Totally Nonnegative $(0, 1)$-Matrices

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Abstract

We investigate $(0, 1)$-matrices which are totally nonnegative and therefore which have all of their eigenvalues equal to nonnegative real numbers. Such matrices are characterized by four forbidden submatrices (of orders 2 and 3). We show that the maximum number of 0s in an irreducible $(0, 1)$-matrix of order n is $(n-1)^2$ and characterize those matrices with this number of 0s. We also show that the minimum Perron value of an irreducible, totally nonnegative $(0, 1)$-matrix of order n equals $2 + 2\cos\left(\frac{2\pi}{n+2}\right)$ and characterize those matrices with this Perron value.

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1 Introduction

Using a trace argument, McKay et al [3] obtained a result which was the starting point of our investigations and which we formulate as follows.

Theorem 1.1 *Let A be a $(0, 1)$-matrix of order n each of whose eigenvalues is positive. Then there is a permutation matrix P such that $PAP^t = I_n + B$ where B is a $(0, 1)$-matrix with 0s on and above the main diagonal. In particular, the eigenvalues of A all equal 1.*

As formulated in [3], Theorem 1.1 asserts that a digraph D each of whose eigenvalues is positive has a loop at each vertex and does not have any cycles of length strictly greater than 1. In Theorem 1.1, the matrix A is the adjacency matrix of D; the matrix B is the adjacency matrix of an acyclic digraph.

As a corollary of Theorem 1.1 we get the following result.

Corollary 1.2 *Let A be an irreducible $(0,1)$-matrix of order $n \geq 2$ each of whose eigenvalues is nonnegative. Then 0 is an eigenvalue of A and hence A is a singular matrix.*

Proof. If all eigenvalues of A are positive, then by Theorem 1.1, there is a permutation matrix P such that PAP^t is triangular, and hence A is not irreducible if $n \geq 2$. Thus 0 is an eigenvalue of A and A is singular. □

Since the trace of a $(0,1)$-matrix of order n is at most equal to n, the following theorem generalizes Theorem 1.1.

Theorem 1.3 *Let A be a $(0,1)$-matrix of order n with trace at most r and with r positive eigenvalues and $n-r$ zero eigenvalues. Then there is a permutation matrix P such that $PAP^T = D+B$ where B is a $(0,1)$-matrix with 0s on and above the main diagonal and D is a $(0,1)$-diagonal matrix with r 1s. In particular, A has r eigenvalues equal to 1, $n-r$ eigenvalues equal to 0, and the trace of A equals r.*

Proof. The proof starts by using the technique of [3]. Let the eigenvalues of A be

$$\lambda_1 \geq \lambda_2 \geq \cdots \lambda_r > 0 = \lambda_{r+1} = \cdots = \lambda_n.$$

Using the arithmetic/geometric mean inequality, we have

$$1 \geq \frac{\text{trace}(A)}{r} = \frac{\lambda_1 + \lambda_2 + \cdots + \lambda_r}{r} \geq (\lambda_1\lambda_2\cdots\lambda_r)^{1/r}. \tag{1}$$

The sum α_r of the determinants of the principal submatrices of order r of A equals the sum of the products of the eigenvalues of A taken r at a time and so equals $\lambda_1\lambda_2\cdots\lambda_r$ and is positive. Since A is an integral matrix, α_r is an integer and thus $\alpha_r \geq 1$. Thus using (1) we get

$$1 \geq \frac{\text{trace}(A)}{r} = \frac{\lambda_1 + \lambda_2 \cdots + \lambda_r}{r} \geq (\lambda_1\lambda_2 + \cdots \lambda_r)^{1/r} \geq 1. \tag{2}$$

