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A matrix realization of spectral bounds

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A B S T R A C T

We give a unified and systematic way to find bounds for the largest real eigenvalue of a nonnegative matrix by considering its modified quotient matrix. We leverage this insight to identify the unique matrix whose largest real eigenvalue is maximum among all $(0, 1)$-matrices with a specified number of ones. This result resolves a problem that was posed independently by R. Brualdi and A. Hoffman, as well as F. Friedland, back in 1985.

1. Introduction

1.1. *Spectral radius of a nonnegative matrix*

All vectors and matrices in this paper are over the field of real numbers. Let $C = (c_{ij})$ be an $n \times n$ matrix. The *spectral radius* of C is defined to be $\rho(C) := \{|\lambda| : \ \lambda \text{ is an eigenvalue of } C\}$, where $|\lambda|$ is the magnitude of complex number λ. Let $\rho_r(C)$ denote the largest real eigenvalue of C and $\rho_r(C) = \infty$ if C has no real eigenvalues. A vector $(v_1, v_2, \ldots, v_n)$ is called *rooted* if $v_i \geq v_n \geq 0$ for $1 \leq i \leq n-1$. If $r_i := \sum_{j=1}^{n} c_{ij}$

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for $1 \leq i \leq n$, the tuple $(r_1, r_2, \ldots, r_n)$ is called the *row-sum vector* of C. Our first main theorem is the following.

Theorem A. *Let $M = (m_{ab})$ be an $\ell \times \ell$ matrix whose first $\ell - 1$ columns and row-sum vector are all rooted. If $C = (c_{ij})$ is an $n \times n$ nonnegative matrix and there exists a partition $\Pi = (\pi_1, \pi_2, \ldots, \pi_\ell)$ of $[n] := \{1, 2, \ldots, n\}$ such that*

$$\max_{i\in\pi_a} \sum_{j\in\pi_b} c_{ij} \leq m_{ab} \quad \text{and} \quad \max_{i\in\pi_a} \sum_{j=1}^{n} c_{ij} \leq \sum_{c=1}^{\ell} m_{ac}$$

for $1 \leq a \leq \ell$ and $1 \leq b \leq \ell - 1$, then $\rho(C) \leq \rho_r(M)$.

The cases $\ell = n$ and $c_{ij} \leq m_{ij}$ for all i, j, and the case $\ell = 1$ in Theorem A are two well-known applications of Perron-Frobenius Theorem, cf. Lemma 2.2 and Lemma 2.3 in Section 2. A very special situation of the case $\ell = n = 2$ is

$$\rho \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix} \leq \rho_r \begin{pmatrix} 5 & 2 \\ 4 & -1 \end{pmatrix} = 2 + \sqrt{17}$$

for nonnegative numbers c_{11}, c_{12}, c_{21}, c_{22} satisfying $c_{11} \leq 5$, $c_{21} \leq 4$, $c_{11} + c_{12} \leq 7$ and $c_{21}+c_{22} \leq 3$. The above upper bound $2+\sqrt{17}$ is smaller than the upper bound 7 obtained by taking the maximum row-sum of C, which is a well-known upper bound by Perron-Frobenius Theorem. Indeed using $\ell = 2$ in Theorem A to compute $\rho(M)$ for a particular M, a lot of existing spectral bounds of nonnegative square matrices of arbitrary orders which involve square roots in their expressions can be easily reproved, cf. the results in [2,4,6,11,12,14,18,19,23,25] to name a few. The matrices C with $\rho(C) = \rho_r(M)$ in Theorem A are also determined. Corollary 5.2 will give the detailed description.

Theorem A has a dual version that deals with lower bounds. In addition to the above results, Lemma 3.1, Lemma 3.2 are of independent interest in matrix theory.

1.2. Nonnegative matrices with prescribed sum of entries

In 1964, B. Schwarz [24] discussed matrices obtained by rearranging the entries of a nonnegative matrix, focusing on the matrices with maximum and minimum spectral radius, respectively. Motivated by this seminal paper, the problem of finding the maximum spectral radius of $(0, 1)$-matrices with precisely e ones was proposed by R. Brualdi and A. Hoffman in 1976 [1, p. 438], and ten years later they gave the following conjecture in 1985 [2].

Conjecture B. *If*

$$e = \frac{c(c-1)}{2} + t, \qquad \text{where } t < c,$$

the maximum spectral radius of an undirected graph with e edges and without isolated vertices is attained by taking the complete graph K_c with c vertices and adding a new vertex which is joined to t of the vertices of K_c.

Conjecture B is partially solved by F. Friedland in 1985 [9] and R. Stanley in 1987 [23], and totally solved by P. Rowlinson in 1988 [21]. For the directed graph situation, R. Brualdi and A. Hoffman [2] and F. Friedland [9] believed the following conjecture.

Conjecture C. *Let $\mathscr{S}(n,e)$ denote the set of $n\times n$ $(0,1)$-matrices having exactly $e=c^2+t$ ones, where $2\le t\le 2c$. If $A\in\mathscr{S}(n,e)$ attains the maximum spectral radius, then there exists a permutation matrix P such that PAP^T or PA^TP^T has the form*

$$\begin{pmatrix} & J_c & & J_{\lfloor\frac{t}{2}\rfloor\times 1} \\ & & & O_{(c-\lfloor\frac{t}{2}\rfloor)\times 1} \\ J_{1\times\lceil\frac{t}{2}\rceil} & O_{1\times(c-\lceil\frac{t}{2}\rceil)} & & 0 \end{pmatrix}\oplus O_{n-c-1}, \tag{1.1}$$

if $t\neq 2c-3$; and has the form

$$\begin{pmatrix} J_{c-1} & J_{(c-1)\times 2} \\ J_{2\times(c-1)} & O_2 \end{pmatrix}\oplus O_{n-c-1} \tag{1.2}$$

if $t=2c-3$, where $J_{s\times t}$ is the $s\times t$ all-one matrix, $O_{s\times t}$ is the $s\times t$ zero matrix, $J_s=J_{s\times s}$, $O_s=O_{s\times s}$ and $\oplus$ is the direct sum operation of two matrices.

The extremal matrices A in cases $t=0$ and $t=1$ have been found in [2] when Conjecture C was proposed: $PAP^T=J_c\oplus O_{n-c}$ when $t=0$; $PAP^T=(J_c\oplus O_{n-c})+E_{ij}$ when $t=1$, where ij is a position that $(J_c\oplus O_{n-c})_{ij}=0$ and E_{ij} is the $n\times n$ matrix with all zero entries except for a 1 in the ij position. The cases $t=2c$, $t=2c-3$ and other t much smaller than c in Conjecture C was solved by F. Friedland [9]. Snellman proved Conjecture C for relatively large t by using combinatorial reciprocity theorem in 2003 [22]. We will apply Theorem A to prove Conjecture C in Section 6.1.

Conjecture B has a generalized version that deals with $(0,1)$-matrices with zero trace. This line of study is usually parallel to the study of Conjecture C. More recent result is in 2015 [15], when Y. Jin and X. Zhang consider the case that t is much smaller than c. We solve this completely in Section 6.2.

We hope the method developed in this paper provides an efficient way of solving more extremal problems related to graphs and their spectral radii.

1.3. Organization of the paper

The paper is organized as follows. In Section 2 we give some preliminaries. Theorem 3.4 in Section 3 is our key tool, which is not easy to apply since rooted eigenvectors are involved. In Section 4 we provide a method to construct matrices having rooted eigenvectors. In Section 5, we prove Corollary 5.2, which is a strengthening of Theorem A. In Section 6 we provide the following three applications of Theorem A:

1. Prove Conjecture C;
2. Prove the nonsymmetric matrix version of Conjecture B;
3. Determine the matrix whose spectral radius is maximum among nonnegative matrices with the largest diagonal (resp. off diagonal) element d (resp. f) and prescribed sum of their entries.

2. Preliminaries

Our study is based on the well-known Perron-Frobenius Theorem. Here we review the necessary parts of the theorem.

Theorem 2.1 *([3, Theorem 2.2.1], [13, Corollary 8.1.29, Theorem 8.3.2]). If C is a nonnegative square matrix, then the following hold.*

(i) *The spectral radius $\rho(C)$ is an eigenvalue of C with a corresponding nonnegative right eigenvector and a corresponding nonnegative left eigenvector.*
(ii) *If there exists a column vector $v > 0$ and a nonnegative number λ such that $Cv \leq \lambda v$, then $\rho(C) \leq \lambda$.*
(iii) *If there exists a column vector $v \geq 0$, $v \neq 0$ and a nonnegative number λ such that $Cv \geq \lambda v$, then $\rho(C) \geq \lambda$.*

Moreover, if C is irreducible, then the eigenvalue $\rho(C)$ in (i) has multiplicity 1 and its corresponding left eigenvector and right eigenvector can be chosen to be positive, and any nonnegative left or right eigenvector of C is only corresponding to the eigenvalue $\rho(C)$. □

Unless specified otherwise, by eigenvector we always mean the right eigenvector. The following two lemmas are well-known consequences of Theorem 2.1. We provide their proofs since they motivate our proofs of results.

Lemma 2.2 *([3, Theorem 2.2.1]). If $0 \leq C \leq C'$ are square matrices, then $\rho(C) \leq \rho(C')$. Moreover, if C' is irreducible, then $\rho(C') = \rho(C)$ if and only if $C' = C$.*

Proof. Let v be a nonnegative eigenvector of C for $\rho(C)$. From the assumption, $C'v \geq Cv = \rho(C)v$. By applying Theorem 2.1(iii) with $(C, \lambda) = (C', \rho(C))$, we have $\rho(C') \geq \rho(C)$. Clearly $C' = C$ implies $\rho(C') = \rho(C)$. If $\rho(C') = \rho(C)$ and C' is irreducible, then $\rho(C){v'}^T v = \rho(C'){v'}^T v = {v'}^T C'v \geq {v'}^T Cv = \rho(C){v'}^T v$, where ${v'}^T$ is a positive left eigenvector of C' for $\rho(C')$. Hence ${v'}^T C'v = {v'}^T Cv$. As ${v'}^T$ is positive, $C'v = Cv$

and $\rho(C')v = \rho(C)v = Cv = C'v$. Since v is a nonnegative eigenvector of irreducible nonnegative matrix C', v is positive and $C' = C$. □

The matrix C' in Lemma 2.2 is a *matrix realization* of the upper bound $\rho(C')$ of $\rho(C)$ as stated in the title. We shall provide other matrix realizations. The next one is via a 1×1 matrix.

