

Maximizing the numerical radii of matrices by permuting their entries

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Dedicated to Professor Pei Yuan Wu.

Abstract

Let A be an $n \times n$ complex matrix such that every row and every column has at most one nonzero entry. We determine permutations of the nonzero entries of A so that the resulting matrix has maximum numerical radius. Extension of the results to operators acting on separable Hilbert spaces are also obtained. Related results and additional problems are also mentioned.

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1 Introduction

Let $B(H)$ be the set of bounded linear operators acting on a Hilbert space H equipped with the inner product (\cdot, \cdot) . If H has dimension n , we identify H with \mathbb{C}^n and $B(H)$ with M_n , the set of $n \times n$ complex matrices; the inner product $(x, y) = y^*x$ will be used. The *numerical range* of $T \in B(H)$ and the *numerical radius* are defined by

$$W(T) = \{(Tx, x) : x \in H, (x, x) = 1\} \quad \text{and} \quad w(T) = \sup\{|\mu| : \mu \in W(T)\},$$

which have been studied extensively; see [6, 7, 8].

Suppose $\{E_{11}, E_{12}, \dots, E_{nn}\}$ is the standard basis for M_n , and $a_1, \dots, a_{n-1} \in \mathbb{C}$. Then a weighted shift operator in M_n has the form $T = a_1E_{12} + \dots + a_{n-1}E_{n-1,n}$. Professor Pei Yuan Wu and his colleagues have obtained many interesting properties of weighted shift operators (see [10, 11, 12]) and raised the following.

Problem A *Determine a permutation σ of $(1, \dots, n-1)$ so that $T_\sigma = a_{\sigma(1)}E_{12} + \dots + a_{\sigma(n-1)}E_{n-1,1}$ will yield the maximum numerical radius.*

Wu and his collaborators verified that for $n \leq 7$, the maximum numerical radius will occur at T_σ such that

$$|a_{\sigma(1)}| \leq |a_{\sigma(n-1)}| \leq |a_{\sigma(2)}| \leq |a_{\sigma(n-2)}| \leq \dots$$

For example, if $(a_1, \dots, a_6) = (1, 2, 3, 4, 5, 6)$, then the weighted shift with maximum numerical radius is attained at the matrix

$$T_\sigma = \begin{pmatrix} 0 & 1 & & & & \\ & 0 & 3 & & & \\ & & 0 & 5 & & \\ & & & 0 & 6 & \\ & & & & 0 & 4 \\ & & & & & 0 & 2 \\ & & & & & & 0 \end{pmatrix}.$$

In [2], the authors confirmed the above result is true for general n , and also described the permutation σ of $(1, \dots, n)$ so that a cyclic weighted shift matrix

$$A_\sigma = a_{\sigma(1)}E_{12} + \dots + a_{\sigma(n-1)}E_{n-1,1} + a_{\sigma(n)}E_{n,1}$$

will yield the maximum numerical radius. Furthermore, they extended their results to (unilateral or bilateral) weighted shifts operators acting on separable Hilbert spaces.

In this paper, we consider a more general class of matrices, and solve the following.

Problem B *Suppose $A \in M_n$ is such that every row and every column has at most one nonzero entry. Determine the permutation(s) of the nonzero entries so that the resulting matrix will yield the maximum numerical radius.*

We will extend the results to operators acting on separable Hilbert spaces. Note that the numerical range of zero-one matrices such that every row and every column has at most one nonzero entry was studied in [9].

Our paper is organized as follows. In Section 2, we present some preliminary results which allow us to reduce the general study to simple special cases, and introduce some graph theory and optimization problem results that are helpful to our study. The main theorem and other auxiliary results of independent interest are presented in Section 3. Related results and questions are mentioned in Section 4.

2 Preliminary

2.1 Reduction of the problem to nonnegative symmetric matrices

For $A = (a_{ij}) \in M_n$, denote by $|A| = (|a_{ij}|)$, and $\lambda_1(A + A^*)$ the largest eigenvalue of the Hermitian matrix $A + A^*$. We have the following well known fact. We give a short proof for completeness.

Lemma 2.1 *Let $A \in M_n$. Then*

$$w(A) \leq w(|A|) = \lambda_1(|A| + |A|^t)/2.$$

Proof. The statement follows from the fact that

$$|x^* Ax| \leq |x|^* |A| |x| = |x|^* \left(\frac{|A| + |A|^t}{2} \right) |x| \leq \lambda_1 \left(\frac{|A| + |A|^t}{2} \right) |x|$$

for any unit vector $x \in \mathbb{C}^n$. ■

Proposition 2.2 *Suppose $A \in M_n$ is such that every row and every column of A has at most one nonzero entries. Then A is permutationally similar to a direct sum of A_1, \dots, A_m and a diagonal matrix D such that every A_j is either a weighted shift or a weighted cyclic matrix. Moreover, we have*

$$w(A) = w(|A|) = \lambda_1(|A| + |A|^t)/2.$$

Proof. Suppose that every row and every column of $A \in M_n$ has at most one nonzero entry. We can associate with the matrix $A = (a_{ij}) \in M_n$ a directed graph $\Gamma(A)$ with vertices $1, \dots, n$, such that there is an arc from vertex i to vertex j if $a_{ij} \neq 0$. Then $\Gamma(A)$ consists of directed cycles, directed paths, self-loops, and null (isolated) vertices. Every directed cycle corresponds to a weighted cyclic principal submatrix, every directed path corresponds to a weighted shift principal submatrix, and grouping the self-loops and null vertices will give rise to the diagonal principal submatrix. Thus, we get the first statement.