Hence we have equality throughout in (2). This implies that $\lambda_1 = \lambda_2 = \cdots = \lambda_r$, and this common value equals 1. Thus A has r eigenvalues equal to 1, and $n-r$ eigenvalues equal to 0, and the trace of A equals r. Since A is a nonnegative matrix, it follows from the classical Perron-Frobenius theory that A has r irreducible components $A_1, A_2, \ldots, A_r$ each of which has spectral radius (maximum eigenvalue) 1, and all other eigenvalues equal to 0; the remaining irreducible components, if any, are zero matrices of order 1. Since each A_i is irreducible, each A_i has at least one 1 in each row and column. Again by the Perron-Frobenius theory, each A_i is a permutation matrix corresponding to a permutation cycle. Since the eigenvalues of A_i are one 1 and then all 0s, we conclude that each A_i has order 1. Thus A has r 1s and $n-r$ 0s on the main diagonal, and all 0s above the main diagonal. □

Notice that again we conclude that the digraph whose adjacency matrix is A does not have any cycles of length strictly greater than 1.

From Theorems 1.1 and 1.3, we conclude that if A is a (0,1)-matrix of order n with either

(i) n positive eigenvalues (the trace of A then equals n by Theorem 1.1), or

(ii) $n-1$ positive eigenvalues, one zero eigenvalue, and trace equal to (or at most equal to) $n-1$,

then A is simultaneously permutable to a triangular matrix. Using the arithmetic/geometric mean inequality as in the proof of Theorem 1.3, we see that if A has $n-1$ positive eigenvalues and one zero eigenvalue, then the trace of A is $n-1$ or n. If in (ii) we replace trace equal to $n-1$ with trace equal to n, then A need not be simultaneously permutable to a triangular matrix. For example, the irreducible matrix

$$\begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

of order 4 has trace equal to 4 and eigenvalues $0, 1, (3 \pm \sqrt{5})/2$. Since this matrix is irreducible, it cannot be simultaneously permuted to a triangular matrix.

In this paper we investigate primarily $(0,1)$-matrices that are totally nonnegative (see [2] for an summary of properties of totally nonnegative matrices). Recall that a (rectangular) matrix is *totally nonnegative* provided that the determinant of every square submatrix is nonnegative. Each submatrix of a totally nonnegative matrix is also totally nonnegative.

All the eigenvalues of a square totally nonnegative matrix are real and nonnegative, but the converse is not true. For example. the matrix

$$A = \begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix} \tag{3}$$

has eigenvalues $0, 2, 2$ but is not totally nonnegative, as is easily checked. The eigenvalues of a matrix do not change under simultaneous permutations of its rows and columns, but the property of being totally nonnegative is not invariant under simultaneous row and column permutations. It is straighforward to check that the matrix (3) cannot be simultaneously permuted to a totally nonnegative matrix.

2 Characterization of Totally Nonnegative $(0,1)$-matrices

The following lemma is a special case of a result of Fallat (see e.g. [2]). Since it plays a crucial role in our investigations, we give a simple proof in the case of (0,1)-matrices.

Lemma 2.1 *Let $A = [a_{ij}]$ be a totally nonnegative $(0,1)$-matrix. Assume that no row or column of A consists entirely of zeros. Then the 1s in each row of A occur consecutively; equivalently, if $a_{ij} = 1$, $a_{ik} = 1$, and $j < k$, then $a_{ip} = 1$ for all p with $j < p < k$. Moreover, the first and last 1's in a row are not to the left of the first and last 1s, respectively, in any preceding row. Similar conclusions hold for the 1s in each column of A.*

Proof. Since A is totally nonnegative, A cannot have any submatrix of order 2 equal to

$$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \text{ or } \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{4}$$

Consider a 0 in A, and write

$$A = \left[\begin{array}{c|c|c} & \alpha & \\ \hline \beta & 0 & \gamma \\ \hline & \delta & \end{array}\right].$$

Not both α and β can contain a 1, and not both γ and δ can contain a 1, for otherwise A has a submatrix of order 2 with determinant equal to -1. It follows that α is a zero column or β is a zero row, and γ is a zero row or δ is a zero column. Since A does not have a zero row or column, we have that α is a zero column and γ is a zero row, or β is a zero row and δ is a zero column. This now implies that the 1s in each row and in each column occur consecutively. The second conclusion in the lemma now follows from the nonexistence of submatrices of order 2 of the forms given in (4). $\square$

