lfloor \frac{t+2s-2}{2} \right\rfloor}}{2} \\
=& \phi\left(s-1, s-1, \left\lfloor \frac{t+2s-2}{2} \right\rfloor, 0\right),
\end{aligned}$$

where the second inequality follows from the increasing of its previous term as a function of k when $k \leq \sqrt{e+\frac{1}{2}}$ and $k = s-1$ is in this range.

On the other hand, for $k = s-1$ and $k = s$, define

$$\begin{aligned}
\alpha :=& \phi\left(s-1, s-1, \left\lfloor \frac{t+2s-2}{2} \right\rfloor, 0\right) = \frac{(s-2)+\sqrt{(s-2)^2+4\left\lfloor \frac{t+2s-2}{2} \right\rfloor}}{2}; \\
\beta :=& \phi\left(s, s, \left\lfloor \frac{t}{2} \right\rfloor, 0\right) = \frac{(s-1)+\sqrt{(s-1)^2+4\left\lfloor \frac{t}{2} \right\rfloor}}{2}.
\end{aligned}$$

Since

$$2(\beta-\alpha)(\beta+\alpha-s+2) = \sqrt{(s-1)^2+4\left\lfloor \frac{t}{2} \right\rfloor} - s + 1 > 0$$

and

$$\beta+\alpha = \frac{(s-1)+\sqrt{(s-1)^2+4\left\lfloor \frac{t}{2} \right\rfloor}}{2} + \frac{(s-2)+\sqrt{s^2+4\left\lfloor \frac{t}{2} \right\rfloor}}{2} > s-2,$$

so $\beta > \alpha$ and hence $\phi(k,k,e_1,0)$ reaches the maximum when $k = s$ and $e_1 = \left\lfloor \frac{t}{2} \right\rfloor$ □

Lemma 5.4. *We have*

$$\max\left\{\phi(s,\ell,e_1,0) \mid 1 \leq e_1 \leq \ell \leq s, \ell + e_1 = t\right\} = \phi\left(s, \left\lceil \frac{t}{2} \right\rceil, \left\lfloor \frac{t}{2} \right\rfloor, 0\right).$$

Proof. For $\ell \leq s-1$, recall that $\phi(s,\ell,e_1,0)$ is the maximum real root of the following function

$$\lambda^3 - (s-2)\lambda^2 - (e_1+s-1)\lambda + e_1(s-\ell-1),$$

and the maximum real root of a cubic polynomial with positive leading coefficient is increasing when the constant term decreases. Consider the constant term of this equation,

$$\begin{aligned} e_1(s-\ell-1) &= (e-s(s-1)-\ell)(s-\ell-1) \\ &= \ell^2+((s-1)^2-e)\ell+(s-1)t, \end{aligned}$$

which is a quadratic polynomial of ℓ and has the minimum value when $\ell = \frac{e-(s-1)^2}{2}$, so we can narrow down the range of ℓ to $\ell \in [\frac{e-s(s-1)}{2}, \frac{e-(s-1)^2}{2}]$.

Let (e_1, ℓ_1) and (e_2, ℓ_2) be two pairs which satisfy the condition of e_1 and ℓ above and assume $e_1 > e_2$ (and hence $1 \leq e_2 < e_1 \leq \ell_1 < \ell_2 \leq s-1$). Then we have two polynomials:

$$\begin{aligned} f(\lambda) &= \lambda^3-(s-2)\lambda^2-(e_1+s-1)\lambda+e_1(s-\ell_1-1), \\ g(\lambda) &= \lambda^3-(s-2)\lambda^2-(e_2+s-1)\lambda+e_2(s-\ell_2-1), \end{aligned}$$

and

$$f(\lambda)-g(\lambda) = (e_2-e_1)\lambda+(e_1-e_2)(s-1)+e_2\ell_2-e_1\ell_1.$$

Let λ_0 be the root of $f(\lambda)-g(\lambda)$, then

$$\begin{aligned} \lambda_0 &= \frac{(e_1-e_2)(s-1)+e_2\ell_2-e_1\ell_1}{(e_1-e_2)} \\ &= \frac{(e_1-e_2)(s-1)+(e_1-e_2)(e_1-\ell_2)}{(e_1-e_2)} \\ &= s-1+e_1-\ell_2 > 0. \end{aligned}$$

and then

$$\begin{aligned} f(\lambda_0) &= \lambda_0^3-(s-2)\lambda_0^2-(e_1+s-1)\lambda_0+e_1(s-\ell_1-1) \\ &= {\lambda_0}^2(e_1-\ell_2)+\lambda_0(e_1-\ell_2)-e_1(e_1-\ell_2+\ell_1) \\ &= {\lambda_0}^2(e_1-\ell_2)+\lambda_0(e_1-\ell_2)-e_1e_2 \ < \ 0. \end{aligned}$$

Since $f(\lambda_0) < 0$, the maximum real root α of $f(\lambda)$ is larger than λ_0. Then $f(\alpha)-g(\alpha) < 0$ and $g(\alpha) > 0$, hence the maximum real root of $g(\lambda)$ is less than $f(\lambda)$. And we have

$$\phi(s,\ell,e_1,0) \leq \phi\left(s, \left\lceil\frac{t}{2}\right\rceil, \left\lfloor\frac{t}{2}\right\rfloor, 0\right)$$

for $\ell \leq s-1$.