Note that a weighted shift matrix $B = \sum_{j=1}^r b_j E_{j,j+1}$ is unitarily similar to $|B|$ via a diagonal unitary matrix $U = \text{diag}(u_1, \dots, u_{r+1})$ such that $u_j \bar{u}_{j+1} b_j = |b_j|$ for $j = 1, \dots, r$, with $u_1 = 1$. Also, if $B = \sum_{j=1}^{r-1} b_j E_{j,j+1} + b_r E_{r,1}$ is weighted cyclic matrix such that $\det(B) = \rho e^{i\theta}$ with $\rho > 0$ and $\theta \in [0, 2\pi)$, then B is unitarily similar to $e^{i\theta/r} |B|$ via a unitary matrix $U = \text{diag}(u_1, \dots, u_r)$ such that $u_j \bar{u}_{j+1} b_j = e^{i\theta/r} |b_j|$ for $j = 1, \dots, r$ with $u_{r+1} = u_1 = 1$. Thus, $w(A_j) = w(|A_j|)$ for $j = 1, \dots, m$, and hence

$$\begin{aligned} w(A) &= \max(\{w(A_j) : j = 1, \dots, m\} \cup \{w(D)\}) \\ &= \max(\{w(|A_j|) : j = 1, \dots, m\} \cup \{w(|D|)\}) = w(|A|). \end{aligned} \quad \blacksquare$$

By the above proposition, to determine the permutation σ of the nonzero entries of a matrix A with at most one nonzero entry in each row and column to get A_σ which attains the maximum numerical radius, we may assume that the weights are nonnegative and focus on

$$w(A_\sigma) = \lambda_1(A_\sigma + A_\sigma^t)/2,$$

when A_σ is a diagonal matrix, weighted shift matrix, or a weighted cyclic matrix.

Clearly, if A is a diagonal matrix, then $w(A_\sigma)$ are the same for any permutation of the nonzero diagonal entries. We will consider the permutation of nonzero weights to yield maximum numerical radius when A is a direct sum of weighted shift matrices, or when A is a direct sum of weighted cyclic matrices in the next two sections. Since $w(A_\sigma) = \lambda_1(A_\sigma + A_\sigma^t)/2$, we will focus on the problem of maximizing the largest eigenvalue of a nonnegative symmetric matrix by permuting its nonzero entries.

2.2 Connection to graph theory and optimization problems

We can associate an undirected graph $G(A)$ to every symmetric matrix $A = (a_{ij}) \in M_n$ with vertices $1, \dots, n$ and there is an edge between vertex i and vertex j if $a_{ij} = a_{ji} \neq 0$. On the other hand, we can construct an adjacency matrix $A(G) \in M_n$ for every graph with n vertices $1, 2, \dots, n$, so that the (i, j) th entry and (j, i) th entry of $A(G)$ equal one if there is an edge joining vertex i and vertex j .

It turns out that our study is closely related to the following.

Problem C Suppose $A \in M_n$ is the adjacency matrix associate with the path graph G consisting of edges $(1, 2), (2, 3), \dots, (n-1, n)$ so that

$$A = \sum_{j=1}^{n-1} (E_{j,j+1} + E_{j+1,j}) = \begin{pmatrix} 0 & 1 & & & \\ 1 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & 1 & \\ & & & & 1 & 0 \end{pmatrix}.$$

For a given vector $x = (x_1, \dots, x_n)^t$ with nonnegative entries, determine the permutation P such that

$$x^t P^t A P x \geq x^t Q^t A Q x \quad \text{for any permutation } Q \in M_n.$$

Clearly, the above problem can be formulated as follows. For a vector $x = (x_1, \dots, x_n)^t$ with nonnegative entries, determine the permutations σ of $(1, \dots, n)$ that yield the maximum quadratic form

$$\sum_{j=1}^{n-1} x_{\sigma(j)} x_{\sigma(j+1)}.$$

It is known that the permutation σ attaining the maximum must satisfy

$$x_{\sigma(1)} \leq x_{\sigma(n)} \leq x_{\sigma(2)} \leq x_{\sigma(n-1)} \leq \dots, \quad \text{or} \quad x_{\sigma(n)} \leq x_{\sigma(1)} \leq x_{\sigma(n-1)} \leq x_{\sigma(2)} \leq \dots;$$

[3, Theorem 1.4] (see also [1, Lemma 2.1] and [2, Lemma 2.3]).

As we will see in the subsequent discussion, it is convenient to relabel the vertices of the path graph so that the adjacency matrix has the form

$$E_{12} + E_{21} + \sum_{j=3}^n (E_{j-2,j} + E_{j,j-2}) = \begin{pmatrix} 0 & 1 & 1 & & & \\ 1 & 0 & 0 & 1 & & \\ & 1 & 0 & \ddots & \ddots & \ddots \\ & & \ddots & \ddots & \ddots & \ddots & 1 \\ & & & \ddots & \ddots & \ddots & 0 \\ & & & & 1 & 0 & 0 \end{pmatrix},$$

and restate the above result as follows.