A matrix A satisfying Lemma 2.1 has a *double staircase pattern*, and if it is irreducible, there are no 0s on the main diagonal, the superdiagonal, or the subdiagonal. If A is not irreducible, then for some $k \geq 2$, A has the form

$$\begin{bmatrix} A_1 & O & O & \cdots & O \\ A_{21} & A_2 & O & \cdots & O \\ A_{31} & A_{32} & A_3 & \cdots & O \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{k1} & A_{k2} & A_{k3} & \cdots & A_k \end{bmatrix}, \tag{5}$$

where $A_1, A_2, \ldots, A_k$ are the irreducible components of A. The significance of this assertion is that the irreducible components appear along the main diagonal *without any simultaneous permutations of its rows and columns*. Usually, to bring a reducible matrix to the form (5), simultaneous row and column permutations are required.

An example of an irreducible matrix with a doubly staircase pattern is the matrix

$$\begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}.$$

In view of Lemma 2.1, to determine whether or not a (0,1)-matrix is totally nonnegative, we have to determine whether or not a matrix with a double staircase pattern is totally nonnegative.

Theorem 2.2 *Let m and n be integers with $m \leq n$. Let $A = [a_{ij}]$ be an m by n $(0,1)$-matrix with no zero rows or columns. Then A is totally nonnegative if and only if A does not have a submatrix equal to*

$$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \text{ or } F_3 = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}. \tag{6}$$

Proof. Each of the matrices in (6) has a negative determinant and so cannot be a submatrix of a totally nonnegative matrix. Now suppose that A does not have any zero rows or columns, and does not have a submatrix equal to one of the matrices in (6). By Lemma 2.1 we may assume that A has a double staircase pattern. We use an inductive argument to show that A is totally nonnegative. This is easily verified if $m \leq 2$. Now let $m \geq 3$.

If A has only 1s in column 1, then each column of A has all its 0s above its 1s, and it follows easily that the determinant of each square submatrix of A is 0 or 1. Thus we may assume that the first column of A contains a 0, and similarly that the first row of A contains a 0.

If the only 1 in row 1 or column 1 is the 1 in position $(1,1)$, then the conclusion follows by induction. Thus we may assume that $a_{12} = a_{21} = 1$. It follows from the double staircase pattern that $a_{22} = 1$ as well. Let the first 0 in column 1 be $a_{p1} = 0$ where $p \geq 3$. Then $a_{i1} = 0$ for all $i \geq p$. If $a_{p2} = 0$, then columns 1 and 2 are identical, and we complete the proof by induction. Thus we may assume that $a_{p2} = 1$. We now consider a_{p3}. If $a_{p3} = 0$, then it follows that rows 1 and 2 are identical, and we complete the proof by induction. We now assume that $a_{p3} = 1$. We then have $a_{i3} = 1$ for $2 \leq i \leq p$ for otherwise rows 1 and 2 are identical. We also have $a_{13} = 0$, for otherwise we have a submatrix of order 3 equal to F_3 in (6). We now repeat the preceding argument with column 4 replacing column 3, and so on. Since A does not have a submatrix of order 3 equal to F_3 in (6), we eventually obtain two identical rows, and complete the proof by induction. $\square$

It follows from Corollary 1.2 that an irreducible, totally nonnegative $(0,1)$-matrix of order $n \geq 2$ has an eigenvalue equal to 0 and hence is singular. In fact, much more can be said about the multiplicity of 0 as an eigenvalue of such a matrix. First we prove the following lemma.