Lemma 2.3 *([13, Theorem 8.1.22]). If an $n \times n$ matrix $C = (c_{ij})$ is nonnegative with row-sum vector $(r_1, r_2, \ldots, r_n)$ satisfying $r_1 \geq r_i \geq r_n$ for $1 \leq i \leq n$, then*

$$r_n \leq \rho(C) \leq r_1.$$

Moreover, if C is irreducible, then $\rho(C) = r_1$ (resp. $\rho(C) = r_n$) if and only if C has constant row-sum.

We provide a proof of the following generalized version of Lemma 2.3, which is due to Ellingham and Zha [8].

Lemma 2.4 *([8]). If an $n \times n$ matrix C (not necessary to be nonnegative) with row-sum vector $(r_1, r_2, \ldots, r_n)$, where $r_1 \geq r_i \geq r_n$ for $1 \leq i \leq n$, has a nonnegative left eigenvector $v^T = (v_1, v_2, \ldots, v_n)$ for θ, then*

$$r_n \leq \theta \leq r_1.$$

Moreover, $\theta = r_1$ (resp. $\theta = r_n$) if and only if $r_i = r_1$ (resp. $r_i = r_n$) for the indices i with $v_i \neq 0$. In particular, if v^T is positive, $\theta = r_1$ (resp. $\theta = r_n$) if and only if C has constant row-sum.

Proof. Without loss of generality, let $\sum_{i=1}^{n} v_i = 1$. Then

$$\theta = \theta v^T J_{n\times 1} = v^T C J_{n\times 1} = \sum_{i=1}^{n} v_i r_i.$$

So θ is a convex combination of those r_i with indices i satisfying $v_i > 0$, and the result follows. □

The following matrix notation will be adopted in the paper. For a matrix $C = (c_{ij})$ and subsets α, β of row indices and column indices respectively, we use $C[\alpha|\beta]$ to denote the submatrix of C with size $|\alpha| \times |\beta|$ that has entries c_{ij} for $i \in \alpha$ and $j \in \beta$, and define $C[\alpha|\beta) := C[\alpha|\overline{\beta}]$, where $\overline{\beta}$ is the complement of β in the set of column indices. We define $C(\alpha|\beta]$ and $C(\alpha|\beta)$ similarly. We use i to denote the subset $[i] = \{1, 2, \ldots, i\}$ to reduce the double use of parentheses. For example, $C[i|i] := C[[i]|[i]]$ and $C[i|i) := C[[i]|[i])$.

Let $\Pi = \{\pi_1, \pi_2, \ldots, \pi_\ell\}$ be a partition of $[n]$ and let C be an $n \times n$ matrix. We define an $\ell \times \ell$ matrix $\Pi(C) := (p_{ab})$, where p_{ab} equals the average row-sum of the submatrix $C[\pi_a|\pi_b]$ of C. In matrix notation,

$$\Pi(C) = (S^T S)^{-1} S^T C S, \tag{2.1}$$

where $S = (s_{jb})$ is the $n \times \ell$ *characteristic matrix* of Π, i.e.,

$$s_{jb} = \begin{cases} 1, & \text{if } j \in \pi_b; \\ 0, & \text{otherwise} \end{cases}$$

for $1 \le j \le n$ and $1 \le b \le \ell$. The matrix $\Pi(C)$ is referred to as the *quotient matrix* of C with respect to Π. Moreover if

$$p_{ab} = \sum_{j \in \pi_b} c_{ij} \qquad (1 \le a, b \le \ell)$$

holds for every $i \in \pi_a$, then Π is called an *equitable partition* of C, and $\Pi(C)$ is called an *equitable quotient matrix* of C. Note that Π is an equitable partition of C if and only if

$$S\Pi(C) = CS. \tag{2.2}$$

Similarly for a column vector $u = (u_1, u_2, \ldots, u_n)^T$, we define a vector $\Pi(v) = (p_a)$ of length ℓ, where p_a equals the average value of entries of v with indices in π_a. If $u = S\Pi(u)$ then Π is an *equitable partition* of u, and $\Pi(u)$ is called an *equitable quotient vector* of u.

Lemma 2.5 *([3, Lemma 2.3.1]). If an $n \times n$ matrix C has an equitable partition $\Pi = \{\pi_1, \pi_2, \ldots, \pi_\ell\}$ with characteristic matrix S, and λ is an eigenvalue of $\Pi(C)$ with eigenvector u, then λ is an eigenvalue of C with eigenvector Su.*

The following are some useful properties of equitable quotient matrices.

Proposition 2.6 *([10, Lemma 5.2.2(b)]). Let C be an $n \times n$ matrix having a left eigenvector v^T for eigenvalue λ, and Π an equitable partition of C with characteristic matrix S. If $v^T S \neq 0$, then λ is also an eigenvalue of $\Pi(C)$.*

Proof. From (2.2), we have $v^T S\Pi(C) = v^T CS = \lambda v^T S$. Then $v^T S \neq 0$ is an eigenvector of $\Pi(C)$ for λ. $\square$

Remark 2.7. In [10, Lemma 5.2.2(b)], the author only considered symmetric $(0, 1)$-matrices, but the same idea proves the general case.

Corollary 2.8 *([10, Corollary 5.2.3]). If C is an $n \times n$ nonnegative matrix and Π is an equitable partition of C, then $\rho(C) = \rho(\Pi(C))$.* $\square$

3. Spectral bound via a same size matrix

In this section we develop the key tool in this paper.

3.1. A generalization of Lemma 2.2

We generalize Lemma 2.2 in the sense of Lemma 2.4 that the matrices considered are not necessarily nonnegative.

Lemma 3.1. *Let $C = (c_{ij})$, $C' = (c'_{ij})$, P and Q be $n \times n$ matrices. Assume that*

(i) *$PCQ \le PC'Q$;*
(ii) *C' has an eigenvector Qu for λ', where u is a nonnegative column vector and $\lambda' \in \mathbb{R}$;*
(iii) *C has a left eigenvector $v^T P$ for λ, where v^T is a nonnegative row vector and $\lambda \in \mathbb{R}$; and*
(iv) *$v^T PQu > 0$.*

Then $\lambda \le \lambda'$. Moreover, $\lambda = \lambda'$ if and only if

$$(PC'Q)_{ij} = (PCQ)_{ij} \qquad \text{for } 1 \le i, j \le n \text{ with } v_i \ne 0 \text{ and } u_j \ne 0. \tag{3.1}$$

Proof. Multiplying the nonnegative vector u given in (ii) to the right of both terms of (i), we have

$$PCQu \le PC'Qu = \lambda' PQu. \tag{3.2}$$

Multiplying the nonnegative row vector v^T given in (iii) to the left of all terms in (3.2), we have

$$\lambda v^T PQu = v^T PCQu \le v^T PC'Qu = \lambda' v^T PQu. \tag{3.3}$$

Now we delete the positive term $v^T PQu$ to obtain $\lambda \le \lambda'$ and finish the proof of the first part.

Assume that $\lambda = \lambda'$. Then the inequality in (3.3) is an equality. Especially $(PCQu)_i = (PC'Qu)_i$ for any i with $v_i \ne 0$. Hence $(PCQ)_{ij} = (PC'Q)_{ij}$ for any i, j with $v_i \ne 0$ and $u_j \ne 0$.

Conversely, (3.1) implies $v^T PCQu = v^T PC'Qu$. Then $\lambda = \lambda'$ by (3.3). □

Let I_n denote the identity matrix of order n. If C is nonnegative and $P = Q = I_n$, then Lemma 3.1 becomes Lemma 2.2 with an additional assumption $v^T u > 0$ which immediately holds if C or C' is irreducible by Theorem 2.1.

In the sequels, we shall call two statements that resemble each other by switching $\le$ and $\ge$ and corresponding variables, like $\theta \ge r_n$ and $\theta \le r_1$, as *dual statements*. Two proofs are called *dual proofs* if one proof is obtained from the other by simply switching each of $\leq$ and $\geq$ to the other. The following is a dual version of Lemma 3.1 which is proved by a dual proof.

Lemma 3.2. *Let $C = (c_{ij})$, $C' = (c'_{ij})$, P and Q be $n \times n$ matrices. Assume that*

(i) *$PCQ \geq PC'Q$;*
(ii) *C' has an eigenvector Qu for λ', where u is a nonnegative column vector and $\lambda' \in \mathbb{R}$;*
(iii) *C has a left eigenvector $v^T P$ for λ, where v^T is a nonnegative row vector and $\lambda \in \mathbb{R}$; and*
(iv) *$v^T PQu > 0$.*

Then $\lambda \geq \lambda'$. Moreover, $\lambda = \lambda'$ if and only if

$$(PC'Q)_{ij} = (PCQ)_{ij} \qquad \text{for } 1 \leq i, j \leq n \quad \text{with } v_i \neq 0 \text{ and } u_j \neq 0. \quad \square$$

3.2. The special case $P = I_n$ and a particular Q

We shall apply Lemma 3.1 and Lemma 3.2 by letting $P = I_n$ and

$$Q = I_n + \sum_{i=1}^{n-1} E_{in} = \begin{pmatrix} I_{n-1} & J_{(n-1)\times 1} \\ O_{1\times(n-1)} & 1 \end{pmatrix}. \tag{3.4}$$

Hence for $n \times n$ matrix $C' = (c'_{ij})$, the matrix $PC'Q$ in Lemma 3.1(i) is

$$C'Q = \begin{pmatrix} & & & & r'_1 \\ & & & & r'_2 \\ & C'[n-1|n-1] & & & \vdots \\ & & & & r'_{n-1} \\ c'_{n1} & c'_{n2} & \cdots & c'_{nn-1} & r'_n \end{pmatrix}, \tag{3.5}$$

where $(r'_1, r'_2, \ldots, r'_n)$ is the row-sum vector of C'.

Recall that a column vector $v' = (v'_1, v'_2, \ldots, v'_n)^T$ is said to be rooted if $v'_j \geq v'_n \geq 0$ for $1 \leq j \leq n-1$.