Proposition 2.3 Suppose $H_{n-1} = E_{12} + E_{21} + \sum_{j=3}^n (E_{j-2,j} + E_{j,j-2})$, and suppose $x = (x_1, \dots, x_n)^t$ with $x_1 \geq \dots \geq x_n \geq 0$. Then a permutation matrix P satisfies

$$2 \left(x_1 x_2 + \sum_{j=3}^n x_{j-2} x_j \right) = x^t P^t H_{n-1} P x \geq x^t Q^t H_{n-1} Q x \quad \text{for any permutation } Q \in M_n \quad (2.1)$$

if and only if $Px = (x_1, \dots, x_n)^t$.

For example, suppose $x = (1, 2, 3, 4, 5, 6, 7)^t$. If the adjacency matrix of the path graph with 7 vertices is depicted as

$$A = \sum_{j=1}^6 (E_{j,j+1} + E_{j+1,j}) = \begin{pmatrix} 0 & 1 & & & & & \\ 1 & 0 & 1 & & & & \\ & 1 & 0 & 1 & & & \\ & & 1 & 0 & 1 & & \\ & & & 1 & 0 & 1 & \\ & & & & 1 & 0 & 1 \\ & & & & & 1 & 0 \end{pmatrix},$$

then $x^t P^t A P x$ attains the maximum value if and only if

$$P x = (1, 3, 5, 7, 6, 4, 2)^t \quad \text{or} \quad P x = (2, 4, 6, 7, 5, 3, 1)^t.$$

On the other hand, if we relabel the vertices and use the adjacency matrix

$$H_6 = E_{12} + E_{21} + \sum_{j=2}^5 (E_{j-1,j+1} + E_{j+1,j-1}) = \begin{pmatrix} 0 & 1 & 1 & & & & \\ 1 & 0 & 0 & 1 & & & \\ 1 & 0 & 0 & 0 & 1 & & \\ & 1 & 0 & 0 & 0 & 1 & \\ & & 1 & 0 & 0 & 0 & 1 \\ & & & 1 & 0 & 0 & 0 \\ & & & & 1 & 0 & 0 \end{pmatrix},$$

then $x^t P H_6 P x$ attains the maximum if and only if $P x = (6, 5, 4, 3, 2, 1)^t$.

3 Main Results

In the following discussion, we always use the following matrices in M_n :

$$H_1 = E_{12} + E_{12}, \quad \text{and} \quad H_j = H_{j-1} + (E_{j-1,j+1} + E_{j+1,j-1}) \quad \text{for} \quad j = 2, \dots, n-1. \quad (3.1)$$

For example, if $n = 5$, then

$$H_1 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad H_2 = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad H_3 = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad H_4 = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}.$$

3.1 Weighted shift matrices

We begin with a slight extension of the Proposition 2.3. Denote by $r(A)$ the *spectral radius* of $A \in M_n$. Note that if A is nonnegative, then $r(A)$ is actually an eigenvalue of A , and is called the *Perron eigenvalue* or the *Perron root* of A ; the corresponding unit eigenvector with nonnegative entries is called the *Perron eigenvector*.

Proposition 3.1 *Let $S(n, k)$, where $1 \leq k < n$, be the set of matrices $A \in M_n$ with sum of entries equal to $2k$ such that A is a direct sum of A_1, \dots, A_m and the zero matrix such that each A_j is*

the adjacency matrix of a path graph. Suppose H_1, \dots, H_{n-1} are defined as in (3.1). Then for any vector $x = (x_1, \dots, x_n)^t$ with $x_1 \geq \dots \geq x_n > 0$,

$$x^t H_k x \geq x^t A x \quad \text{for any } A \in S(n, k).$$

Consequently,

$$r(H_k) \geq r(A) \quad \text{for all } A \in S(n, k).$$

The above proposition asserts that among the adjacency matrices of graphs with n vertices and k edges forming disjoint paths, the optimal quadratic form will attain at an adjacency matrix with a single path with k edges.

Proof. Suppose $A \in S(n, k)$ is the adjacency matrix of a path with k edges together with some isolated vertices if $k < n - 1$. Then there is a $(k + 1) \times (k + 1)$ principal submatrix \hat{A} of A corresponding to the path, and $\tilde{x} = (x_{i_1}, \dots, x_{i_{k+1}})^t$, where i_1, \dots, i_{k+1} are distinct elements in $\{1, \dots, n\}$, and a permutation $P \in M_k$

$$x^t A x = \tilde{x}^t \hat{A} \tilde{x} \leq \tilde{x}^t P^t \hat{H}_k P \tilde{x} \leq x^t H_k x$$

by Proposition 2.3, where \hat{H}_k is the leading principal submatrix of H_k of size $k + 1$.