Moreover, if $t \geq s$, then $\phi(s,s,t-s,0) \leq \phi(s,\ell,e_1,0)$ and the equality holds when $t = 2s-1$, $\ell = s = \lceil \frac{t}{2} \rceil$ and $e_1 = s-1 = \lfloor \frac{t}{2} \rfloor$. So we conclude that for $1 \leq e_1 \leq \ell \leq s$ and $e_1 + \ell = t$, $\phi(s,\ell,e_1,0)$ has the maximum when $e_1 = \lfloor \frac{t}{2} \rfloor$ and $\ell = \lceil \frac{t}{2} \rceil$. $\square$

Lemma 5.5. *Let $e = s(s-1)+t$, $2s-7 \leq t \leq 2s-4$. Then*

(i) $\phi(k,k-1,e_1,0) \leq \phi(s,\lceil \frac{t}{2} \rceil,\lfloor \frac{t}{2} \rfloor,0)$ for $1 \leq k \leq s-1$ and $e_1 \leq \left\lfloor \frac{e-k(k-1)}{2} \right\rfloor$;

(ii) $\phi(k,k,e_1,0) \leq \phi(s,\lceil \frac{t}{2} \rceil,\lfloor \frac{t}{2} \rfloor,0)$ for $1 \leq k \leq s-2$ and $e_1 \leq \left\lfloor \frac{e-k(k-1)}{2} \right\rfloor$.

Proof. Let $\beta := \phi\left(s-1,s-2,\left\lfloor \frac{e-(s-1)(s-2)}{2} \right\rfloor,0\right)$, which is the maximum real root of

$$f(\lambda) = \lambda^3 - (s-3)\lambda^2 - \left(\left\lfloor \frac{t}{2} \right\rfloor + 2s - 3\right)\lambda.$$

Then

$$\beta = \frac{s-3+\sqrt{(s-3)^2+4(\lfloor \frac{t}{2} \rfloor + 2s-3)}}{2}.$$

Note that $\phi(s,\lceil \frac{t}{2} \rceil,\lfloor \frac{t}{2} \rfloor,0)$ is the maximum real root of

$$g(\lambda) = \lambda^3 - (s-2)\lambda^2 - (\left\lfloor \frac{t}{2} \right\rfloor + s - 1)\lambda + \left\lfloor \frac{t}{2} \right\rfloor (s - \left\lceil \frac{t}{2} \right\rceil - 1).$$

Consider the following equation:

$$f(\lambda) - g(\lambda) = \lambda^2 - (s-2)\lambda - \left\lfloor \frac{t}{2} \right\rfloor (s - \left\lceil \frac{t}{2} \right\rceil - 1)$$

which has the maximum real root

$$\alpha := \frac{s-2+\sqrt{(s-2)^2+4(\lfloor \frac{t}{2} \rfloor (s - \lceil \frac{t}{2} \rceil - 1))}}{2}.$$

Since $2s-7 \leq t \leq 2s-4$, then

$$\begin{aligned}
&4(\beta+\alpha-(s-3))(\beta-\alpha) \\
&= (2\beta-(s-3))^2 - (2\alpha-(s-3))^2 \\
&= 6s - 8 - 4\left\lfloor \frac{t}{2} \right\rfloor \left(s - \left\lceil \frac{t}{2} \right\rceil - 2\right) - 2\sqrt{(s-2)^2 + 4\left(\left\lfloor \frac{t}{2} \right\rfloor \left(s - \left\lceil \frac{t}{2} \right\rceil - 1\right)\right)} \\
&> 0.
\end{aligned}$$

Note that $\beta+\alpha > (s-3)$ and $(\beta+\alpha-(s-3))(\beta-\alpha) > 0$, so $\beta > \alpha$. Since $f(\lambda)-g(\lambda) > 0$ for $\lambda > \alpha$, we have

$$-g(\beta) = f(\beta) - g(\beta) > 0,$$

hence $g(\beta) < 0$ and the maximum real root of $g(\lambda)$ is larger than which of $f(\lambda)$. On the other hand,

$$\phi\left(s-1, s-2, \left\lfloor \frac{e-(s-1)(s-2)}{2} \right\rfloor, 0\right) = \phi\left(s-2, s-2, \left\lfloor \frac{e-(s-2)(s-3)}{2} \right\rfloor, 0\right).$$