Lemma 3.3. *Let $u = (u_1, u_2, \ldots, u_n)^T$ be a column vector and Q be as in (3.4). Then the following (i)-(ii) hold.*

(i) *Qu is rooted if and only if u is nonnegative.*
(ii) *For $1 \leq j \leq n-1$, $(Qu)_j > (Qu)_n$ if and only if $u_j > 0$.*

Proof. (i)-(ii) follow from the observation that $Qu = (u_1 + u_n, u_2 + u_n, \ldots, u_{n-1} + u_n, u_n)^T$. $\square$

The following theorem is immediate from Lemma 3.1 by applying $P = I$, the Q in (3.4), $v' = Qu$ and referring to (3.5) and Lemma 3.3.

Theorem 3.4. *Let $C = (c_{ij})$, $C' = (c_{ij})$ be $n \times n$ matrices with row-sum vectors $(r_1, r_2, \ldots, r_n)$ and $(r'_1, r'_2, \ldots, r'_n)$ respectively. Assume the following (i)-(iv).*

(i) $C[n|n-1] \le C'[n|n-1]$ *and* $(r_1, r_2, \ldots, r_n) \le (r'_1, r'_2, \ldots, r'_n)$.
(ii) C' *has a rooted eigenvector* $v' = (v'_1, v'_2, \ldots, v'_n)^T$ *for* $\lambda' \in \mathbb{R}$;
(iii) C *has a nonnegative left eigenvector* $v^T = (v_1, v_2, \ldots, v_n)$ *for* $\lambda \in \mathbb{R}$;
(iv) $v^T v' > 0$.

Then $\lambda \le \lambda'$. Moreover, $\lambda = \lambda'$ if and only if the following (a), (b) hold.

(a) *If* $v'_n \neq 0$, *then* $r_i = r'_i$ *for* $1 \le i \le n$ *with* $v_i \neq 0$.
(b) $c'_{ij} = c_{ij}$ *for* $1 \le i \le n, 1 \le j \le n-1$ *with* $v_i \neq 0$ *and* $v'_j > v'_n$. □

Note that (a), (b) in Theorem 3.4 are from (3.1) in Lemma 3.1. The first part of assumption (i) in Theorem 3.4 indicates that in some sense the last column is *irrelevant* in the comparison of C and C'. The following theorem is the dual version of Theorem 3.4 which is proved by a dual proof.

Theorem 3.5. *Let $C = (c_{ij})$, $C' = (c_{ij})$ be $n \times n$ matrices with row-sum vectors $(r_1, r_2, \ldots, r_n)$ and $(r'_1, r'_2, \ldots, r'_n)$ respectively. Assume the following (i)-(iv).*

(i) $C[n|n-1] \ge C'[n|n-1]$ *and* $(r_1, r_2, \ldots, r_n) \ge (r'_1, r'_2, \ldots, r'_n)$, *where* $(r_1, r_2, \ldots, r_n)$ *and* $(r'_1, r'_2, \ldots, r'_n)$ *are the row-sum vectors of* C *and* C', *respectively.*
(ii) C' *has a rooted eigenvector* $v' = (v'_1, v'_2, \ldots, v'_n)^T$ *for* $\lambda' \in \mathbb{R}$;
(iii) C *has a nonnegative left eigenvector* $v^T = (v_1, v_2, \ldots, v_n)$ *for* $\lambda \in \mathbb{R}$;
(iv) $v^T v' > 0$.

Then $\lambda \ge \lambda'$. Moreover, $\lambda = \lambda'$ if and only if the following (a)-(b) hold.

(a) *If* $v'_n \neq 0$, *then* $r_i = r'_i$ *for* $1 \le i \le n$ *with* $v_i \neq 0$.
(b) $c'_{ij} = c_{ij}$ *for* $1 \le i \le n, 1 \le j \le n-1$ *with* $v_i \neq 0$ *and* $v'_j > v'_n$. □

Example 3.6. Consider the following three matrices

$$C'_\ell = \begin{pmatrix} 3 & 1 & 1 \\ 0 & 0 & 3 \\ 0 & 1 & 2 \end{pmatrix}, \quad C = \begin{pmatrix} 3 & 1 & 1 \\ 1 & 0 & 2 \\ 1 & 1 & 1 \end{pmatrix}, \quad C'_r = \begin{pmatrix} 3 & 2 & 0 \\ 1 & 2 & 0 \\ 1 & 2 & 0 \end{pmatrix}$$

with $C'_\ell[3|2] \le C[3|2] \le C'_r[3|2]$, and the same row-sum vector $(5, 3, 3)$. Note that C'_ℓ has a rooted eigenvector $v'_\ell = (1, 0, 0)^T$ for $\lambda'_\ell = 3$ and C'_r has a rooted eigenvector

$v'_r = (2,1,1)^T$ for $\lambda'_r = 4$. Since C is irreducible, it has a positive left eigenvector (v_1, v_2, v_3) for $\rho(C)$. Hence assumptions (i)-(iv) in Theorem 3.4 and Theorem 3.5 hold, and we conclude that $\lambda'_\ell \le \rho(C) \le \lambda'_r$. Since $[3] \times [1]$ is the set of the pairs (i, j) described in Theorem 3.4(b) and Theorem 3.5(b), by simple comparison of the first columns $C'_\ell[3|1] < C[3|1] = C'_r[3|1]$ of these three matrices, we easily conclude that $3 = \lambda'_\ell < \rho(C) = \lambda'_r = 4$ by the second part of Theorem 3.4 and that of Theorem 3.5.

4. Matrix with a rooted eigenvector

To apply Theorem 3.4 and Theorem 3.5, we need to construct C' which possesses a rooted eigenvector for some λ'. The following lemma comes directly.

Lemma 4.1. *If an $n \times n$ matrix C' has a rooted eigenvector for λ', then $C' + dI_n$ also has the same rooted eigenvector for $\lambda' + d$, where d is any constant.* □

The definition of a rooted column vector is generalized to a rooted matrix as follows.

Definition 4.2. An $n \times n$ matrix $C' = (c'_{ij})$ is called *rooted* if there is a constant d such that the first $n-1$ columns and the row-sum vector of $C' + dI_n$ are all rooted.

The matrix Q in (3.4) is invertible with

$$Q^{-1} = I_n - \sum_{i=1}^{n-1} E_{in} = \begin{pmatrix} I_{n-1} & -J_{(n-1)\times 1} \\ O_{1\times(n-1)} & 1 \end{pmatrix}.$$

Multiplying Q^{-1} to the left of $C'Q$ in (3.5), we have $Q^{-1}C'Q$ as

$$\begin{pmatrix} c'_{11} - c'_{n1} & c'_{12} - c'_{n2} & \cdots & c'_{1\ n-1} - c'_{nn-1} & r'_1 - r'_n \\ c'_{21} - c'_{n1} & c'_{22} - c'_{n2} & \cdots & c'_{2\ n-1} - c'_{nn-1} & r'_2 - r'_n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ c'_{n-1\ 1} - c'_{n1} & c'_{n-1\ 2} - c'_{n2} & \cdots & c'_{n-1\ n-1} - c'_{nn-1} & r'_{n-1} - r'_n \\ c'_{n1} & c'_{n2} & \cdots & c'_{nn-1} & r'_n \end{pmatrix}. \tag{4.1}$$

From (4.1), C' is rooted if and only if $Q^{-1}(C' + dI_n)Q$ is nonnegative for some constant d. Moreover, v' is an eigenvector of C' for λ' if and only if $u = Q^{-1}v'$ is an eigenvector of $Q^{-1}C'Q$ for λ'.

Lemma 4.3. *If $C' = (c'_{ij})$ is an $n \times n$ rooted matrix, then $\rho_r(C') < \infty$ and C' has a rooted eigenvector v' for $\rho_r(C')$. Moreover, for any eigenvalue λ with a rooted eigenvector $v' = (v'_1, v'_2, \ldots, v'_n)^T$ of C', the following (i), (ii) hold.*

(i) *If row vector $(c'_{n1}, c'_{n2}, \ldots, c'_{nn-1})$ is positive, then v' is positive.*
(ii) *If $v'_n > 0$ and $r'_i > r'_n$ for some $1 \le i \le n-1$, then $v'_i > v'_n$.*

Proof. If C' is a rooted matrix, then $Q^{-1}(C'+dI_n)Q$ is nonnegative for some constant d. By Theorem 2.1, there is a nonnegative eigenvector u of $Q^{-1}(C'+dI_n)Q$ for $\rho(Q^{-1}(C'+dI_n)Q) = \rho_r(C') + d$. Therefore, C' has a rooted eigenvector $v' = Qu$ for $\rho_r(C')$.

(i) Suppose that $(c'_{n1}, c'_{n2}, \ldots, c'_{nn-1})$ is positive and $v'_n = 0$. Then

$$\sum_{j=1}^{n-1} c'_{nj}v'_j = \sum_{j=1}^{n} c'_{nj}v'_j = (C'v')_n = \lambda v'_n = 0.$$

Hence v' is a zero vector, a contradiction. So $v'_n > 0$ and $v' > 0$ since v' is rooted.

(ii) Note that the row-sum vector $(r'_1, r'_2, \ldots, r'_n)^T$ of C' is rooted, and there exists a constant d such that $\lambda + d > 0$ and $C' + dI_n = (c''_{ij})$ satisfies $c''_{ij} \geq c''_{nj}$ for $1 \leq i \leq n, 1 \leq j \leq n-1$. From the computation

$$\begin{aligned}
(\lambda + d)v'_i &= \sum_{j=1}^{n} c''_{ij}v'_j \\
&= \sum_{j=1}^{n} c''_{nj}v'_j + \sum_{j=1}^{n}(c''_{ij} - c''_{nj})v'_j \\
&\geq \sum_{j=1}^{n} c''_{nj}v'_j + \sum_{j=1}^{n}(c''_{ij} - c''_{nj})v'_n \\
&= (\lambda + d)v'_n + (r'_i + d - r'_n - d)v'_n > (\lambda + d)v'_n,
\end{aligned}$$

and deleting $\lambda + d$, we have $v'_i > v'_n$. □

By Lemma 2.5 and Lemma 4.3, we have the following lemma.