Suppose $A \in S(n, k)$ corresponds to a graph with at least 2 disjoint paths. Let A_1 and A_2 be two principal submatrices of A corresponding to disjoint paths with $p - 1$ edges and $q - 1$ edges, respectively. Then there are two vectors $v_1 = (x_{i_1}, \dots, x_{i_p})^t$ and $v_2 = (x_{j_1}, \dots, x_{j_q})^t$ such that (i_1, \dots, i_p) and (j_1, \dots, j_q) are increasing subsequences of $(1, \dots, n)$ with no common terms satisfying

$$x^t A x = v_1^t A_1 v_1 + v_2^t A_2 v_2 + \Delta,$$

where Δ is the sum of the rest of the terms in the quadratic form. Suppose $i_p \leq j_q$. Then

$$\begin{aligned} x^t A x &= v_1^t A_1 v_1 + v_2^t A_2 v_2 + \Delta \\ &\leq 2(x_{i_1} x_{i_2} + \sum_{\ell=3}^p x_{i_{\ell-2}} x_{i_\ell}) + 2(x_{j_1} x_{j_2} + \sum_{\ell=3}^q x_{j_{\ell-2}} x_{j_\ell}) + \Delta \\ &\leq 2(x_{i_1} x_{i_2} + \sum_{\ell=3}^p x_{i_{\ell-2}} x_{i_\ell}) + 2(x_{j_1} x_{j_2} + \sum_{\ell=3}^{q-1} x_{j_{\ell-2}} x_{j_\ell} + x_{j_{q-2}} x_{i_p}) + \Delta \\ &= x^t \tilde{A} x, \end{aligned}$$

where $\tilde{A} \in S(n, k)$ is obtained from A by replacing the two principal submatrices A_1 and A_2 by \tilde{A}_0 corresponding to a path with $p + q - 2$ edges connecting the vertices

$$i_{p-1}, i_{p-3}, \dots, i_{p-2}, i_p, j_{q-2}, j_{q-4}, \dots, j_{q-3}, j_{q-1}.$$

If \tilde{A} corresponds to a graph with a single path, then $x^t \tilde{A} x \leq x^t H_k x$. Otherwise, we can repeat the argument to show that $x^t \tilde{A} x \leq x^t \hat{A} x$ where \hat{A} has one fewer path. Repeating this process, we see that $x^t A x \leq x^t B x$ for some adjacency matrix B corresponding to a graph consisting of a path with k edges. By the conclusion in the first paragraph of the proof, we see that $x^t B x \leq x^t H_k x$.

For any $A \in S(n, k)$, there is a nonnegative eigenvector x of unit length such that

$$\lambda_1(A) = x^* Ax \leq x^* P^t H_k P x \leq \lambda_1(H_k),$$

where P is a permutation matrix so that Px has entries arranged in descending order. The last assertion follows. \blacksquare

Next, we determine the optimal quadratic form of an adjacency matrix of a weighted path.

Theorem 3.2 *Let $a_1 \geq \dots \geq a_{n-1} > 0$, and let*

$$A = a_1(E_{12} + E_{21}) + \sum_{j=2}^{n-1} a_j(E_{j-1,j+1} + E_{j+1,j-1}) = \begin{pmatrix} 0 & a_1 & a_2 & & & \\ a_1 & 0 & 0 & a_3 & & \\ a_2 & 0 & 0 & 0 & \ddots & \\ a_3 & 0 & 0 & 0 & 0 & a_{n-1} \\ & & \ddots & 0 & 0 & 0 \\ & & & a_{n-1} & 0 & 0 \end{pmatrix}.$$

Then for any $x = (x_1, \dots, x_n)^t$ with nonnegative entries arranged in descending order, and for any permutation matrix P , we have

$$x^t Ax \geq x^t P^t A P x.$$

Consequently, if σ is a permutation of $(1, \dots, n-1)$, and

$$A_\sigma = a_{\sigma(1)}(E_{12} + E_{21}) + \dots + \sum_{j=2}^{n-1} a_{\sigma(j)}(E_{j-1,j+1} + E_{j+1,j-1}),$$

then

$$r(A) \geq r(A_\sigma);$$

the equality holds if and only if $A = A_\sigma$.

Note that A_σ in the above theorem can be expressed as $\sum_{j=1}^{n-1} \gamma_j A_j$, where

- $\gamma_j = a_j - a_{j+1}$ for $j = 1, \dots, n-2$, $\gamma_{n-1} = a_{n-1}$,
- $A_{n-1} = (E_{12} + E_{21}) + \sum_{j=2}^{n-1} (E_{j-1,j+1} + E_{j+1,j-1})$, and
- A_j is obtained from A_{j+1} by removing a pair of ones in two symmetric positions for $j = n-2, \dots, 1$.

For example,

$$A = \begin{pmatrix} 0 & 3 & 8 & 0 & 0 \\ 3 & 0 & 0 & 1 & 0 \\ 8 & 0 & 0 & 0 & 5 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 5 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} + 2 \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} + 2 \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} + 3 \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Thus, Theorem 3.2 can be restated and proved in the following equivalent form.

Theorem 3.3 Suppose A_{n-1} is the adjacency matrix of a length $n-1$ path joining n vertices, and A_j is obtained from A_{j+1} by removing a pair of ones in two symmetric positions for $j = n-2, \dots, 1$. Let H_1, \dots, H_{n-1} be defined as in (3.1). Then for any vector $x = (x_1, \dots, x_n)^t$ with $x_1 \geq \dots \geq x_n > 0$, and any nonnegative numbers $\gamma_1, \dots, \gamma_{n-1}$,

$$x^t \left(\sum_{j=1}^{n-1} \gamma_j H_j \right) x \geq x^t \left(\sum_{j=1}^{n-1} \gamma_j A_j \right) x. \quad (3.2)$$

Suppose $\gamma_{n-1} > 0$ and x is the Perron vector for $\sum_{j=1}^{n-1} \gamma_j H_j$, the equality holds if and only if

$$\sum_{j=1}^{n-1} \gamma_j H_j = \sum_{j=1}^{n-1} \gamma_j A_j.$$

Proof. The inequality (3.2) follows from Theorem 3.1. To prove the last assertion, suppose $\gamma_{n-1} > 0$ and x is the Perron vector for $\hat{H} = \sum_{j=1}^{n-1} \gamma_j H_j$. Then

$$x^t \left(\sum_{j=1}^{n-1} \gamma_j H_j \right) x = x^t \left(\sum_{j=1}^{n-1} \gamma_j A_j \right) x. \quad (3.3)$$

only if $\gamma_j x^t H_j x = \gamma_j x^t A_j x$ for all $k = 1, \dots, n-1$.