Then by Lemma 5.1 and 5.3,

$$\max\left\{\phi(k, k-1, e_1, 0) \mid 1 \leq k \leq s-1, e_1 \leq \left\lfloor \frac{e-k(k-1)}{2} \right\rfloor\right\} \leq \phi\left(s, \left\lceil \frac{t}{2} \right\rceil, \left\lfloor \frac{t}{2} \right\rfloor, 0\right),$$

and

$$\max\left\{\phi(k, k, e_1, 0) \mid 1 \leq k \leq s-2, e_1 \leq \left\lfloor \frac{e-k(k-1)}{2} \right\rfloor\right\} \leq \phi\left(s, \left\lceil \frac{t}{2} \right\rceil, \left\lfloor \frac{t}{2} \right\rfloor, 0\right),$$

for $2s-7 \leq t \leq 2s-4$. □

6 $\rho(D)$ for $2s-7 \leq t \leq 2s-3$, $t \neq 0, 1$

For $D \in \mathscr{D}^{**}(e)$, Lemma 4.1 showed that ϕ is an upper bound of $\rho(D)$, and we have investigated some properties for ϕ in Section 5: Lemma 5.1 and 5.3 showed that ϕ is increasing as a function of k when D is in $\mathscr{D}_2$ and $\mathscr{D}_4 \cup \mathscr{D}_6$, respectively; Lemma 5.2 showed that ϕ of $D \in \mathscr{D}_3 \cup \mathscr{D}_5$ is less than which of $D \in \mathscr{D}_2$; Lemma 5.4 showed that ϕ has the maximum when $\ell - e_1 \leq 1$ for $k(D) = s$. Now we use these upper bounds to prove Conjecture 1.1 for $e = s(s-1)+t$, where $2s-7 \leq t \leq 2s-3$, $t \neq 0, 1$.

Fix $e = s(s-1)+t$ for $2 \leq t \leq 2s-1$, define D^* to be the digraph which is obtained from a clique of order s by adding a new vertex and t arcs from the new vertex to the clique with at most one arc being single-direction which is pointing to the clique.

Lemma 6.1. *Let $e = s(s-1)+t$ be a positive integer with $2 \leq t \leq 2s-1$. Then for any digraph D in $\mathscr{D}^{**}(e)$ with $k(D) = s$, we have $\rho(D) \leq \rho(D^*)$ and equality holds if and only if $D \in \{D^*, D^{*t}\}$.*

Proof. Let ℓ' (resp. e_1') denote the number of arcs in D which are from $\{s+1\}$ to $[s]$ (resp. from $[s]$ to $\{s+1\}$). And we might assume $\ell' \geq e_1'$ by considering D^t if necessary. Let ℓ (resp. e_1) denote the number of arcs from $V(D)-[s]$ to $[s]$ (resp. from $[s]$ to $V(D)-[s]$). Note that $\ell' \leq \ell$, $e_1' \leq e_1$ and $\ell + e_1 = t$ since $k(D) = s$. Then by Lemma 5.4,

$$\rho(D) \leq \phi(s, \ell', e_1, 0) \leq \phi(s, \ell, e_1, 0) \leq \rho(D^*).$$

Note that $\ell = \ell'$ if and only if $D = D^*$ since the diagraphs are strongly connected. □

Theorem 6.2. *Let $e = s(s-1)+t$ be a positive integer with $t = 2s-3$ and $t \neq 1$. Then $\rho(e) = \frac{(s-2)+\sqrt{(s+2)^2-12}}{2}$. Moreover, for $D \in \mathscr{D}(e)$, $\rho(D) = \rho(e)$ if and only if $D \in \{D^*, D^{*t}\}$.*

Proof. Since $e = s(s-1)+2s-3$ and $s \neq 2$, $\mathscr{D}_1 = \emptyset$. For a digraph in $\mathscr{D}_2$, the maximum upper bound $\phi\left(s, s-1, \left\lfloor \frac{e-s(s-1)}{2} \right\rfloor, 0\right)$ can be attained by D^* since $s-1 = \lceil \frac{t}{2} \rceil$. And by Lemma 5.2, $\rho(D) < \phi\left(s, s-1, \left\lfloor \frac{e-s(s-1)}{2} \right\rfloor, 0\right) = \rho(D^*)$ for $D \in \mathscr{D}_3 \cup \mathscr{D}_5$. On the other hand, for the digraph in $\mathscr{D}_4 \cup \mathscr{D}_6$ with clique number $k = s-1$, the maximum upper bound $\phi\left(s-1, s-1, \left\lfloor \frac{e-(s-1)(s-2)}{2} \right\rfloor, 0\right)$ is equal to $\phi\left(s, s-1, \left\lfloor \frac{e-s(s-1)}{2} \right\rfloor, 0\right) = \rho(D^*)$ (notice that this upper bound can't be attained by the digraph in $\mathscr{D}_4 \cup \mathscr{D}_6$). Then by Lemma 5.3 and 6.1, $\rho(D) < \rho(D^*)$ for $D \in \mathscr{D}_4 \cup \mathscr{D}_6$.

Hence $\rho(D) \leq \rho(D^*) = \frac{(s-2)+\sqrt{(s+2)^2-12}}{2}$ for D with e arcs, where $e = s(s-1)+2s-3$, $t \neq 0, 1$. That is, $\rho(e) = \frac{(s-2)+\sqrt{(s+2)^2-12}}{2}$. Moreover, by Theorem 3.4, $\rho(D) = \rho(e) = \frac{(s-2)+\sqrt{(s+2)^2-12}}{2}$ if and only if $D \in \{D^*, D^{*t}\}$.