Lemma 4.4. *If C' is an $n \times n$ matrix, $\Pi = \{\pi_1, \ldots, \pi_\ell\}$ is an equitable partition of C' with $n \in \pi_\ell$ and $\Pi(C')$ is a rooted matrix, then C' has a rooted eigenvector Su for $\rho_r(\Pi(C'))$, where S is the characteristic matrix of Π and u is a rooted eigenvector of $\Pi(C')$ for $\rho_r(C')$.* □

Lemma 4.3 and Lemma 4.4 will be useful to construct matrix C' with a rooted eigenvector, while the following lemma will help us reduce the size of C' for computing $\rho_r(C')$.

Lemma 4.5. *Let C' be an $n \times n$ rooted matrix and $\Pi = \{\pi_1, \ldots, \pi_\ell\}$ be an equitable partition of ${C'}^T$ with $\pi_\ell = \{n\}$. Then $\rho_r(C') = \rho_r(\Pi({C'}^T))$.*

Proof. By Lemma 4.3, C' has a rooted eigenvector v' for $\rho_r(C')$. Then ${C'}^T$ has a nonnegative eigenvector ${v'}^T$ for $\rho_r(C')$. Hence ${v'}^T S \neq 0$, where S is the characteristic matrix of Π. By Proposition 2.6 $\rho_r(C')$ is also an eigenvalue of $\Pi({C'}^T)$. Then $\rho_r(\Pi({C'}^T)) = \rho_r(C')$ by Lemma 2.5. □

The following matrix is a special rooted matrix which will be used to obtain certain bounds of the spectral radius of a nonnegative matrix.

For $d, f_1, f_2, r_1, r_2, \ldots, r_n \geq 0$ with $f_1 \geq f_2$ and $r_j \geq r_n$ with $1 \leq j \leq n-1$, define

$$M_n := \begin{pmatrix} f_1 J_{n-1} + (d - f_1) I_{n-1} & \begin{matrix} r_1 - d - (n-2)f_1 \\ r_2 - d - (n-2)f_1 \\ \vdots \\ r_{n-1} - d - (n-2)f_1 \end{matrix} \\ f_2 J_{1\times(n-1)} & r_n - (n-1)f_2 \end{pmatrix}. \tag{4.2}$$

Lemma 4.6. *Referring to the notation of M_n in (4.2), the following (i), (ii) hold.*

(i) *The matrix M_n has a rooted eigenvector v' for the largest real eigenvalue $\rho_r(M_n)$ of M_n.*
(ii) *If $f_2 > 0$, then $v' > 0$.*

Proof. Since M_n is rooted, (i) follows from the first part of Lemma 4.3, and (ii) follows from Lemma 4.3(i). □

Lemma 4.7. *Referring to the notation of M_n in (4.2), the following (i)-(iii) hold.*

(i) *The largest real eigenvalue $\rho_r(M_n)$ of M_n is*

$$\begin{aligned} &\frac{1}{2}(r_n + d - f_2 + (n-2)(f_1 - f_2)) \\ &+ \frac{1}{2}\sqrt{(r_n - d + f_2 - (n-2)(f_1 - f_2))^2 + 4f_2 \sum_{i=1}^{n-1}(r_i - r_n)}. \end{aligned} \tag{4.3}$$

In particular $\rho_r(M_n) \geq \max(d - f_2, r_n)$.

(ii) *If $f_1 = f_2 = f$ and $r_n = 0$, then*

$$\rho_r(M_n) = \frac{d - f + \sqrt{(d-f)^2 + 4fm}}{2},$$

where $m := \sum_{i=1}^{n-1} r_i$ is the sum of all entries of M_n.

(iii) *If $f_1 = f_2$ and $r_t = r_{t+1} = \cdots = r_n$ for some $t \leq n$, then $\rho_r(M_t) = \rho_r(M_n)$.*

Proof. Note that $\Pi = \{\{1, 2, \ldots, n-1\}, \{n\}\}$ is an equitable partition of M_n^T, and

$$\Pi(M_n^T) = \begin{pmatrix} d + (n-2)f_1 & f_2 \\ \sum_{i=1}^{n-1}(r_i - (d + (n-2)f_1)) & r_n - (n-1)f_2) \end{pmatrix}.$$

By Lemma 4.5 and direct computation, we find $\rho_r(M) = \rho_r(\Pi(M_n^T))$ as the expression in (4.3). The rest of (i), (ii) and (iii) follow from (4.3) immediately. □

5. The proof of Theorem A

The following theorem is a strengthening of Theorem A.

Theorem 5.1. *Let $M = (m_{ab})$ be an $\ell \times \ell$ rooted matrix. If $C = (c_{ij})$ is an $n \times n$ nonnegative matrix and there exists a partition $\Pi = \{\pi_1, \pi_2, \ldots, \pi_\ell\}$ of $[n]$ such that*

$$\max_{i \in \pi_a} \sum_{j \in \pi_b} c_{ij} \leq m_{ab} \quad \text{and} \quad \max_{i \in \pi_a} \sum_{j=1}^{n} c_{ij} \leq \sum_{c=1}^{\ell} m_{ac}$$

for $1 \leq a \leq \ell$ and $1 \leq b \leq \ell - 1$, then $\rho(C) \leq \rho_r(M)$. Moreover, let $u = (u_1, \ldots, u_\ell)$ be a rooted eigenvector of M for $\rho_r(M)$. If C is irreducible, then $\rho(C) = \rho_r(M)$ if and only if the following (a), (b) hold.

(a) *If $u_\ell \neq 0$, then $\sum_{j=1}^{n} c_{ij} = \sum_{c=1}^{\ell} m_{ac}$ for $1 \leq a \leq \ell, i \in \pi_a$.*
(b) *$\sum_{j \in \pi_b} c_{ij} = m_{ab}$ for $1 \leq a \leq \ell, 1 \leq b \leq \ell - 1, i \in \pi_a$ with $u_b > u_\ell$.*

Proof. Rearranging the indices of C if necessary, we might assume $n \in \pi_\ell$. We first consider the case that the row vector $(m_{\ell 1}, m_{\ell 2}, \ldots, m_{\ell \ell-1})$ is positive. We construct an $n \times n$ matrix C' such that the conditions in Theorem 3.4(i) hold, and Π is an equitable partition of C' with $\Pi(C') = M$. Indeed, C' is obtained from C by increasing entries in $C[n|n-1]$ such that each row of the submatrix $C'[\pi_a|\pi_b]$ of C' has the same row-sum m_{ab} for $1 \leq a \leq \ell, 1 \leq b \leq \ell - 1$, and the last column of C' is filled to make the i-th row-sum of C' equals $\sum_{c=1}^{\ell} m_{ac}$ for each i, where $i \in \pi_a$. By Lemma 4.3 and Lemma 4.4, $\rho_r(M)$ is an eigenvalue of C' with a positive and rooted eigenvector v'. Let v^T be a nonnegative left eigenvector of C for $\rho(C)$. Then $v^T v' > 0$ and the conditions (i)-(iv) in Theorem 3.4 hold. From the conclusion of Theorem 3.4 with $\lambda = \rho(C)$ and $\lambda' = \rho_r(M)$, we find $\rho(C) \leq \rho_r(M)$.

In general, let $\epsilon > 0$ and $M_\epsilon := M + \epsilon J_\ell$. Note that M_ϵ is rooted and $M[\{\ell\}|\{\ell\})$ is positive. Then by the argument above, we have $\rho(C) \leq \rho_r(M_\epsilon)$. Hence

$$\rho(C) \leq \lim_{\epsilon \to 0^+} \rho_r(M_\epsilon) = \rho_r(M)$$

by the continuity of the eigenvalues [7,20].

For the second part, assume C is irreducible. Then C has a positive left eigenvector v^T for $\rho(C)$. To prove the sufficiency in the second part, assume that (a), (b) hold. Let S be the characteristic matrix of π. Then by Lemma 4.4 $v' = (v'_1, \ldots, v'_n)^T = Su$ is a rooted eigenvector of above C' for $\rho_r(M)$ and clearly Theorem 3.4 (a) holds, for $1 \leq i \leq n, 1 \leq j \leq n-1$ with $v'_j > v'_n$. Let $i \in \pi_a$ and $j \in \pi_b$. Then $u_b = v'_j > v'_n = u_\ell$

and $\sum_{j'\in\pi_b} c_{ij'} = m_{ab} = \sum_{j'\in\pi_b} c'_{ij'}$ by (b) here. Hence for $j' \in \pi_b$, $c_{ij'} = c'_{ij'}$ since $c_{ij'} \le c'_{ij'}$, and $c_{ij} = c'_{ij}$. Thus Theorem 3.4 (b) holds and $\rho(C) = \rho_r(M)$ by Theorem 3.4.

To prove the necessity, assume that $\rho(C) = \rho_r(M)$. Then clearly Theorem 3.4 (a) implies (a) here since $v'_n = u_\ell$. For $1 \le a \le \ell, 1 \le b \le \ell - 1, i \in \pi_a$ with $u_b > u_\ell$, from Theorem 3.4 (b), we have $\sum_{j\in\pi_b} c_{ij} = \sum_{j\in\pi_b} c'_{ij} = m_{ab}$. Then (b) holds and the proof is completed. □

To characterize when the equality holds in Theorem 5.1, we need certain information about the eigenvector of M. With additional conditions, we now give an eigenvector-free version of Theorem 5.1. A vector $(v_1, v_2, \ldots, v_\ell)$ is *strictly rooted* if $v_i > v_\ell > 0$ for every $i \le \ell$.

Corollary 5.2. *Let $M = (m_{ab})$ be an $\ell \times \ell$ rooted matrix. If $C = (c_{ij})$ is an $n \times n$ nonnegative matrix and there exists a partition $\Pi = \{\pi_1, \pi_2, \ldots, \pi_\ell\}$ of $[n]$ such that*

$$\max_{i\in\pi_a} \sum_{j\in\pi_b} c_{ij} \le m_{ab} \quad \textit{and} \quad \max_{i\in\pi_a} \sum_{j=1}^{n} c_{ij} \le \sum_{c=1}^{\ell} m_{ac}$$

for $1 \le a \le \ell$ and $1 \le b \le \ell - 1$, then $\rho(C) \le \rho_r(M)$. Moreover, if C is irreducible, the row vector $(m_{\ell 1}, m_{\ell 2}, \ldots, m_{\ell \ell-1})$ is positive, and the row-sum vector of M is strictly rooted, then $\rho(C) = \rho_r(M)$ if and only if Π is an equitable partition of C and $\Pi(C) = M$.