Let us first analyze the Perron vector $x = (x_1, \dots, x_n)^t$ where $x_1 \geq \dots \geq x_n > 0$. Let $a_k = \gamma_k + \dots + \gamma_{n-1}$ for $k = 1, \dots, n$.

1. Writing $x^t \hat{H} x = 2(a_1 x_1 x_2 + a_2 x_1 x_3 + a_3 x_2 x_4 + \Delta)$, we see that if $x_1 = x_2$ then $a_2 x_3 = a_3 x_4$ and hence $x_3 = x_4$ and $a_2 = a_3$.

In fact, if $a_2 x_3 > a_3 x_4$, then for $\hat{x}_1 = \sqrt{x_1^2 + \varepsilon}$ and $\hat{x}_2 = \sqrt{x_2^2 - \varepsilon}$ with a sufficiently small $\varepsilon > 0$, we have

$$a_1 \hat{x}_1 \hat{x}_2 + a_2 \hat{x}_1 x_3 + a_3 \hat{x}_2 x_4 > a_1 x_1 x_2 + a_2 x_1 x_3 + a_3 x_2 x_4,$$

contradicting the fact that $x^t \hat{H} x \geq y^t \hat{H} y$ for all unit vector y .

We will use a similar reasoning in the next few cases.

2. Writing $x^t \hat{H} x = 2(a_{n-2} x_{n-3} x_{n-1} + a_{n-1} x_{n-2} x_n + \Delta)$, we see that if $x_{n-1} = x_n$ then $a_{n-2} x_{n-3} = a_{n-1} x_{n-2}$ and hence $x_{n-3} = x_{n-2}$ and $a_{n-2} = a_{n-1}$.
3. Writing $x^t \hat{H} x = 2(a_{i-1} x_{i-2} x_i + a_{i+1} x_i x_{i+2} + a_i x_{i-1} x_{i+1} + a_{i+2} x_{i+1} x_{i+3} + \Delta)$, we see that if $x_i = x_{i+1}$ then $a_{i-1} x_{i-2} + a_{i+1} x_{i+2} = a_i x_{i-1} + a_{i+2} x_{i+3}$ and hence $x_{i-2} = x_{i-1}$, $x_{i+2} = x_{i+3}$, $a_{i-1} = a_i$ and $a_{i+1} = a_{i+2}$ for $i = 2, \dots, n-3$.
4. Writing $x^t \hat{H} x = 2(a_{n-3} x_{n-4} x_{n-2} + a_{n-1} x_{n-2} x_n + a_{n-2} x_{n-3} x_{n-1} + \Delta)$, we see that it is impossible to have $x_{n-2} = x_{n-1}$.

5. If $a_i = a_{i+1}$ then the partial sum $a_{i+1}x_i x_{i+2} + a_i x_{i-1} x_{i+1}$ will be greater if we replace $(x_{i-1}, x_i, x_{i+1}, x_{i+2})$ by

$$\left(\sqrt{(x_{i-1}^2 + x_i^2)/2}, \sqrt{(x_{i-1}^2 + x_i^2)/2}, \sqrt{(x_{i+1}^2 + x_{i+2}^2)/2}, \sqrt{(x_{i+1}^2 + x_{i+2}^2)/2} \right),$$

for $i = 2, 3, \dots, n-2$.

We can deduce the following:

- (a) If n is even and $a_1 \geq a_2 = a_3 \geq a_4 = a_5 \geq \dots \geq a_{n-2} = a_{n-1}$, then $x_1 = x_2 > x_3 = x_4 > x_5 = x_6 > \dots > x_{n-1} = x_n$.
- (b) If n is odd and $a_1 = a_2 \geq a_3 = a_4 \geq a_5 = a_6 \geq \dots \geq a_{n-2} = a_{n-1}$, then $x_1 > x_2 = x_3 > x_4 = x_5 > \dots > x_{n-1} = x_n$.
- (c) If n is even and $a_{2k} \neq a_{2k+1}$ for some k , or n is odd and $a_{2k-1} \neq a_{2k}$ for some k , then $x_1 > x_2 > \dots > x_n$.

Translating the above observation in terms of γ 's, we have:

If $\gamma_{n-2} = \gamma_{n-4} = \gamma_{n-6} = \dots = 0$, then $x_n = x_{n-1} < x_{n-2} = x_{n-3} < \dots$.

Otherwise, we have $x_1 > x_2 > \dots > x_n$.