□

Let $e = s(s-1)+t$, for $2s-7 \leq t \leq 2s-4$, $t \neq 0, 1$. Then by Lemmas 5.2, 5.5 and 6.1, we only need to consider D^* and the digraphs $D \in \mathscr{D}_4 \cup \mathscr{D}_6$, with $k(D) = s-1$ for this problem. On the other hand, according to the proof of [5, Lemma 3.2], they showed that when $k(D) = s$, we may assume that $\mid V(D) \mid = s+1$, and we can also prove the same result for $k(D) = s-1$ by a similar proof. So for the following four theorems, we only consider the digraphs with $s+1$ vertices.

Theorem 6.3. *Let $e = s(s-1)+t$ be a positive integer with $t = 2s-4$ and $t \neq 0$. Then $\rho(e) = \phi(s, s-2, s-2, 0)$, i.e. $\rho(e)$ is equal to the maximum real root of*

$$\lambda^3 - (s-2)\lambda^2 - (2s-3)\lambda + (s-2).$$

Moreover for $D \in \mathscr{D}(e)$, $\rho(D) = \rho(e)$ if and only if $D \in \{D^*, D^{*t}\}$.

Proof. The digraph $D \in \mathscr{D}_4 \cup \mathscr{D}_6$ with $k(D) = s-1$ and $\mid V(D) \mid = s+1$ is unique, which has the spectral radius $\rho(D) = \phi(s-1, s-1, 2s-4, 0)$. Recall that $\rho(D)$ is the maximum real root of

$$f(\lambda) = \lambda^2 - (s-2)\lambda - (2s-4),$$

and $\phi\left(s, \left\lceil \frac{t}{2} \right\rceil, \left\lfloor \frac{t}{2} \right\rfloor, 0\right) = \phi(s, s-2, s-2, 0)$ is the maximum real root of

$$g(\lambda) = \lambda^3 - (s-2)\lambda^2 - (2s-3)\lambda + (s-2).$$

Consider the following function

$$\lambda f(\lambda) - g(\lambda) = \lambda - (s-2)$$

which has the root $s-2$. Since $s > 1$, $s-2 \leq \rho(D)$. Then $-g(\rho(D)) = \rho(D)f(\rho(D)) - g(\rho(D)) > 0$ and $g(\rho(D)) < 0$, hence $\phi(s, s-2, s-2, 0) > \rho(D)$. We conclude that for $D \in \mathscr{D}(e)$, $\rho(D) \leq \phi(s, s-2, s-2, 0)$. Moreover, by Theorem 3.4 $\rho(D) = \phi(s, s-2, s-2, 0) = \rho(e)$ if and only if $D \in \{D^*, D^{*t}\}$. □

Definition 6.4. Let $A^{(i)}$ denote an $(s-1)$-dimensional column vector with the first i entries be 1, and 0 otherwise. Let $A_{(j)}$ denote an $(s-1)$-dimensional row vector with the first j entries be 1, and 0 otherwise.

Theorem 6.5. *Let $e = s(s-1)+t$ be a positive integer with $t = 2s-5$ and $t \neq 1$. Then $\rho(e) = \phi(s, s-2, s-3, 0)$, i.e. $\rho(e)$ is the maximum real root of*

$$\lambda^3 - (s-2)\lambda^2 - (2s-4)\lambda + (s-3).$$

Moreover for $D \in \mathscr{D}(e)$, $\rho(D) = \rho(e)$ if and only if $D \in \{D^*, D^{*t}\}$.

Proof. There are two non-isomorphic digraphs D_1, D_2 in $\mathscr{D}_4 \cup \mathscr{D}_6$ with $k(D_1), k(D_2) = s-1$ and $\mid V(D_1) \mid = \mid V(D_2) \mid = s+1$, where

$$A(D_1) = \begin{pmatrix} J_{s-1} - I_{s-1} & A^{(s-2)} & A^{(s-3)} \\ A_{(s-1)} & 0 & 0 \\ A_{(s-1)} & 0 & 0 \end{pmatrix}, \quad A(D_2) = \begin{pmatrix} J_{s-1} - I_{s-1} & A^{(s-2)} & A^{(s-2)} \\ A_{(s-1)} & 0 & 0 \\ A_{(s-2)} & 0 & 0 \end{pmatrix}.$$

Moreover,

$$\rho(D_1) = \phi(s-1, s-1, 2s-5, 0)$$
$$\rho(D_2) = \phi(s-1, s-2, 2s-4, 1),$$

Compare $\rho(D^*)$, $\rho(D_1)$ and $\rho(D_2)$. Recall that $\rho(D^*)$, $\rho(D_1)$ and $\rho(D_2)$ are the maximum real roots of $f(\lambda)$, $g(\lambda)$ and $h(\lambda)$, respectively, where

$$f(\lambda) = \lambda^3 - (s-2)\lambda^2 - (2s-4)\lambda + (s-3);$$
$$g(\lambda) = \lambda^2 - (s-2)\lambda - (2s-5);$$
$$h(\lambda) = \lambda^3 - (s-3)\lambda^2 - (3s-6)\lambda - (s-2).$$

For $\rho(D^*)$ and $\rho(D_1)$, consider the following equation

$$f(\lambda) - \lambda g(\lambda) = -\lambda + (s-3) = 0,$$

which has a root $s-3$ and $\rho(D_1) > s-3$. Then $f(\rho(D_1)) - \rho(D_1)g(\rho(D_1)) < 0$ and $f(\rho(D_1)) < 0$. Hence $\rho(D^*) > \rho(D_1)$.