Proof. It remains to prove the second part. To prove the sufficiency, assume that Π is an equitable partition of C and $\Pi(C) = M$. Then $\rho(C) = \rho(M) = \rho_r(M)$ by Proposition 2.8.

To prove the necessity, assume that C is irreducible, the row vector $(m_{\ell 1}, m_{\ell 2}, \ldots, m_{\ell \ell-1})$ is positive, the row-sum vector of M is strictly rooted, and $\rho(C) = \rho_r(M)$. Then M has a strictly rooted eigenvector $u = (u_1, u_2, \ldots, u_\ell)^T$ for $\rho_r(M)$ by Lemma 4.3. By the second part of Theorem 5.1, we have that the row-sum vectors of C and C' are equal and $C[n|\pi_\ell) = C'[n|\pi_\ell)$. Hence $\Pi(C) = \Pi(C') = M$. □

We provide an example to explain Theorem 5.1 and its proof.

Example 5.3. Consider the following matrices C, C' and M from left to right appearing in the assumption and proof of Theorem 5.1:

$$\left(\begin{array}{ccc|cc|cc} 2 & 1 & 3 & 3 & 3 & 12 & 0 \\ 4 & 2 & 1 & 4 & 2 & 6 & 4 \\ 2 & 3 & 1 & 4 & 1 & 8 & 3 \\ \hline 3 & 5 & 3 & 1 & 1 & 3 & 4 \\ 5 & 6 & 1 & 1 & 0 & 3 & 3 \\ \hline 0 & 2 & 1 & 2 & 2 & 6 & 0 \\ 2 & 2 & 0 & 2 & 1 & 1 & 4 \end{array}\right), \left(\begin{array}{ccc|cc|cc} 2 & 2 & 3 & 3 & 3 & 12 & -1 \\ 4 & 2 & 1 & 4 & 2 & 6 & 5 \\ 2 & 3 & 2 & 4 & 2 & 8 & 3 \\ \hline 4 & 5 & 3 & 1 & 1 & 3 & 3 \\ 5 & 6 & 1 & 1 & 1 & 3 & 3 \\ \hline 1 & 2 & 1 & 2 & 2 & 6 & -1 \\ 2 & 2 & 0 & 2 & 2 & 1 & 4 \end{array}\right), \begin{pmatrix} 7 & 6 & 11 \\ 12 & 2 & 6 \\ 4 & 4 & 5 \end{pmatrix},$$

with corresponding row-sum vectors

$$(24, 23, 22|20, 19|13, 12), \quad (24, 24, 24|20, 20|13, 13), \quad (24, 20, 13),$$

where the separating lines are according to the equitable partition $\Pi = \{\{1, 2, 3\}, \{4, 5\}, \{6, 7\}\}$ of the middle matrix C'. Notice that C' is not rooted, so we can not apply Lemma 4.3 and then Theorem 3.4 directly. Since M is rooted and by Theorem 5.1, we have $\rho(C) \le \rho_r(M) \approx 18.6936$. If we apply Lemma 2.2 with C' the following nonnegative matrix C^* using the same equitable partition Π:

$$C^* = \left(\begin{array}{ccc|cc|cc} 2 & 2 & 3 & 3 & 3 & 12 & 0 \\ 4 & 2 & 1 & 4 & 2 & 6 & 6 \\ 2 & 3 & 2 & 4 & 2 & 8 & 4 \\ \hline 4 & 5 & 3 & 1 & 1 & 3 & 4 \\ 5 & 6 & 1 & 1 & 1 & 3 & 4 \\ \hline 1 & 2 & 1 & 2 & 2 & 6 & 0 \\ 2 & 2 & 0 & 2 & 2 & 2 & 4 \end{array}\right), \qquad \Pi(C^*) = \begin{pmatrix} 7 & 6 & 12 \\ 12 & 2 & 7 \\ 4 & 4 & 6 \end{pmatrix},$$

then the upper bound $\rho(C^*) = \rho(\Pi(C^*)) \approx 19.4$ of $\rho(C)$ is larger than the previous one.

Theorem 5.4, due to X. Duan and B. Zhou [6], generalizes the results in [2,4,11,12, 18,23,25] and relates to the results in [14,19,23]. Theorem 5.4 can be easily reproved by using Corollary 5.2.

Theorem 5.4 *([6]). Let $C = (c_{ij})$ be a nonnegative $n \times n$ matrix with row-sums $r_1 \ge r_2 \ge \cdots \ge r_n$, $f := \max_{1\le i\ne j\le n} c_{ij}$ and $d := \max_{1\le i\le n} c_{ii}$. Then*

$$\rho(C) \le \frac{r_\ell + d - f + \sqrt{(r_\ell - d + f)^2 + 4f\sum_{i=1}^{\ell-1}(r_i - r_\ell)}}{2} \tag{5.1}$$

for $1 \le \ell \le n$. Moreover, if C is irreducible, then the equality holds in (5.1) if and only if $r_1 = r_n$ or for $1 \le t \le \ell$ with $r_{t-1} \ne r_t = r_\ell$, we have $r_t = r_n$ and

$$c_{ij} = \begin{cases} d, & \text{if } i = j \le t-1; \\ f, & \text{if } i \ne j \text{ and } 1 \le i \le n,\ 1 \le j \le t-1. \end{cases}$$

Proof. The inequality in (5.1) is obtained by applying Corollary 5.2 with $\Pi = \{\{1\}, \{2\}, \ldots, \{\ell-1\}, \{\ell, \ell+1, \ldots, n\}\}$ and $M = \Pi(C')$, where $C' = M_\ell$ is the matrix described in (4.2) with $n = \ell$, $f_1 = f_2 = f$. For the equality case, we apply Lemma 4.7(iii) and the second part of Corollary 5.2 by choosing the least t such that $r_t = r_\ell$. □

Remark 5.5. From our method in Corollary 5.2, the assumptions f and d in Theorem 5.4 can be replaced by smaller numbers $f = \max_{1\le i\le n, 1\le j\le \ell-1, i\ne j} c_{ij}$ and $d =$

$\max_{1\le i\le \ell-1} c_{ii}$, respectively. Furthermore, by Lemma 4.7(i) the upper bound could be replaced by

$$\frac{1}{2}(r_n + d - f_2 + (n-2)(f_1 - f_2)) \\ + \frac{1}{2}\sqrt{(r_n - d + f_2 - (n-2)(f_1-f_2))^2 + 4f_2\sum_{i=1}^{n-1}(r_i - r_n)},$$

where

$$f_1 = \max_{i\in[n], j\in[\ell-1], i\neq j} c_{ij},\ \ f_2 = \max_{\ell\le i\le n, j\in[\ell-1]} c_{ij},\ \ d = \max_{i\in[\ell-1]} c_{ii}.$$

The following is the dual theorem of Corollary 5.2, but its proof is not completely dual.

Theorem 5.6. *Let $M = (m_{ab})$ be an $\ell\times\ell$ rooted matrix. If $C = (c_{ij})$ is an $n\times n$ nonnegative matrix and there exists a partition $\Pi = \{\pi_1, \pi_2, \ldots, \pi_\ell\}$ of $[n]$ such that*

$$\min_{i\in\pi_a}\sum_{j\in\pi_b} c_{ij} \ge m_{ab} \quad \textit{and} \quad \min_{i\in\pi_a}\sum_{j=1}^{n} c_{ij} \ge \sum_{c=1}^{\ell} m_{ac}$$

for $1\le a\le \ell$ and $1\le b\le \ell-1$, then $\rho(C)\ge \rho_r(M)$. Moreover, if C is irreducible, the row vector $(m_{\ell 1}, m_{\ell 2}, \ldots, m_{\ell\ell-1})$ is positive, and the row-sum vector of M is strictly rooted, then $\rho(C) = \rho_r(M)$ if and only if Π is an equitable partition of C and $\Pi(C) = M$.

Proof. The second part of the statement follows from a dual proof of Corollary 5.2. To prove the first part, without assuming the row vector $(m_{\ell 1}, m_{\ell 2}, \ldots, m_{\ell\ell-1})$ being positive and referring to (3.5), we construct C' similarly as in the proof of Theorem 5.1 by changing the operation of increasing entries to decreasing entries in $C[n|n-1]$ to have $CQ \ge C'Q \ge 0$ and $\Pi(C') = M$. Since M is rooted, there is a rooted eigenvector v' of C' for $\lambda' = \rho(M)$ by Lemma 4.4. Then $u = Q^{-1}v'$ is nonnegative and we have $Cv' = CQu \ge C'Qu = C'v' = \lambda' v'$. Since v' is nonnegative, $\rho(C)\ge\rho(M)$ by Theorem 2.1(iii). □

6. Applications

We provide three applications of our matrix realization of spectral bounds in this section.

6.1. The proof of Conjecture C

Throughout this subsection, we assume $e = c^2 + t$, where $2\le t\le 2c$. Recall that $\mathscr{S}(n,e)$ is the set of $n\times n$ $(0,1)$-matrices having exactly e 1's. Let $\mathscr{S}^*(n,e)$ denote the subset of $\mathscr{S}(n,e)$ which collects matrices $A = (a_{ij})$ satisfying

$$\text{if } a_{ij} = 1, \text{ then } a_{hk} = 1 \text{ for } h \le i,\ k \le j.$$

We need the following lemma.