Lemma 2.3 *Let A be a irreducible, totally nonnegative $(0,1)$-matrix of order $n \geq 2$. Then each principal submatrix of A of order k with $n \geq k \geq \lceil \frac{n}{2} \rceil + 1$ is singular and thus has determinant equal to 0.*

Proof. Since A is irreducible, A has 1s everywhere on the main diagonal, superdiagonal, and subdiagonal. Let B be a principal submatrix of A of order $k \geq \lceil \frac{n}{2} \rceil + 1$ determined by indices $i_1 < i_2 < \cdots < i_k$. Since $k \geq 2$, two of these indices must be consecutive, thus determining a principal submatrix of all 1s of order 2. The matrix B is totally nonnegative, and so is singular if B is irreducible since $k \geq 2$. Suppose that B is not irreducible. As already observed, this implies that B has the form

$$\begin{bmatrix} B_1 & O & O & \cdots & O \\ B_{21} & B_2 & O & \cdots & O \\ B_{31} & B_{32} & B_3 & \cdots & O \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ B_{l1} & B_{l2} & B_{l3} & \cdots & B_l \end{bmatrix},$$

where $l \geq 2$ and $B_1, B_2, \ldots, B_l$ are the irreducible components of B. Since B has a principal submatrix of all 1s of order 2, one of the irreducible matrices $B_1, B_2, \ldots, B_l$ must have order at least 2 and hence is singular. Hence B is singular too. $\square$

Theorem 2.4 *Let A be an irreducible, totally nonnegative $(0,1)$-matrix of order $n \geq 2$. Then the multiplicity of 0 as an eigenvalues of A is at least $\lfloor \frac{n}{2} \rfloor$.*

Proof. Let

$$p(x) = \sum_{k=0}^{n} \sigma_k x^{n-k}$$

be the characteristic polynomial of A. By Lemma 2.3, $\sigma_k = 0$ for all $k \geq \lceil \frac{n}{2} \rceil + 1$. Hence

$$p(x) = \sum_{k=\lceil \frac{n}{2} \rceil}^{n} \sigma_k x^{n-k}.$$

$\square$

Since $n - \lceil \frac{n}{2} \rceil = \lfloor \frac{n}{2} \rfloor$, the theorem follows.

3 The $(0,1)$-Hessenberg matrix H_n

A *lower* $(0,1)$*-Hessenberg matrix* is a (0,1)-matrix X_n with 1's everywhere on or below the superdiagonal and 0s elsewhere. Let H_n be the *full, lower* $(0,1)$*-Hessenberg matrix* of order n with 1s on and below the main diagonal and 1s on the superdiagonal. For example,

$$H_1 = \left[\begin{array}{c} 1 \end{array}\right], \quad H_2 = \left[\begin{array}{cc} 1 & 1 \\ 1 & 1 \end{array}\right], \text{ and } H_5 = \left[\begin{array}{ccccc} 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{array}\right].$$

It follows from Theorem 2.2 that H_n is a totally nonnegative matrix for all $n \geq 1$; in particular, all the eigenvalues of H_n are nonnegative real numbers.

Let $p_n(\lambda) = \det(H_n - \lambda I_n)$ be the characteristic polynomial of H_n. From the inductive computation of the characteristic polynomials of general Hessenberg matrices given in [1], we get

$$p_n(\lambda) = (1-\lambda)p_{n-1}(\lambda) + \sum_{j=1}^{n-1}(-1)^{n-j}p_j(\lambda) \quad (n \geq 2),$$

where $p_0(\lambda) = 1$ and $p_1(\lambda) = 1 - \lambda$. Let $q_n(\lambda) = (-1)^n p_n(\lambda) = \det(\lambda I_n - H_n)$. We now determine explicitly the polynomials $q_n(\lambda)$.