For $\rho(D^*)$ and $\rho(D_2)$, consider the following function

$$f(\lambda) - h(\lambda) = -\lambda^2 + (s-2)\lambda + (2s-5),$$

which has the same maximum real root as $g(\lambda)$, i.e. such a maximum real root is equal to $\rho(D_1)$. So $f(\lambda) - h(\lambda) < 0$ for $\lambda > \rho(D_1)$. Since $\rho(D^*) > \rho(D_1)$, $f(\rho(D^*)) - h(\rho(D^*)) < 0$ and $h(\rho(D^*)) > 0$. Hence the maximum real root $\rho(D_2)$ of $h(\lambda)$ is less than $\rho(D^*)$. We conclude that for $D \in \mathscr{D}(e)$, $\rho(D) \leq \rho(D^*) = \phi(s, s-2, s-3, 0)$. Moreover, by Theorem 3.4 $\rho(D) = \phi(s, s-2, s-3, 0) = \rho(e)$ if and only if $D \in \{D^*, D^{*t}\}$. □

Theorem 6.6. *Let $e = s(s-1)+t$ be a positive integer with $t = 2s-6$ and $t \neq 0$. Then $\rho(e) = \phi(s, s-3, s-3, 0)$, i.e. $\rho(e)$ is the maximum real root of the following function*

$$\lambda^3 - (s-3)\lambda^2 - (2s-4)\lambda + 2(s-3).$$

Moreover, for $D \in \mathscr{D}(e)$, $\rho(D) = \rho(e)$ if and only if $D \in \{D^*, D^{*t}\}$.

Proof. Assume that all of the digraphs have $s+1$ vertices, then there are three non-isomorphic digraphs D_1, D_2 and D_3 in $\mathscr{D}_4 \cup \mathscr{D}_6$ with $k(D_1), k(D_2), k(D_3) = s-1$, where

$$A(D_1) = \begin{pmatrix} J_{s-1} - I_{s-1} & A^{(s-2)} & A^{(s-4)} \\ A_{(s-1)} & 0 & 0 \\ A_{(s-1)} & 0 & 0 \end{pmatrix}, \quad A(D_2) = \begin{pmatrix} J_{s-1} - I_{s-1} & A^{(s-3)} & A^{(s-3)} \\ A_{(s-1)} & 0 & 0 \\ A_{(s-1)} & 0 & 0 \end{pmatrix},$$

$$A(D_3) = \begin{pmatrix} J_{s-1} - I_{s-1} & A^{(s-2)} & A^{(s-3)} \\ A_{(s-1)} & 0 & 0 \\ A_{(s-2)} & 0 & 0 \end{pmatrix},$$

and

$$\rho(D_1) = \rho(D_2) = \phi(s-1, s-1, 2s-6, 0) = \frac{s-2+\sqrt{(s+2)^2-24}}{2}.$$

Compare $\rho(D^*)$ and $\rho(D_1)$, and recall that $\rho(D^*) = \phi(s, s-3, s-3, 0)$ and $\rho(D_1) = \phi(s-1, s-1, 2s-6, 0)$ are the maximum real roots of $f(\lambda)$ and $g(\lambda)$, respectively, where

$$f(\lambda) = \lambda^3 - (s-2)\lambda^2 - (2s-4)\lambda + 2(s-3);$$
$$g(\lambda) = \lambda^2 - (s-2)\lambda - (2s-6).$$

Consider the following function

$$f(\lambda) - \lambda g(\lambda) = -2\lambda + (2s-6) = 0,$$

which has the root $s-3$ and for $\lambda > s-3$, $f(\lambda) - \lambda g(\lambda) < 0$. Since $\rho(D_1) > s-3$, $f(\rho(D_1)) < 0$ and hence $\rho(D_1)$ is less than the maximum real root of $f(\lambda) = 0$, i.e. $\rho(D_1) < \rho(D^*)$.

Next, we compare $\rho(D^*)$ and $\rho(D_3)$. The adjacency matrix of D^* is

$$A(D^*) = \begin{pmatrix} J_{s-1} - I_{s-1} & A^{(s-1)} & A^{(s-3)} \\ A_{(s-1)} & 0 & 0 \\ A_{(s-3)} & 0 & 0 \end{pmatrix}.$$

Since $A(D^*)$ and $A(D_3)$ are nonnegative and irreducible, by Perron-Frobenius theorem, there exist a positive column vector $u = (u_1, u_2, \ldots, u_{s+1})^T$ and a positive row vector $v^T = (v_1, v_2, \ldots, v_{s+1})$ such that $A(D_3)u = \rho(D_3)u$ and $v^T A(D^*) = \rho(D^*)v^T$. Then

$$\begin{aligned}(\rho(D^*) - \rho(D_3))v^T u =& v^T(A(D^*) - A(D_3))u \\ =& v^T \begin{pmatrix} 0 & A^{(s-1)} - A^{(s-2)} & 0 \\ 0 & 0 & 0 \\ A^{(s-3)} - A^{(s-2)} & 0 & 0 \end{pmatrix} u \\ =& u_s v_{s-1} - u_{s-2} v_{s+1} \\ =& u_s(v_{s-1} - v_{s+1}) > 0,\end{aligned}$$

so $\rho(D^*) - \rho(D_3) > 0$, and hence $\rho(D^*) > \rho(D_3)$. We conclude that for $D \in \mathscr{D}(e)$, $\rho(D) \leq \rho(D^*) = \phi(s, s-3, s-3, 0)$. Moreover, by Theorem 3.4, $\rho(D) = \phi(s, s-3, s-3, 0) = \rho(e)$ if and only if $D \in \{D^*, D^{*t}\}$. □