Lemma 6.1 *([9]). If $A \in \mathscr{S}(n,e)$ attains the maximum spectral radius, then there exists a permutation matrix P such that $PAP^T \in \mathscr{S}^*(n,e)$ and PAP^T has the form $A[k|k] \oplus O_{n-k}$ for some k and the submatrix $A[k|k]$ is irreducible.*

Proof of Conjecture C. Let A_0 be the matrix in (1.1), and A'_0 be the matrix in (1.2) in the case $t = 2c-3$. Observe that $A_0, A'_0 \in \mathscr{S}^*(n,e)$. To prove Conjecture C, by using Lemma 6.1, we only need to show $\rho(A) < \rho(A_0)$ for every $A \in \mathscr{S}^*(n,e) - \{A_0, A_0^T\}$ if $t \neq 2c-3$; and $\rho(A) < \rho(A_0)$ for every $A \in \mathscr{S}^*(n,e) - \{A_0, A_0^T, A'_0\}$ and $\rho(A_0) < \rho(A'_0)$ if $t = 2c-3$. Fix a matrix $A \in \mathscr{S}^*(n,e) - \{A_0, A_0^T\}$. By considering A^T if necessary, we might assume that the number of 1's in $A[c|c)$ is no larger than that in $A(c|c]$. Let $(r_1, r_2, \ldots, r_n)$ denote the row-sum vector of A. Since $e \ge c^2+2$, $A[c+1 \mid c+1]$ is irreducible by Lemma 6.1, so $0 < r_{c+1} < \max(c+1, t)$. Let $s := r_{c+1}$. Applying Corollary 5.2 with $\ell = c+1$, $C = A$, partition $\Pi = \{\{1\}, \{2\}, \ldots, \{c\}, \{c+1, c+2, \ldots, n\}\}$, and the following $(c+1)\times(c+1)$ rooted matrix

$$M = \begin{pmatrix} J_s & J_{s\times(c-s)} & \begin{matrix} r_1 - c \\ r_2 - c \\ \vdots \end{matrix} \\ J_{(c-s)\times s} & J_{c-s} & r_c - c \\ J_{1\times s} & O_{1\times(c-s)} & 0 \end{pmatrix},$$

we have $\rho(A) \le \rho_r(M)$. To find $\rho_r(M)$, we consider the partition $\Pi_1 = \{\{1, 2, \ldots, s\}, \{s+1, \ldots, c\}, \{c+1\}\}$ of $[c+1]$, and observe that Π_1 is an equitable partition of M^T. According to $s = c$ or $s < c$, the equitable quotient matrix $\Pi_1(M^T)$ has one of the following two forms

$$\begin{pmatrix} c & 1 \\ a & 0 \end{pmatrix}, \quad \begin{pmatrix} s & c-s & 1 \\ s & c-s & 0 \\ a & b & 0 \end{pmatrix}, \tag{6.1}$$

respectively, where $a = \sum_{i=1}^{s}(r_i - c)$, $\quad b = \sum_{i=s+1}^{c}(r_i - c)$. Observe that the first matrix is the *degenerated* case of the second: the -1 value and the two eigenvalues of the first matrix form the three eigenvalues of the second matrix in the special case $s = c$ and $b = 0$.

Note that $A = A_0$ implies $s = \lceil \frac{t}{2} \rceil$, $a = \lfloor \frac{t}{2} \rfloor$ and $b = 0$. The converse is also true: Notice that

$$a + b + s + \sum_{i=c+2}^{n} r_i = t$$

holds generally in A. The conditions $s = \lceil \frac{t}{2} \rceil$, $a = \lfloor \frac{t}{2} \rfloor$ and $b = 0$ imply $A(c+1|c] = O_{(n-c-1)\times c}$ and $A[\{s+1, s+2, \ldots, c\}|c) = O_{(c-s)\times(n-c)}$, and $A(c+1|c] = O_{(n-c-1)\times c}$ also implies $A[c|c+1) = O_{c\times(n-c-1)}$ from the shape of A described in Lemma 6.1, so $A = A_0$ follows.

We will provide important constraints between s, a, b and t. Let r denote the number of zeros in $A[c|c]$. Then $a + b + r$ is the number of 1's in $A[c|c)$. From the assumption in the beginning, we have $a + b + r \leq (e - (c^2 - r))/2 = (t + r)/2$. Since the integer a is at most the number of 1's in $A[s|c)$, we have

$$a \leq a + b + r \leq (t + r)/2. \tag{6.2}$$

In particular, $a + b \leq (t - r)/2$ and

$$2a + b \leq t. \tag{6.3}$$

Since the number of 1's in $A(c|s]$ is $e - (c^2 - r) - (a + b + r) = t - a - b$, we have

$$s \leq t - a - b. \tag{6.4}$$

Since $\rho_r(M) = \rho_r(\Pi_1(M^T))$ by Lemma 4.5, it suffices to show $\rho(\Pi_1(M^T)) < \rho(A_0)$. The characteristic polynomial of $\Pi_1(M^T)$ in (6.1) is $f(x)/(x+1)$ or $f(x)$ according to $s = c$ or $s < c$, where

$$f(x) = x^3 - cx^2 - ax + a(c - s) - sb. \tag{6.5}$$

We use Calculus to study the shape of the polynomial $f(x)$. The derivative of $f(x)$ is $f'(x) = 3x^2 - 2cx - a$. If $x > c$, then

$$f'(x) > c(3c - 2c) - a = c^2 - a \geq c^2 - \frac{t + r}{2} \geq c^2 - \frac{2c + (c-1)^2}{2} \geq 0$$

by (6.2). Hence $f(x)$ is increasing in the interval (c, ∞). Since $\rho(A_0) > \rho(J_c) = c$, to prove $\rho_r(M) < \rho(A_0)$, it suffices to show that $f(\rho(A_0)) > 0$. Setting $s = a = \lceil \frac{t}{2} \rceil$ and $b = 0$ in (6.5), $\rho(A_0)$ is the largest zero of

$$g(x) := x^3 - cx^2 - \left\lfloor \frac{t}{2} \right\rfloor x + \left\lfloor \frac{t}{2} \right\rfloor \left(c - \left\lceil \frac{t}{2} \right\rceil \right). \tag{6.6}$$

Then

$$\begin{aligned} f(\rho(A_0)) =& f(\rho(A_0)) - g(\rho(A_0)) \\ =& \left(\left\lfloor \frac{t}{2} \right\rfloor - a \right) (\rho(A_0) - c) - s\,(a + b) + \left\lfloor \frac{t}{2} \right\rfloor \left\lceil \frac{t}{2} \right\rceil. \end{aligned} \tag{6.7}$$

If $a \leq \lfloor \frac{t}{2} \rfloor$, then we immediately have $f(\rho(A_0)) \geq 0$ from (6.7), since $s + a + b \leq t$ in (6.4) implies $s(a + b) \leq \lfloor \frac{t}{2} \rfloor \lceil \frac{t}{2} \rceil$; and indeed $f(\rho(A_0)) > 0$, since $f(\rho(A_0)) = 0$ only happens when $a = \lfloor \frac{t}{2} \rfloor = a + b$ and $s = \lceil \frac{t}{2} \rceil$, a contradiction to $A \neq A_0$. We assume $a > \lfloor \frac{t}{2} \rfloor$ for the remaining. By (6.3) and (6.4), we have $\max(2a+b+1, s+a+b+1) \leq t+1$, so

$$\begin{aligned} a + s(a+b) &\leq \begin{cases} a(a+b+1), & \text{if } s < a; \\ s(a+b+1), & \text{if } s \geq a \end{cases} \\ &\leq \left\lfloor \frac{t+1}{2} \right\rfloor \left\lceil \frac{t+1}{2} \right\rceil \\ &= \begin{cases} \left\lfloor \frac{t}{2} \right\rfloor + \left\lfloor \frac{t}{2} \right\rfloor \left\lceil \frac{t}{2} \right\rceil + 1, & \text{if } t \text{ is odd;} \\ \left\lfloor \frac{t}{2} \right\rfloor + \left\lfloor \frac{t}{2} \right\rfloor \left\lceil \frac{t}{2} \right\rceil, & \text{if } t \text{ is even.} \end{cases} \end{aligned}$$

Putting this information to (6.7) and using $\rho(A_0) < \rho(J_{c+1}) = c+1$, we have $f(\rho(A_0)) > 0$, except that t is odd, $s = a = (t+1)/2$, and $b = -1$. There is only one such matrix

$$A = \begin{pmatrix} J_{s\times s} & J_{s\times(c-1-s)} & J_{s\times 1} & J_{s\times 1} \\ J_{(c-1-s)\times s} & J_{(c-1-s)\times(c-1-s)} & J_{(c-1-s)\times 1} & O_{(c-1-s)\times 1} \\ J_{1\times s} & J_{1\times(c-1-s)} & 0 & 0 \\ J_{1\times s} & O_{1\times(c-1-s)} & 0 & 0 \end{pmatrix} \oplus O_{n-c-1},$$

where $s = (t+1)/2$. Thus $2 \leq t = 2s - 1 \leq 2c - 3$ and $c \geq 3$. To compute $\rho(A) = \rho(A[c+1|c+1])$, observe that $\Pi_2 := \{\{1, \ldots, s\}, \{s+1, \ldots, c-1\}, \{c\}, \{c+1\}\}$ is an equitable partition of $A[c+1|c+1]$ and the quotient matrix $\Pi_2(A[c+1|c+1])$ is

$$\begin{pmatrix} s & c-1-s & 1 & 1 \\ s & c-1-s & 1 & 0 \\ s & c-1-s & 0 & 0 \\ s & 0 & 0 & 0 \end{pmatrix},$$

which has characteristic polynomial

$$h(x) = x^4 - (c-1)x^3 + (1-c-s)x^2 + s(c-1-s)x + s(c-1-s).$$

For $x \geq c$, the derivative of $h(x)$ satisfies

$$\begin{aligned} h'(x) =& 4x^3 - 3(c-1)x^2 + 2(1-c-s)x + s(c-1-s) \\ \geq& x((4x - 3(c-1))x + 2(1-c-s)) \\ >& c((4c - 3(c-1))c + 2(1-c-(c-2))) \\ \geq& c((c+3)c - 4c + 6) > 0. \end{aligned}$$

Then $h(x)$ is strictly increasing in the interval (c, ∞). Using the polynomial g in (6.6),

$$h(x) - (x+1)g(x) = (c-1-s)x + c - 2s.$$

If $t \leq 2c-5$, then

$$\begin{aligned} h(\rho(A_0)) =& (c-1-s)\rho(A_0) + c - 2s \\ >& (c-1-(c-2))c + c - 2(c-2) = 4 > 0, \end{aligned}$$

concluding $\rho(A) < \rho(A_0)$, since $\rho(A_0) \in (c, \infty)$. If $2 \leq t = 2c-3$, then $s = c-1$, $A = A_0'$ and $h(\rho(A_0)) = c - 2(c-1) = -c+2 < 0$. Hence $\rho(A_0) < \rho(A_0')$. $\square$

Remark 6.2. The above proof also shows that in the case $t = 2c-3$, A_0 is the unique graph in $\mathscr{S}^*(n,e)$ attaining the second largest spectral radius.