If $\gamma_j = 0$ then $\gamma_j H_j = \gamma_j A_j$. If $\gamma_j \neq 0$ then $x^t H_j x = x^t A_j x$, hence A_j must be an adjacency matrix to attain the maximum, and the 1's have to be assigned to the edges corresponding to the largest $x_i x_j$'s, and thus $H_j = A_j$. ■

We have the following simple corollary.

Corollary 3.4 *Suppose we are going to assign weights $a_1 \geq a_2 \geq \dots \geq a_{n-1} \geq 0$ to a collection of paths of different lengths in order to maximize the numerical radius of the adjacency matrix, then we should assign the largest a_j 's to the path with maximal length in the way as in Theorem 3.2.*

3.2 Weighted Cyclic Matrices

We can determine the optimal quadratic form of an adjacency matrix of a weighted cycle. In this subsection, we always assume that $n \geq 3$.

Theorem 3.5 *Let $a_1 \geq \dots \geq a_n > 0$, and let*

$$\begin{aligned} A &= a_1(E_{12} + E_{21}) + \sum_{j=2}^{n-1} a_j(E_{j-1,j+1} + E_{j+1,j-1}) + a_n(E_{n-1,n} + E_{n,n-1}) \\ &= \begin{pmatrix} 0 & a_1 & a_2 & & & \\ a_1 & 0 & 0 & a_3 & & \\ a_2 & 0 & 0 & 0 & \ddots & \\ & a_3 & 0 & 0 & 0 & a_{n-1} \\ & & \ddots & 0 & 0 & a_n \\ & & & a_{n-1} & a_n & 0 \end{pmatrix}. \end{aligned}$$

Then for any $x = (x_1, \dots, x_n)^t$ with nonnegative entries arranged in descending order, and for any permutation matrix P , we have

$$x^t A x \geq x^t P^t A P x.$$

Consequently, if σ is a permutation of $(1, \dots, n)$, and

$$A_\sigma = a_{\sigma(1)}(E_{12} + E_{21}) + \dots + \sum_{j=2}^{n-1} a_{\sigma(j)}(E_{j-1,j+1} + E_{j+1,j-1}) + a_{\sigma(n)}(E_{n-1,n} + E_{n,n-1}),$$

then

$$r(A) \geq r(A_\sigma);$$

the equality holds if and only if $A = A_\sigma$.

We can reformulate Theorem 3.5 and prove it using Theorem 3.3. We will make use of the matrices H_1, \dots, H_{n-1} in (3.1) together with the matrix

$$H_n = H_{n-1} + E_{n-1,n} + E_{n,n-1} = \begin{pmatrix} 0 & 1 & 1 & & & \\ 1 & 0 & 0 & 1 & & \\ & 1 & 0 & 0 & \ddots & \\ & & \ddots & 0 & 0 & 1 \\ & & & 1 & 1 & 0 \end{pmatrix}. \quad (3.4)$$

Theorem 3.6 Suppose A_n is the adjacency matrix of a cycle joining n vertices, and A_j is obtained from A_{j+1} by removing a pair of ones in two symmetric positions for $j = n-1, \dots, 1$. Let H_1, \dots, H_n be defined as in (3.1) and (3.4). Then for any vector $x = (x_1, \dots, x_n)^t$ with $x_1 \geq \dots \geq x_n > 0$, and any nonnegative numbers $\gamma_1, \dots, \gamma_n$,

$$x^t \left(\sum_{j=1}^n \gamma_j H_j \right) x \geq x^t \left(\sum_{j=1}^n \gamma_j A_j \right) x. \quad (3.5)$$

Proof. By Theorem 3.3,

$$x^t \left(\sum_{j=1}^{n-1} \gamma_j H_j \right) x \geq x^t \left(\sum_{j=1}^{n-1} \gamma_j A_j \right) x$$

and

$$x^t A_n x = \tilde{x}^t A_{n-1} \tilde{x} + 2x_n \sum_{j=1}^n x_j - 2nx_n^2 \leq \tilde{x}^t H_{n-1} \tilde{x} + 2x_n \sum_{j=1}^n x_j - 2nx_n^2 = x^t H_n x,$$

where $\tilde{x} = (x_1 - x_n, \dots, x_{n-1} - x_n, 0)^t$. Thus, $x^t \left(\sum_{j=1}^n \gamma_j A_j \right) x \leq x^t \left(\sum_{j=1}^n \gamma_j H_j \right) x$. ■

We have the following corollary similar to Corollary 3.4

Corollary 3.7 *Suppose we are going to assign $a_1 \geq a_2 \geq \dots \geq a_n \geq 0$ to a collection of cycles of different lengths in order to maximize the numerical radius of the adjacency matrix. Then we should assign the largest a_j 's to the cycle with minimal size in the way as in Theorem 3.6.*

Proof. It suffices to show that $r(A_n) \leq r(A_{n-1})$ where

$$A_k = a_1(E_{12} + E_{21}) + \sum_{j=2}^{k-1} a_j(E_{j-1,j+1} + E_{j+1,j-1}) + a_k(E_{k-1,k} + E_{k,k-1}).$$

To this end, we see that the Perron eigenvalue of A_n is of the form

$$R = 2(a_{n-1}x_{n-2}x_n + a_nx_{n-1}x_n + \Delta)$$

where $x_1 \geq \dots \geq x_{n-2} \geq x_{n-1} \geq x_n > 0$ and $x = (x_1, x_2, \dots, x_n)^t$ is the Perron vector. Note that $R \geq 2a_n$ (consider the vector $\frac{1}{\sqrt{n}}(1, \dots, 1)^t$).