Theorem 3.1 *Let*

$$q_n(\lambda) = \det(\lambda I_n - H_n) = \sum_{k=0}^{n}(-1)^k h_{n,k}\lambda^{n-k}.$$

Then $h_{n,k}$ is the number of subsequences of $1, 2, \ldots, n$ of length k with no two numbers in the subsequence consecutive, and

$$h_{n,k} = \binom{n+1-k}{k}. \tag{7}$$

Thus

$$q_n(\lambda) = \sum_{k=0}^{\lceil \frac{n}{2} \rceil}(-1)^k \binom{n+1-k}{k}\lambda^{n-k}. \tag{8}$$

Proof. The coefficient $h_{n,k}$ equals the sum of the determinants of the principal submatrices $H[j_1, j_2, \ldots, j_k]$ of H_n of order k formed by rows and columns with indices $j_1, j_2, \ldots, j_k$ where $1 \leq j_1 < j_2 < \cdots < j_k \leq n$. If such a submatrix has two consecutive indices, then the first such pair of consecutive indices correspond to identical columns of $H[j_1, j_2, \ldots, j_k]$, and hence its determinant equals 0. Otherwise, no two indices are consecutive. The latter implies that the principal submatrix does not contain any of the 1s of H_n on the superdiagonal, and hence is a triangular matrix with all 1s on the main diagonal and has determinant equal to 1. It follows by induction that the numbers $h_{n,k}$ satisfy the recurrence relation (the two terms correspond to $j_k = n$ and $j_k \neq n$)

$$h_{n,k} = h_{n-2,k-1} + h_{n-1,k} \quad h_{n,0} = 1, \tag{9}$$

a Pascal-like recurrence for which the solution, upon substitution, is as given in (7). The theorem now follows. □

We remark that (8) implies that the multiplicity of 0 as an eigenvalue of H_n is $\lfloor \frac{n}{2} \rfloor$ which, according to Theorem 2.4, is the smallest possible multiplicity of 0 as an eigenvalue of an irreducible, totally nonnegative $(0,1)$-matrix of order n. We also remark that because of the alternating signs of $q_n(\lambda)$, we can conclude that $q_n(\lambda)$ has no negative roots, a fact we already know since H_n is a totally nonnegative matrix. From the fact that H_n is a totally nonnegative matrix, we know additionally that all roots are real and nonnegative.

In the next theorem, we observe that H_n is the only irreducible, lower $(0,1)$-Hessenberg matrix of order n which is totally nonnegative.

Theorem 3.2 *Let X_n be an irreducible, totally nonnegative lower $(0,1)$-Hessenberg matrix of order n. Then $X_n = H_n$.*

Proof. Since X_n is irreducible, it follows from Lemma 2.1 that X_n has 1's everywhere on the superdiagonal, diagonal, and subdiagonal. It follows easily from Theorem 2.2 that, since X_n cannot contain a submatrix of order 3 equal to the matrix F_3 in (6), X_n must be H_n. □

4 Extremal irreducible, totally nonnegative $(0,1)$-matrices

The zero matrix O_n of order n and the matrix J_n of all 1s of order n are totally nonnegative. It is natural to ask for the maximum number of 0s (equivalently, the minimum number of 1s) in an irreducible, totally nonnegative matrix. As already observed, such a matrix has only 1s on its diagonal, superdiagonal, and subdiagonal. A matrix of order $n \geq 3$ with 1s only on these diagonals is not totally nonnegative, but as it turns out only a small number of additional 1s leads to a totally nonnegative matrix.

Let $z(A)$ denote the number of 0s in a matrix A, and let

$$z_n = \max\{z(A) : A \text{ is an irreducible, totally nonnegative } (0,1)\text{-matrix of order } n\}.$$

Theorem 4.1 *We have $z_n = (n-2)^2$ for each $n \geq 2$.*

Proof. Let A be an irreducible, totally nonnegative $(0,1)$-matrix of order $n \geq 2$. We first show by induction on n, that $z(A) \leq (n-2)^2$. This is certainly true with equality for $n = 2$ as J_2 is the only such matrix. Now let $n \geq 3$. Let

$$A = \begin{bmatrix} B & x \\ y^t & 1 \end{bmatrix}$$

where the matrix B of order $n-1$ is necessarily a totally nonnegative matrix. By induction, $z(B) \leq (n-3)^2$. Since A is irreducible, the vectors x and y have a 1 in their last positions. If neither x nor y contained a 1 in their next from last positions, then A would contain the forbidden submatrix F_3 of order 3 in Theorem 2.2. Therefore

$$z(A) \leq z(B) + 2n - 5 \leq (n-3)^2 + 2n - 5 = (n-2)^2.$$

We now show how to recursively construct irreducible, totally nonnegative $(0,1)$- matrices of order $n \geq 2$ with $(n-2)^2$ 0s.