6.2. $(0,1)$*-matrices with zero trace*

In this subsection, we study $(0,1)$-matrices with zero trace. This study is parallel to proving Conjecture C. For easier comparison, we suppress the meaning of $\mathscr{S}(n,e)$ in Conjecture C and let $\mathscr{S}(n,e)$ denote the set of $n \times n$ $(0,1)$-matrices with zero trace having exactly e ones. We will prove the following theorem.

Theorem 6.3. *If $e = c(c-1) + t$, where $2 \leq t \leq 2c-1$ are integers, and $A \in \mathscr{S}(n,e)$ attains the maximum spectral radius, then there exists a permutation matrix P such that PAP^T or PA^TP^T has the form*

$$A_0 = \begin{pmatrix} \multicolumn{2}{c}{J_c - I_c} & \begin{matrix} J_{\lfloor \frac{t}{2} \rfloor \times 1} \\ O_{(c-\lfloor \frac{t}{2} \rfloor)\times 1} \end{matrix} \\ J_{1\times\lceil \frac{t}{2}\rceil} \quad O_{1\times(c-\lceil \frac{t}{2}\rceil)} & & 0 \end{pmatrix} \oplus O_{n-c-1}. \tag{6.8}$$

For the not mentioned cases $t = 0$ and $t = 1$ in Theorem 6.3, Y. Jin and X. Zhang [15] proved that $PAP^T = (J_c - I_c) \oplus O_{n-c}$ if $t = 0$; $PAP^T = ((J_c - I_c) \oplus O_{n-c}) + E_{ij}$ if $t = 1$, where $i > c$ or $j > c$, and an additional situation in $e = 3$ $(c = 2, t = 1)$,

$$PAP^T = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \oplus O_{n-3}$$

is also possible. Y. Jin and X. Zhang [15] also proved Theorem 6.3 in the cases that t is relatively small.

Let $\mathscr{S}^*(n,e)$ denote the subset of $\mathscr{S}(n,e)$ which collects matrices $A = (a_{ij})$ satisfying

$$\text{if } a_{ij} = 1, \text{ then } a_{hk} = 1 \text{ for } h \leq i,\ k \leq j \text{ and } h \neq k.$$

The following lemma is similar to Lemma 6.1.

Lemma 6.4 *([15]). If $e = c(c-1)+t$, where $2 \le t \le 2c-1$, and $A \in \mathscr{S}(n,e)$ attains the maximum spectral radius, then there exists a permutation matrix P such that $PAP^T \in \mathscr{S}^*(n,e)$ and PAP^T has the form $A[k|k] \oplus O_{n-k}$ for some k and the submatrix $A[k|k]$ is irreducible.*

Proof of Theorem 6.3. Let $e = c(c-1)+t$, where $2 \le t \le 2c-1$. The matrix A_0 in (6.8) is in $\mathscr{S}^*(n,e)$. We will show that $\rho(A) < \rho(A_0)$ for every $A \in \mathscr{S}^*(n,e) - \{A_0, A_0^T\}$. Then Theorem 6.3 is proved by Lemma 6.4. The proof is almost a copy of the proof of Conjecture C. For the interested reader to check, we also provide the details. Other reader might go to the next section directly without missing important background.

By considering A^T if necessary, we might assume that the number of 1's in $A[c|c)$ is no larger than that in $A(c|c]$. Let $(r_1, r_2, \ldots, r_n)$ denote the row-sum vector of A. Since $A[c+1 \mid c+1]$ is irreducible by Lemma 6.4, $0 < r_{c+1} < \max(c+1, t)$. Let $s := r_{c+1}$. Applying Corollary 5.2 with $\ell = c+1$, $C = A$, partition $\Pi = \{\{1\}, \{2\}, \ldots, \{c\}, \{c+1, c+2, \ldots, n\}\}$, and the following $(c+1)\times(c+1)$ rooted matrix

$$M = \begin{pmatrix} J_s - I_s & J_{s\times(c-s)} & \begin{matrix} r_1 - c + 1 \\ r_2 - c + 1 \\ \vdots \end{matrix} \\ J_{(c-s)\times s} & J_{c-s} - I_{c-s} & r_c - c + 1 \\ J_{1\times s} & O_{1\times(c-s)} & 0 \end{pmatrix},$$

we have $\rho(A) \le \rho_r(M)$. To find $\rho_r(M)$, we consider the partition $\Pi_1 = \{\{1, 2, \ldots, s\}, \{s+1, \ldots, c\}, \{c+1\}\}$ of $[c+1]$, and observe that Π_1 is an equitable partition of M^T. According to $s = c$ or $s < c$, the equitable quotient matrix $\Pi_1(M^T)$ has one of the following two forms

$$\begin{pmatrix} c-1 & 1 \\ a & 0 \end{pmatrix}, \quad \begin{pmatrix} s-1 & c-s & 1 \\ s & c-s-1 & 0 \\ a & b & 0 \end{pmatrix}, \tag{6.9}$$

respectively, where $a = \sum_{i=1}^{s}(r_i - c + 1),\ b = \sum_{i=s+1}^{c}(r_i - c + 1)$. Observe that the first matrix is the degenerated case of the second. Note that $A = A_0$ implies $s = \lceil \frac{t}{2} \rceil$, $a = \lfloor \frac{t}{2} \rfloor$ and $b = 0$. The converse is also true: Notice that

$$a + b + s + \sum_{i=c+2}^{n} r_i = t$$

holds generally in A. The conditions $s = \lceil \frac{t}{2} \rceil$, $a = \lfloor \frac{t}{2} \rfloor$ and $b = 0$ imply $A(c+1|c] = O_{(n-c-1)\times c}$ and $A[\{s+1, s+2, \ldots, c\}|c) = O_{(c-s)\times(n-c)}$, and $A(c+1|c] = O_{(n-c-1)\times c}$ also implies $A[c|c+1) = O_{c\times(n-c-1)}$ from the shape of A described in Lemma 6.4, so $A = A_0$ follows.

We will provide important constraints between s, a, b and t, which are exactly the same as in Section 6.1. Let r denote the number of off-diagonal zeros in $A[c|c]$. Then $a+b+r$ is the number of 1's in $A[c|c)$. From the assumption in the beginning, we have $a+b+r \leq (t+r)/2$. Since the integer a is at most the number of 1's in $A[s|c)$, we have

$$a \leq a+b+r \leq (t+r)/2. \tag{6.10}$$

In particular, $a+b \leq (t-r)/2$ and

$$2a+b \leq t. \tag{6.11}$$

Since the number of 1's in $A(c|s]$ is $t-a-b$, we have

$$s \leq t-a-b. \tag{6.12}$$

Since $\rho_r(M) = \rho_r(\Pi_1(M^T))$ by Lemma 4.5, it suffices to show $\rho(\Pi_1(M^T)) < \rho(A_0)$. The characteristic polynomial of $\Pi_1(M^T)$ in (6.9) is $f(x)/(x+1)$ or $f(x)$ according to $s = c$ or $s < c$, where

$$f(x) = x^3 - (c-2)x^2 + (1-c-a)x + a(c-s-1) - sb. \tag{6.13}$$

We use Calculus to study the shape of the polynomial $f(x)$. If $x > c-1$, the derivative of $f(x)$ satisfies

$$\begin{aligned} f'(x) =& x(3x+2(2-c)) + 1 - c - a \\ >& (c-1)(3(c-1)+2(2-c)) + 1 - c - a \\ =& (c-1)c - a \geq c(c-1) - \frac{t+r}{2} \\ \geq& c(c-1) - \frac{2c-1+(c-1)(c-2)}{2} \geq 0 \end{aligned}$$

by (6.10). Hence $f(x)$ is increasing in the interval $(c-1, \infty)$. Since $\rho(A_0) > \rho(K_c) = c-1$, to prove $\rho_r(M) < \rho(A_0)$, it suffices to show that $f(\rho(A_0)) > 0$. Setting $s = \lceil \frac{t}{2} \rceil$, $a = \lfloor \frac{t}{2} \rfloor$, and $b = 0$ in (6.13), $\rho(A_0)$ is the largest zero of

$$g(x) := x^3 - (c-2)x^2 + \left(1 - c - \left\lfloor \frac{t}{2} \right\rfloor\right) x + \left\lfloor \frac{t}{2} \right\rfloor \left(c - \left\lceil \frac{t}{2} \right\rceil - 1\right). \tag{6.14}$$

Hence

$$\begin{aligned} f(\rho(A_0)) =& f(\rho(A_0)) - g(\rho(A_0)) \\ =& \left(\left\lfloor \frac{t}{2} \right\rfloor - a\right)(\rho(A_0) - c + 1) - s(a+b) + \left\lfloor \frac{t}{2} \right\rfloor \left\lceil \frac{t}{2} \right\rceil. \end{aligned} \tag{6.15}$$

As in Section 6.1, if $a \le \lfloor \frac{t}{2} \rfloor$, then we immediately have $f(\rho(A_0)) \ge 0$ from (6.15), since $s+a+b \le t$ in (6.12) implies $s(a+b) \le \lfloor \frac{t}{2} \rfloor \lceil \frac{t}{2} \rceil$; and indeed $f(\rho(A_0)) > 0$, since $f(\rho(A_0)) = 0$ only happens when $a = \lfloor \frac{t}{2} \rfloor = a+b$ and $s = \lceil \frac{t}{2} \rceil$, a contradiction to $A \ne A_0$. We assume $a > \lfloor \frac{t}{2} \rfloor$ for the remaining. By (6.11) and (6.12), we have $\max(2a+b+1, s+a+b+1) \le t+1$, so

$$\begin{aligned} a + s(a+b) &\le \begin{cases} a(a+b+1), & \text{if } s < a; \\ s(a+b+1), & \text{if } s \ge a \end{cases} \\ &\le \left\lfloor \frac{t+1}{2} \right\rfloor \left\lceil \frac{t+1}{2} \right\rceil \\ &= \begin{cases} \left\lfloor \frac{t}{2} \right\rfloor + \left\lfloor \frac{t}{2} \right\rfloor \left\lceil \frac{t}{2} \right\rceil + 1, & \text{if } t \text{ is odd;} \\ \left\lfloor \frac{t}{2} \right\rfloor + \left\lfloor \frac{t}{2} \right\rfloor \left\lceil \frac{t}{2} \right\rceil, & \text{if } t \text{ is even.} \end{cases} \end{aligned}$$