Now consider a unit vector $y = \frac{1}{\sqrt{1-x_n^2}}(x_1, x_2, \dots, x_{n-1})^t$ and calculate the quadratic form

$$\begin{aligned} S = y^t A_{n-1} y &= 2 \left(\frac{1}{1-x_n^2} (a_{n-1}x_{n-1}x_{n-2} + \Delta) \right) \\ &= 2 \left(\frac{1}{1-x_n^2} (a_{n-1}x_{n-1}x_{n-2} + R/2 - a_{n-1}x_{n-2}x_n - a_nx_{n-1}x_n) \right). \end{aligned}$$

We have

$$\begin{aligned} \frac{1}{2}(1-x_n^2)(S-R) &= 2^{-1}Rx_n^2 + a_{n-1}x_{n-1}x_{n-2} - a_{n-1}x_{n-2}x_n - a_nx_{n-1}x_n \\ &\geq a_nx_n^2 + a_{n-1}x_{n-1}x_{n-2} - a_{n-1}x_{n-2}x_n - a_nx_{n-1}x_n \\ &= (a_{n-1}x_{n-2} - a_nx_n)(x_{n-1} - x_n) \\ &\geq 0. \end{aligned}$$

Thus the Perron eigenvalue of A_{n-1} is larger. ▀

3.3 Solution of Problem B

Using the results in Subsections 3.1 and 3.2, we have the following.

Proposition 3.8 *For $a_1 \geq a_2 \geq \dots \geq a_n \geq 0$, let $W_1 = [a_1]$,*

$$W_2 = \begin{pmatrix} 0 & a_1 \\ a_2 & 0 \end{pmatrix}, \quad W_3 = \begin{pmatrix} 0 & a_1 & 0 \\ 0 & 0 & a_2 \\ a_3 & 0 & 0 \end{pmatrix}, \quad \dots, \quad W_n = \begin{pmatrix} 0 & a_{n-2} & & & & & & & & \\ & 0 & a_{n-4} & & & & & & & \\ & & 0 & \ddots & & & & & & \\ & & & 0 & \ddots & & & & & \\ & & & & \ddots & a_1 & & & & \\ & & & & & 0 & \ddots & & & \\ & & & & & & \ddots & a_{n-3} & & \\ & & & & & & & 0 & a_{n-1} & \\ a_n & & & & & & & & & 0 \end{pmatrix},$$

if and only if A_σ has a principal submatrix \tilde{A} which is a weighted cyclic matrix satisfying one of the following conditions.

(a) $|\tilde{A}| + |\tilde{A}|^t$ is permutationally similar to $2B$.

(b) \tilde{A} has size less than or equal to k and all its nonzero entries have magnitudes d_1 .

(3) The nonzero direct summands of A are all weighted shift matrices, and the largest one has size ℓ . Then A_σ has maximum numerical radius equal to $w(B)$ with

$$B = \frac{1}{2} \begin{pmatrix} 0 & d_1 & d_2 & & & \\ d_1 & 0 & 0 & d_3 & & \\ d_2 & 0 & 0 & 0 & \ddots & \\ & d_3 & 0 & 0 & 0 & d_{\ell-1} \\ & & \ddots & 0 & 0 & 0 \\ & & & d_{\ell-1} & 0 & 0 \end{pmatrix}$$

if and only if A_σ has a principal submatrix \tilde{A} such that $|\tilde{A}| + |\tilde{A}|^t$ is permutationally similar to $2B$.

Thus, we have the following general strategy for permuting entries of $A \in M_n$ described in Problem B to maximize the numerical radius.

- If A has a nonzero diagonal entry, exchange it with an entry with maximum magnitude.
- If A has no nonzero diagonal entries, search for a principal submatrix \tilde{A} corresponding to a weighted cyclic matrix of minimum size, say, m ; exchange its entries by those with largest magnitudes and arrange the entries so that the resulting matrix has the maximum numerical radius as in Theorem 3.6.
- If the direct summands consist of weighted shift matrices only, then choose the one with maximum size, exchange its entries with entries in A with largest magnitudes and arrange the entries so that the resulting matrix has the maximum numerical radius as in Theorem 3.2.

4 Further remarks and open questions

4.1 Remark on infinite dimensional case

In [2], the authors consider the permutation of the entries of a unilateral weighted shift operator $T = \sum_{j=0}^{\infty} a_j(\cdot, e_{j+1})e_j$, or a bilateral weighted shift operator $T = \sum_{j=-\infty}^{\infty} a_j(\cdot, e_{j+1})e_j$, to get the maximum numerical radius. In either case, they use the weights of the operator T to construct a nonnegative non-increasing sequence $\{d_1, d_2, \dots\}$ as follows. If there are k terms in $\{|a_1|, |a_2|, \dots\}$ with $0 \leq k \leq \infty$ larger than $\limsup\{|a_i| : i = 1, 2, \dots\}$, then arrange the k terms in descending order and set them as $d_1 \geq \dots \geq d_k$, and set $d_j = \limsup\{|a_i| : i = 1, 2, \dots\}$ for all $j > k$ if $k < \infty$. They showed that the maximum numerical radius one can get is equal to $w(\tilde{T})$ with

$$\tilde{T} = \sum_{j=0}^{\infty} d_{2j+1}(\cdot, e_{j+1})e_j + \sum_{j=1}^{\infty} d_{2j}(\cdot, e_{-j+1})e_{-j}.$$