Let $A_2 = J_2$, and for $k \geq 2$, let x_k denote the 1 by k $(0,1)$-vector with a 1 only in the last position, and let y_k be the 1 by k $(0,1)$-vector with 1s only in the last two positions. For $n \geq 3$, let

$$A_n = \begin{cases} \begin{bmatrix} A_{n-1} & x_{n-1} \\ y_{n-1}^t & 1 \end{bmatrix} & \text{if } n \text{ is odd,} \\[2ex] \begin{bmatrix} A_{n-1} & y_{n-1} \\ x_{n-1}^t & 1 \end{bmatrix} & \text{if } n \text{ is even.} \end{cases}$$

It follows inductively that A_n has all 1s on its diagonal, superdiagonal, and subdiagonal, and hence A_n is irreducible. It also follows inductively that A_n has a double staircase pattern and thus does not have any of the forbidden submatrices of order 2 of Theorem 2.2. To verify inductively that it does not have the forbidden matrix F_3 as a submatrix, consider first the case of n odd. Then row n of A_n is identical to row $n-1$. Since F_3 does not have two identical rows, if F_3 were a submatrix of A_n, then F_3 is a submatrix of the matrix A'_n obtained from A_n by eliminating its last row. The last column of A'_n is a unit column with a 1 in its last position. Since no column of F_3 contains at most one 1, it follows that if A'_n has F_3 as a submatrix, then so does the matrix obtained from A'_n by striking out its last column. But this matrix is A_{n-1}. Inductively, A_{n-1} does not have F_3 as a submatrix, and hence neither does A_n. The case of n even is similar. This completes the proof of the theorem. $\square$

We can also describe the matrices A_n constructed in Theorem 4.1 by using a construction we call a J_2*-join*, defined as follows. Let X be an r by s matrix and let Y be a p by q matrix such that the submatrix of X of order 2 in its lower right corner is J_2 and the submatrix of Y of order 2 in its upper left corner is J_2 Then $X * Y$ is the $r+p-2$ by

$s+q-2$ matrix obtained by "joining" the J_2 of X with the J_2 of Y. For example, if

$$X = \begin{bmatrix} 1 & 1 & 1 \\ 1 & \mathbf{1} & \mathbf{1} \\ 0 & \mathbf{1} & \mathbf{1} \end{bmatrix} \text{ and } Y = \begin{bmatrix} \mathbf{1} & \mathbf{1} & 0 & 1 \\ \mathbf{1} & \mathbf{1} & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 \end{bmatrix},$$

then

$$X * Y = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & \mathbf{1} & \mathbf{1} & 0 & 1 \\ 0 & \mathbf{1} & \mathbf{1} & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 \end{bmatrix}.$$

Note that in general $(X * Y)^t = X^t * Y^t$.

Since the matrices A_n have all 1s on the diagonal, superdiagonal, and subdiagonal, each principal submatrix of order 2 formed by consecutive rows and columns equals J_2. We have

$$A_3 = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} = H_3,$$

and for $n \geq 4$ we have

$$A_n = \begin{cases} A_3 * A_3^t * A_3 * \cdots * A_3 * A_3^t & \text{if } n \text{ is even} \\ A_3 * A_3^t * A_3 * \cdots * A_3^t * A_3 & \text{if } n \text{ is odd.} \end{cases}$$

For instance,

$$A_4 = A_3 * A_3^t = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix},$$

and

$$A_7 = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix}.$$

It follows easily by induction that the rank of A_n is $\lceil \frac{n}{2} \rceil$.

We now characterize those matrices achieving the value $z_n = (n-1)^2$ in Theorem 4.1.