Putting this information to (6.15) and using $\rho(A_0) < \rho(J_{c+1} - I_{c+1}) = c$, we have $f(\rho(A_0)) > 0$, except that t is odd, $s = a = (t+1)/2$, and $b = -1$. There are two such matrices A and A^T and they have the same spectral radius, where

$$A = \begin{pmatrix} J_{s\times s} - I_s & J_{s\times(c-1-s)} & J_{s\times 1} & J_{s\times 1} \\ J_{(c-1-s)\times s} & J_{(c-1-s)\times(c-1-s)} - I_{c-1-s} & J_{(c-1-s)\times 1} & O_{(c-1-s)\times 1} \\ J_{1\times s} & J_{1\times(c-2-s)} \quad 0 & 0 & 0 \\ J_{1\times s} & O_{1\times(c-1-s)} & 0 & 0 \end{pmatrix} \oplus O_{n-c-1}.$$

Note that $s = r_{c+1} \le c-2$ in the above A, since a zero in the $(c, c-1)$ position causes a zero in $(c+1, c-1)$ position. To compute $\rho(A) = \rho(A[c+1|c+1])$, observe that $\Pi_2 := \{\{1,\ldots,s\},\{s+1,\ldots,c-1\},\{c\},\{c+1\}\}$ is an equitable partition of $A[c+1|c+1]$ and the quotient matrix $\Pi_2(A[c+1|c+1])$ is

$$\begin{pmatrix} s-1 & c-1-s & 1 & 1 \\ s & c-2-s & 1 & 0 \\ s & c-2-s & 0 & 0 \\ s & 0 & 0 & 0 \end{pmatrix},$$

which has characteristic polynomial

$$h(x) = x^4 - (c-3)x^3 + (4-2c-s)x^2 + ((c-2)(s-1) - s^2)x - s(s-c+2).$$

Since the derivative of $h(x)$ is

$$\begin{aligned} h'(x) =& 4x^3 - 3(c-3)x^2 + 2(4-2c-s)x + (c-2)(s-1) - s^2 \\ =& x(3x(x-(c-3)) + 8 - 4c - 2s) + (x^3 + (c-2)(s-1) - s^2), \end{aligned}$$

for $x \geq c-1 \geq s+1$, we have $h'(x) \geq x(3(c-1)\cdot 2+8-4c-2(c-2)) > 0$. Then $h(x)$ is strictly increasing in the interval $(c-1,\infty)$. Since $\rho(A_0) > \rho(J_c-I_c) = c-1$, to prove $\rho(A_0) > \rho(A)$, it suffices to show $h(\rho(A_0)) > 0$. Since $\rho(A_0)$ is the zero of the polynomial g in (6.14), we first compute

$$h(x)-(x+1)g(x) = (c-1-s)x+c-1-2s,$$

and then find

$$\begin{aligned} h(\rho(A_0)) =&(c-1-s)\rho(A_0)+c-1-2s \\ >&(c-1-(c-2))(c-1)+c-1-2(c-2) = 2. \quad \square \end{aligned}$$

Remark 6.5. If we follow the proof of Theorem 6.3 to symmetric $(0,1)$-matrices with zero trace, the proof will be finished in the middle. Hence this gives an alternative proof of Conjecture B.

6.3. Nonnegative matrices with prescribed sum of entries

We recall an old result in 1987 due to R. Stanley [23].

Theorem 6.6 *([23]). Let $C=(c_{ij})$ be an $n\times n$ symmetric $(0,1)$-matrix with zero trace. Let $2e$ be the number of 1's of C. Then*

$$\rho(C) \leq \frac{-1+\sqrt{1+8e}}{2},$$

with equality if and only if

$$e = \frac{k(k-1)}{2}$$

and there exists a permutation matrix P such that

$$PCP^T = (J_k-I_k)\oplus O_{n-k}$$

for some positive integer k.

The following theorem generalizes Theorem 6.6 to nonnegative matrices, not necessarily symmetric.

Theorem 6.7. *Let $C=(c_{ij})$ be an $n\times n$ nonnegative matrix. Let m be the sum of entries and d (resp. f) be the largest diagonal element (resp. the largest off-diagonal element) of M. Then*

$$\rho(C) \leq \frac{d-f+\sqrt{(d-f)^2+4mf}}{2}. \tag{6.16}$$

Moreover, if $f > 0$ then the equality in (6.16) holds if and only if there exists a permutation matrix P such that

$$PCP^T = (fJ_k + (d-f)I_k) \oplus O_{n-k} \tag{6.17}$$

for some positive integer k.

Proof. If $f = 0$ then the nonzero entries only appear in the diagonal of C, so $\rho(C) \leq d$ and (6.16) holds. Assume $f > 0$. Consider the $(n+1) \times (n+1)$ nonnegative matrix $C^+ = C \oplus O_1$ which has row-sum vector $(r_1, r_2, \ldots, r_n, r_{n+1})$ with $r_{n+1} = 0$ and a nonnegative left eigenvector v^T for $\rho(C^+) = \rho(C)$. Let $C' = M_{n+1}$ defined in (4.2) with $f_1 = f_2 = f$ such that C' has the same row-sum vector as C^+ and $C^+[n|n] \leq C'[n|n] = fJ_n + (d-f)I_n$. Note that C' has a positive rooted eigenvector $v' = (v'_1, v'_2, \ldots, v'_{n+1})^T$ for $\rho_r(C')$ by Lemma 4.6, so $v^T v' > 0$. Hence the assumptions of Theorem 3.4 hold with $(C, \lambda, \lambda') = (C^+, \rho(C^+), \rho_r(C'))$. Now by Theorem 3.4 and Lemma 4.7(ii), we have

$$\rho(C) = \rho(C^+) \leq \rho_r(C') = \frac{d-f+\sqrt{(d-f)^2+4mf}}{2},$$

finishing the proof of the first part.

To prove the sufficiency in the second part, assume $f > 0$ and (6.17). Note that $m = k^2 f + k(d-f)$. Using $\rho(C) = \rho(PCP^T) = \rho(fJ_k + (d-f)I_k)$, we have

$$\rho(C) = kf + (d-f) = \frac{d-f+\sqrt{(d-f)^2+4mf}}{2}.$$

For proving necessity, assume $f > 0$ and $\rho(C) = \rho_r(C')$. Then $C \neq O_n$ and $C^+ \neq O_{n+1}$. We will apply Theorem 3.4 with $C = C^+ = (c^+_{ij})$. Let $v^T = (v_1, v_2, \ldots, v_{n+1})$ be a nonnegative left eigenvector of C^+ for $\rho(C^+)$. Then $v_{n+1} = 0$. By rearranging the indices of C we might assume that for some $k \leq n$, $r_i > 0$ for $1 \leq i \leq k$ and $C^+(k|n+1] = O_{(n+1-k)\times(n+1)}$. Since r_i are also row-sums of C' and by Lemma 4.3(ii), we have $v'_j > v'_{n+1}$ for $1 \leq j \leq k$. By Theorem 3.4(b), we have $c^+_{ij} = c'_{ij}$ for $1 \leq i \leq n$, $1 \leq j \leq k$ with $v_i \neq 0$. With $v[k]^T := (v_1, v_2, \ldots, v_k)$, we have

$$\rho(C)v^T = v^T C^+ = v[k]^T C^+[k|n+1] \tag{6.18}$$

and

$$v[k]^T C^+[k|k] = v[k]^T C'[k|k] = v[k]^T (fJ_k + (d-f)I_k). \tag{6.19}$$

From (6.18) and (6.19), we have

$$\rho(C)v[k]^T = v[k]^T C^+[k|k] = v[k]^T (fJ_k + (d-f)I_k).$$

Since $v[k]^T$ is a left eigenvector of the irreducible matrix $fJ_k+(d-f)I_k$, $v[k]^T$ is positive, so $C[k|k] = C^+[k|k] = C'[k|k] = fI_k + (d-f)I_k$. For $k+1 \leq i \leq n+1$, we have $v_i = 0$ by Theorem 3.4(b), since $0 = c^+_{i1} \neq c'_{i1} = f$. Using (6.18) again, the last $n+1-k$ columns of C^+ are zero. Hence $C^+ = (fJ_k + (d-f)I_k) \oplus O_{n+1-k}$, and consequently $C = (fJ_k + (d-f)I_k) \oplus O_{n-k}$. □

7. Concluding remarks

In this paper, we have developed a tool to obtain both upper and lower bounds for the spectral radius of a nonnegative matrix. This assists obtaining known and new results more visually and also make them easier to improve. The key tool, Theorem 3.4, and the main result, Corollary 5.2, are special cases of Lemma 3.1 when a specific triple (C', P, Q) of square matrices is chosen according to a given square matrix C. Let us consider the simplest case that C is a binary matrix. By choosing $P = I_n$, $Q = I_n + \sum_{i=1}^n E_{in}$, and C' obtained from J_n by changing the entries in its last column to maintain the same row-sums with C, we can check easily at least the condition $PCQ \leq PC'Q$ in Lemma 3.1(i) holds and expect the remaining conditions (ii)-(iv) hold to conclude that $\rho(C) \leq \rho(C')$.

We believe it is worth focusing more on investigating the bounds derived from selecting other triples of (C', P, Q), as this exploration may be helpful in solving many extremal problems related to graphs and their spectral radii. For example, a result of P. Csikvári in 2009 [5] stating that the spectral radius of a symmetric $(0,1)$ matrix C will not be decreased after a *Kelmans transformation* [16] can be reproved by the method in this paper taking $P = I_n + E_{ij} = Q^T$ and C' to be the Kelmans transformation of C from i to j. This result extends to a nonsymmetric matrix with a minor assumption by essentially the same proof [17].

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Data availability

No data was used for the research described in the article.

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