Theorem 6.7. *Let $e = s(s-1) + t$ be a positive integer with $t = 2s - 7$ and $t \neq 1$. Then $\rho(e) = \phi(s, s-3, s-4, 0)$, i.e. $\rho(e)$ is the maximum real root of the following function*

$$\lambda^3 - (s-2)\lambda^2 - (2s-5)\lambda + 2(s-4).$$

Moreover, for $D \in \mathscr{D}(e)$, $\rho(D) = \rho(e)$ if and only if $D \in \{D^*, D^{*t}\}$.

Proof. Assume that all of the digraphs have $s + 1$ vertices, then there are five non-isomorphic digraphs D_1, D_2, D_3, D_4 and D_5 in $\mathscr{D}_5 \cup \mathscr{D}_6$ with $k(D_1), k(D_2), k(D_3), k(D_4), k(D_5) =$

$s-1$, where

$$A(D_1)=\begin{pmatrix} J_{s-1}-I_{s-1} & A^{(s-2)} & A^{(s-5)} \\ A_{(s-1)} & 0 & 0 \\ A_{(s-1)} & 0 & 0 \end{pmatrix},\quad A(D_2)=\begin{pmatrix} J_{s-1}-I_{s-1} & A^{(s-3)} & A^{(s-4)} \\ A_{(s-1)} & 0 & 0 \\ A_{(s-1)} & 0 & 0 \end{pmatrix},$$

$$A(D_3)=\begin{pmatrix} J_{s-1}-I_{s-1} & A^{(s-2)} & A^{(s-4)} \\ A_{(s-1)} & 0 & 0 \\ A_{(s-2)} & 0 & 0 \end{pmatrix},\quad A(D_4)=\begin{pmatrix} J_{s-1}-I_{s-1} & A^{(s-3)} & A^{(s-3)} \\ A_{(s-1)} & 0 & 0 \\ A_{(s-2)} & 0 & 0 \end{pmatrix},$$

$$A(D_5)=\begin{pmatrix} J_{s-1}-I_{s-1} & A^{(s-2)} & A^{(s-3)} \\ A_{(s-1)} & 0 & 0 \\ A_{(s-3)} & 0 & 0 \end{pmatrix},$$

and

$$\rho(D_1)=\rho(D_2)=\phi(s-1,s-1,2s-7,0)=\frac{s-2+\sqrt{(s+2)^2-28}}{2}.$$

Compare $\rho(D^*)$ and $\rho(D_1)$, and recall that $\rho(D^*)=\phi(s,s-3,s-4,0)$ and $\rho(D_1)=\phi(s-1,s-1,2s-7,0)$ are the maximum real roots of $f(\lambda)$ and $g(\lambda)$, respectively, where

$$\begin{aligned} f(\lambda)=&\lambda^3-(s-2)\lambda^2-(2s-5)\lambda+2(s-4); \\ g(\lambda)=&\lambda^2-(s-2)\lambda-(2s-7). \end{aligned}$$

Consider the following function

$$f(\lambda)-\lambda g(\lambda)=-2\lambda+(2s-8),$$

which has the root $s-4$ and for $\lambda>s-4$, $f(\lambda)-\lambda g(\lambda)<0$. Since $\rho(D_1)>s-4$, $f(\rho(D_1))<0$ and hence $\rho(D_1)$ is less than the maximum real root of $f(\lambda)=0$, i.e. $\rho(D_1)<\rho(D^*)$.

Next, we compare $\rho(D_4)$ with $\rho(D_5)$. Since $A(D_4)$ and $A(D_5)$ are nonnegative and irreducible, there exist a positive column vectors y and a positive row vector x^T such that $A(D_4)y=\rho(D_4)y$, $A(D_5)x=x^T\rho(D_5)$. Then

$$(\rho(D_5)-\rho(D_4))x^Ty=x^T(A(D_5)-A(D_4))y>0$$

and hence $\rho(D_5) > \rho(D_4)$.