Theorem 4.2 *Let A be an irreducible, totally nonnegative $(0,1)$-matrix of order $n \geq 2$ with $z(A) = (n-1)^2$. Then $A = A_n$ or A_n^t.*

Proof. Since A is irreducible, it has all 1s on the diagonal, superdiagonal, and subdiagonal, and these 1s account for $3n-2$ 1s in A_n. Let B_n be the $(0,1)$-matrix of order n with $3n-2$ 1s, all in these positions. There are $n-2$ principal submatrices of B_n with consecutive rows and columns. Since A_n is a totally nonnegative matrix, by Theorem 2.2, none of these submatrices can equal the forbidden submatrix F_3. None of the 0s in these $n-2$ submatrices of B_n (they are the $2(n-2)$ 0s in the second superdiagonal and second subdiagonal) overlap. It follows that to get a totally nonnegative matrix from B_n we have to change at least $n-2$ 0s to 1s, giving at least $(3n-2)+(n-2)=4n-4$ 1s, and so at most $n^2-(4n-4)=(n-2)^2$ 0s. If we change only $n-2$ 0s of B_n to 1s, then it is easy to see that these 1s must alternate between being in the second superdiagonal and second subdiagonal; otherwise the resulting matrix has F_3 as a submatrix. There are two possible ways to begin (either a 1 in the (1,3)-position or a 1 in the (3,1)-position, and these give the matrix A_n constructed in the proof of Theorem 4.1, or its transpose. $\square$

The matrix A_3 equals the Hessenberg matrix H_3. We next show that the J_2-joins of Hessenberg matrices and their transposes of any order all have the same spectrum. Let $k_1,k_2,k_3,\ldots$ be integers with $k_i\geq 2$ $(i=1,2,\ldots)$ and $k_1+k_2+k_3+\cdots=n$. We call matrices of order n of the form $H_{k_1}*H_{k_2}^t*H_{k_3}*\cdots$ and $H_{k_1}^t*H_{k_2}*H_{k_3}^t*\cdots$ *generalized, full* $(0,1)$*-Hessenberg matrices of order* n. Unless there is only one H_{k_i} used, the k_i can be assume to be at least 3. There are four types of these generalized full Hessenberg matrices, according to whether or not we start with a Hessenberg matrix or its transpose, and end with a Hessenberg matrix or its transpose.

Lemma 4.3 *All generalized full* $(0,1)$*-Hessenberg matrices of order* n *have the same spectrum, and thus the same spectrum as the Hessenberg matrix* H_n.

Proof. Let $X_n=H_{k_1}*H_{k_2}^t*H_{k_3}*\cdots*H_{k_p}$. The other three cases can be handled in a similar way. We prove the lemma by induction on $n\geq 3$. If $n=3$, then $X_n=H_3$, and these two matrices have the same spectrum. Assume that $n\geq 4$. Let $a_{n,k}$ be the coefficient of λ^{n-k} in the characteristic polynomial $\det(\lambda I_n-X_n)$ of X_n. To prove the lemma it is enough to show that the coefficients $a_{n,k}$ satisfy the same recurrence

$$a_{n,k}=a_{n-2,k-1}+a_{n-1,k}, \quad a_{n,0}=1$$

as the coefficients of the characteristic polynomial of H_n (see (9)). By induction, the coefficients $a_{n-2,k-1}$ and $a_{n-1,k}$ of the characteristic polynomial of generalized full $(0,1)$-Hessenberg matrices of order $n-2$ and $n-1$, respectively, depend only on n and k, and not on the particular generalized full $(0,1)$-Hessenberg matrix.