In fact, if we depict the operator matrix of \tilde{T} using the ordered basis $\{e_0, e_1, e_{-1}, e_2, e_{-2}, \dots\}$ or $\{e_0, e_{-1}, e_1, e_{-2}, e_2, \dots\}$, then the matrix T_σ attaining the maximum numerical radius has the form

$$\frac{1}{2} \begin{pmatrix} 0 & d_1 & d_2 & & \\ d_1 & 0 & 0 & d_3 & \\ d_2 & 0 & 0 & 0 & \ddots \\ & d_3 & 0 & 0 & 0 \\ & & \ddots & 0 & 0 \end{pmatrix},$$

which can be viewed an extension of the result in finite dimensional case in Theorem 3.2.

One easily adapts our results to $T \in B(H)$, whose operator matrix with a suitable countable orthonormal basis has at most one entry in each row and each column so that it is a direct sum of finite cycles, paths (finite or infinite), and diagonal operator (finite or infinite).

4.2 Additional results for matrices

The following was proved in [3, Theorem 2.1].

Theorem 4.1 *Suppose A is the adjacency matrix of a tree. Then there is a permutation P such that*

$$x^t P^t A P x \geq x^t Q^t A Q x$$

for any permutation matrix Q and any nonnegative vector x with entries arranged in descending order if and only if $P^t A P = U + U^t$ with

$$U = e_1 \left(\sum_{1 < j \leq d_1} e_j \right)^t + e_2 \left(\sum_{d_1 < j \leq d_2} e_j \right)^t + \dots + e_k \left(\sum_{d_{k-1} < j \leq d_k} e_j \right)^t,$$

where $d_1 < \dots < d_k = n$ and $d_j - d_{j-1} \geq d_{j+1} - d_j$ for $j = 1, \dots, k-1$.

Note that the nonzero rows of U always add up to the vector $(0, 1, 1, \dots, 1)$, and $d_j - d_{j-1} \geq d_{j+1} - d_j$ simply means that the row sums of U is non-increasing. For example, we may have $A = U + U^t$ with

$$U = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

By Theorem 4.1, if there is no permutation matrix P such that $P^t A P$ has the described form, then for different nonnegative vector with entries in descending order, one needs to choose different Q so that $x^t Q^t A Q x$ attains the maximum among all choices of permutation matrix Q .

For example, if G is obtained by the path $1 - 2 - 3 - 4 - 5$ adding a vertex 6 connected to 2. Then we see that different vector x may lead to different optimal weight assignment. For example, for $x = (7, 6, 5, 4, 3, 2)$, we should assign $(4, 7, 6, 5, 2, 3)$ or $(3, 4, 6, 5, 2, 4)$, where vertex 4 is the third largest; for $x = (10, 5, 4, 3, 2, 1)$, we should assign $(4, 10, 5, 2, 1, 3)$ or $(3, 10, 5, 2, 14)$, vertex 4 is the second smallest.

On the other hand, there may be different permutation matrix P such that P^tAP has the described form. Then for each of these matrices P , x^tP^tAPx will give the maximum values among all choices of permutation matrices.

For a weighted tree having the structure described in Theorem 4.1, we have the following.

Proposition 4.2 *Suppose $A = U + U^t$, where U is in upper triangular form described in Theorem 4.1. For any nonnegative numbers $a_1 \geq \dots \geq a_{n-1}$, we can obtain \tilde{U}^t from U^t by replacing the j th column by $\sum_{d_{j-1} < r \leq d_j} a_r e_r$. Then the resulting matrix $\tilde{A} = \tilde{U} + \tilde{U}^t$ satisfies*

$$x^t \tilde{A} x \geq x^t A_\sigma x$$

for any other assignment of the nonzero entries in A by the a_1, \dots, a_{n-1} (in the symmetric positions).

The following observation is clear.

Proposition 4.3 *Let $a_1 \geq \dots \geq a_{n-1}$. For any nonnegative vector x with nonnegative entries arranged in descending order,*

$$x^t \left(\sum_{j=2}^n a_{j-1} (E_{1j} + E_{j1}) \right) x \geq x^t A x$$

for any adjacency matrix A corresponding to a weighted tree with weights $a_1 \geq \dots \geq a_{n-1}$.

In connection to our study, it would be interesting to study the following general problem.

Problem D *Given a matrix $A = (a_{ij}) \in M_n$, determine the permutation(s) of its entries to maximize/minimize its spectral radius, numerical radius, or spectral norm.*

One may consider special classes of matrices such as adjacency matrices of some special graphs, companion matrices, the complementary basic matrices defined by Fielder [4] (see also [5]).

It is also interesting to study the minimization problems on quadratic forms and numerical radius.

Problem E *Let $A \in M_n$ be a real matrix with some special structure, and let $x = (x_1, \dots, x_n)^t$ be a real vector with entries arranged in descending order. Determine the permutation matrices P such that $x^t P^t A P x$ attain its minimum.*

Problem F *Let $A \in M_n$ with some special structure, say, each row and each column has at most one nonzero entry. Determine the permutations of its nonzero entries that yield the minimum eigenvalue.*

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