Finally, we discuss $\rho(D_3)$, $\rho(D_5)$ and $\rho(D^*)$. The adjacency matrix of D^* is

$$A(D^*) = \begin{pmatrix} J_{s-1} - I_{s-1} & A^{(s-1)} & A^{(s-4)} \\ A_{(s-1)} & 0 & 0 \\ A_{(s-3)} & 0 & 0 \end{pmatrix}.$$

Since $A(D_3)$, $A(D_5)$ and $A(D^*)$ are nonnegative and irreducible, by Perron-Frobenius theorem, there exist two positive column vectors u, w and two positive row vectors v^T, z^T such that $A(D_3)u = \rho(D_3)u$, $A(D_5)w = \rho(D_5)w$ and $v^T A(D^*) = \rho(D^*)v^T$. Then

$$\begin{aligned}(\rho(D^*) - \rho(D_3))v^T u =& v^T(A(D^*) - A(D_3))u > 0;\\ (\rho(D^*) - \rho(D_5))v^T w =& v^T(A(D^*) - A(D_5))w > 0,\end{aligned}$$

so $\rho(D^*) - \rho(D_3) > 0$ and $\rho(D^*) - \rho(D_5) > 0$, and hence $\rho(D^*) > \rho(D_3)$ and $\rho(D^*) > \rho(D_5)$. We conclude that for $D \in \mathscr{D}(e)$, $\rho(D) \leq \rho(D^*) = \phi(s, s-3, s-4, 0)$. Moreover, by Theorem 3.4 $\rho(D) = \phi(s, s-3, s-4, 0) = \rho(e)$ if and only if $D \in \{D^*, D^{*t}\}$. □

7 A lower bound of the spectral radius of the digraph in $\mathscr{D}^{**}(e)$

Definition 7.1. Let B be an $n \times n$ matrix and let $\Pi = \{\pi_1, \pi_1, \ldots, \pi_k\}$ be a partition of $[n]$. Let $B_{a,b}$ be the $|\pi_a| \times |\pi_b|$ submatrix of B formed by the rows in π_a and the columns in π_b, where $1 \leq a, b \leq k$. The $k \times k$ matrix $\Pi(B) := (\pi_{ab})$, where π_{ab} is the average row sum of $B_{a,b}$, is called the *quotient* matrix of B with respect to Π.

With the notation in Definition 7.1, we can write $\Pi(B)$ as

$$\Pi(B) = (S^T S)^{-1} S^T B S,$$

where $S = (s_{ij})$ is an $n \times k$ matrix with

$$s_{ij} = \begin{cases} 1, & \text{if } i \in \pi_j; \\ 0, & \text{otherwise.} \end{cases}$$

It is known that $\rho(\Pi(A)) \leq \rho(A)$ for any symmetric matrix A. For particular types of partition Π and non-symmetric matrix A, we have the following similar result.

Theorem 7.2. *Let $D \in \mathscr{D}^{**}(e)$ with the adjacency matrix A and let $\Pi = \{\{1\}, \{2\}, \ldots, \{k\}, \{k+1, \ldots, n\}\}$ be a partition of $[n]$, where k is the clique number of D. Then $\rho(\Pi(A)) \leq \rho(A)$, where $\Pi(A)$ is the quotient matrix of A with respect to Π.*

Proof. Since $\Pi(A)$ is the quotient matrix of A with respect to Π, $\Pi(A)$ is a $(k+1)\times(k+1)$ matrix and

$$\Pi(A) = (S^T S)^{-1} S^T A S, \tag{12}$$

where $S = (s_{ij})$ is an $n \times (k+1)$ matrix with

$$s_{ij} = \begin{cases} 1, & \text{if } i = j \text{ or } (i \in ([n] - [k]) \text{ and } j = k+1); \\ 0, & \text{otherwise,} \end{cases}$$

Since A is nonnegative and irreducible, by Perron-Frobenius theorem, there exists a positive vector $u = (u_1, u_2, \ldots, u_n)^T$ such that $\rho(A)u = Au$, then $(\rho(A)+1)u = (A+I)u$. By the computation of $(\rho(A)+1)u = (A+I)u$, we have

$$\frac{u_{k+1} + \cdots + u_n}{n-k} \leq \frac{u_{k+1} + \cdots + u_{k+(d_i-k+1)}}{d_i - k + 1}, \tag{13}$$

where d_i is the out-degree of vertex i. Let $u' = (u_1, u_2, \ldots, u_k, \frac{u_{k+1}+\cdots+u_n}{n-k})^T$, multiplying u' to the right of both terms in (12):

$$\Pi(A)u' = (S^T S)^{-1} S^T A S u'. \tag{14}$$

By (13), $ASu' \leq Au$ and then (14) will be

$$\Pi(A)u' = (S^T S)^{-1} S^T A S u' \leq (S^T S)^{-1} S^T A u = \rho(A)(S^T S)^{-1} S^T u. \tag{15}$$

Since $\Pi(A)$ is nonnegative and irreducible, by Perron-Frobenius theorem again, there exists a positive vector $y^T = (y_1, y_2, \ldots, y_{k+1})$ such that $\rho(\Pi(A))y^T = y^T \Pi(A)$. Multiplying y^T to the left of all terms in (15), then

$$\rho(\Pi(A))y^T u' = y^T \Pi(A) u' \leq y^T (S^T S)^{-1} S^T A u = \rho(A) y^T (S^T S)^{-1} S^T u. \tag{16}$$

Note that $y^T u' = y^T (S^T S)^{-1} S^T u$ and it is positive. Deleting this term in both sides of (16) leads to $\rho(\Pi(A)) \leq \rho(A)$ and the proof is completed. $\square$

Corollary 7.3. *Let A be the adjacency matrix of D, where $D \in \mathscr{D}^{**}(e)$. Let $\Pi = \{\{1\}, \{2\}, \ldots, \{k\}, \{k+1, \ldots, n\}\}$ and $\Pi' = \{\{1, 2, \ldots, k\}, \{k+1\}\}$ be partitions of $[n]$ and $[k+1]$, respectively, where k is the clique number of D. Then $\rho(\Pi'(\Pi(A)^T)) \leq \rho(A)$, where $\Pi'(\Pi(A)^T)$ is the quotient matrix of $\Pi(A)^T$ with respect to Π'.*

Proof. Since $\Pi'(\Pi(A)^T)$ is the quotient matrix of $\Pi(A)^T$ with respect to Π', $\Pi'(\Pi(A)^T)$ is a 2×2 matrix and

$$\Pi'(\Pi(A)^T) = (S^T S)^{-1} S^T \Pi(A)^T S, \tag{17}$$

where $S = (s_{ij})$ is a $(k+1) \times 2$ matrix with

$$s_{ij} = \begin{cases} 1, & \text{if } (i, j) \in [k] \times \{1\} \text{ or } (i = k+1 \text{ and } j = 2); \\ 0, & \text{otherwise,} \end{cases}$$

Since $\Pi(A)^T$ is nonnegative and irreducible, by Perron-Frobenius theorem, there exist a positive vector $u = (u_1, u_2, \ldots, u_{k+1})^T$ such that $\Pi(A)^T u = \rho(\Pi(A)^T) u$. Let $u' = (\frac{\sum_{i=1}^{k} u_i}{k}, u_{k+1})^T$. It is easy to see that $\Pi(A)^T S u' \leq \Pi(A)^T u$. Multiplying u' to the right of both terms in (17), we have

$$\Pi'(\Pi(A)^T) u' = (S^T S)^{-1} S^T \Pi(A)^T S u' \leq (S^T S)^{-1} S^T \Pi(A)^T u = \rho(\Pi(A)^T)(S^T S)^{-1} S^T u. \tag{18}$$

Since $\Pi'(\Pi(A)^T)$ is nonnegative and irreducible, by Perron-Frobenius theorem again, there exist a positive y^T such that $\rho(\Pi'(\Pi(A)^T)) y^T = y^T \Pi'(\Pi(A)^T)$. Multiplying y^T to the left of all terms in (18), then

$$\rho(\Pi'(\Pi(A)^T)) y^T u' = y^T \Pi'(\Pi(A)^T) u' \leq \rho(\Pi(A)^T) y^T (S^T S)^{-1} S^T u. \tag{19}$$

Note that $y^T u' = y^T (S^T S)^{-1} S^T u$ and it is positive. Deleting this term in both sides of (18) leads to $\rho(\Pi'(\Pi(A)^T)) \leq \rho(\Pi(A)^T)$, then by Theorem 7.2, we have

$$\rho(\Pi'(\Pi(A)^T)) \leq \rho(\Pi(A)^T) = \rho(\Pi(A)) \leq \rho(A),$$

and finish the proof is completed. □

Remark 7.4. The matrix $\Pi'(\Pi(A)^T)$ in Corollary 7.3 is

$$\begin{pmatrix} k-1 & \frac{\sum\limits_{i=k+1}^{n} d_i}{(n-k)k} \\ \sum\limits_{i=1}^{k}(d_i-k+1) & 0 \end{pmatrix},$$

which has the characteristic polynomial

$$f(\lambda) = \lambda^2 - (k-1)\lambda - \frac{a_1 a_2}{(n-k)k},$$

where

$$a_1 = \sum_{i=1}^{k}(d_i - k + 1), \quad a_2 = \sum_{i=k+1}^{n} d_i.$$

Corollary 7.5. *Let $D \in \mathscr{D}^{**}$ be a digraph with n vertices and $k(D) = k$, then*

$$\rho(D) \geq \frac{k - 1 + \sqrt{(k-1)^2 + 4\frac{a_1 a_2}{(n-k)k}}}{2},$$

where $a_1 = \sum\limits_{i=1}^{k}(d_i - k + 1), a_2 = \sum\limits_{i=k+1}^{n} d_i$.

Proof. This is proved immediately by Corollary 7.3 and Remark 7.4. □

8 Conclusion

In this thesis, we give some upper bounds for the digraphs with e arcs, where $e \in \mathbb{N}$, and compare these bounds to prove that the maximum spectral radius of a simple digraph D with e arcs and without isolated vertices occurs when $D \in \{D^*, D^{*t}\}$ for $e = s(s-1)+t$, $2s - 7 \leq t \leq 2s - 3$ and $t \neq 0, 1$. But for $\sqrt[4]{\frac{s-4}{4}} \leq t \leq 2s - 8$, it remains open. In the last section, we also give a lower bound of the spectral radius of a digraph through the concept of quotient matrix.

In our research, we obtain a weaker restriction of e_1 in Lemma 5.1 and Lemma 5.3, and get larger upper bounds to solve the problem, so there are a few cases for t can be solved.

If we narrow down the range of e_1, we believe that the conjecture can be solved by using Lemma 5.1 and Lemma 5.4 only, but the problem of the increasing of $\phi(k, k-1, e_1, 0)$ should be considered carefully.

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