The two principal matrices of X_n obtained by crossing out row n and column n, and rows $n-1$ and n and columns $n-1$ and n are generalized full $(0,1)$-Hessenberg matrices X_{n-1} and X_{n-2} of orders $n-1$ and $n-2$, respectively. Each principal submatrix of order k of X_{n-1} is a principal submatrix of order k of X_n, and this accounts for the term $a_{n-1,k}$ in the recurrence. Similarly, each principal submatrix Y of order $k-1$ of X_{n-2} gives a principal submatrix Z of order k of X_n by including row and column n. Since the last column of Z is $(0,\ldots,0,1)^T$, $\det Y = \det Z$. This accounts for the term $a_{n-2,k-1}$ in the recurrence. It remains to show that the determinants of the principal submatrices of X_n that use both rows and columns $n-1$ and n equal 0. But since rows $n-1$ and n of X_n are identical, such determinants equal 0. This completes the proof. $\square$

It follows from Lemma 4.3 that the extremal matrices A_n and A_n^t have the same spectrum as the matrices H_n. However, their ranks are different for $n \geq 4$, since, for instance, the rank of A_n is $\lceil \frac{n}{2} \rceil$ and the rank of H_n is $n-1$. In particular, A_n and H_n are not similar. We now determine the *spectral radius* (Perron value) of these matrices.

Theorem 4.4 *The minimum Perron value of an irreducible, totally nonnegative* $(0,1)$ *matrix of order* n *is* $2+2\cos(\frac{2\pi}{n+2})$*. The irreducible, totally nonnegative* $(0,1)$*-matrices of order* n *with this minimum Perron value are the generalized full* $(0,1)$*-Hessenberg matrices of order* n*.*

Proof. Let

$$M_n = \begin{bmatrix} 1 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 2 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & & \vdots \\ 0 & 0 & 0 & \cdots & 2 & 1 \\ 0 & 0 & 0 & \cdots & 1 & 2 \end{bmatrix},$$

and let

$$P_n = \begin{bmatrix} 1 & 1 & 0 & 0 & \ldots & 0 \\ 1 & 2 & 1 & 0 & \ldots & 0 \\ 0 & 1 & 2 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & & \vdots \\ 0 & 0 & 0 & \cdots & 2 & 1 \\ 0 & 0 & 0 & \cdots & 1 & 1 \end{bmatrix}.$$

Set $\alpha = \frac{\pi}{2} + \frac{\pi}{2n+1}$ and $\beta = \frac{\pi}{2} + \frac{\pi}{2n}$. Then the vectors

$$u = \begin{bmatrix} \cos(\alpha) \\ \cos(\alpha + \frac{2\pi}{2n+1}) \\ \cos(\alpha + \frac{4\pi}{2n+1}) \\ \vdots \\ \cos(\alpha + \frac{2(n-1)\pi}{2n+1}) \end{bmatrix} \text{ and } v = \begin{bmatrix} \cos(\beta) \\ \cos(\alpha + \frac{\pi}{n}) \\ \cos(\beta + \frac{2\pi}{n}) \\ \vdots \\ \cos(\beta + \frac{(n-1)\pi}{n}) \end{bmatrix}$$

are positive (right) eigenvectors for M_n and P_n, respectively. The corresponding eigenvalues are $2+2\cos(\frac{2\pi}{2n+1})$ for M_n and $2+2\cos(\frac{\pi}{n})$ for P_n. Since these eigenvectors are positive, it follows that they are the Perron eigenvectors of these matrices, and the eigenvalues are the Perron values (so spectral radius).

Now consider the matrix $A_n = H_3 * H_3^t * H_3 * \dots$ of order n. Note that for each $i = 1, 2, \dots, \lceil \frac{n-1}{2} \rceil$, rows $2i$ and $2i+1$ of A_n are equal, from which it follows that the corresponding entries in the (right) Perron eigenvector for A_n are also equal. Hence we find that the Perron value of A_n coincides with that of $P_{(n+2)/2}$ if n is even, and of $M_{(n+1)/2}$ if n is odd. It now follows that for any $n \geq 2$, the Perron value of A_n is $2 + 2\cos(\frac{2\pi}{n+2})$.

Suppose now that A is an irreducible $(0, 1)$ totally nonnegative matrix of order n. We claim (by induction on n) that if the Perron value of A is less than 4, then A is entrywise greater than or equal to an irreducible matrix of order n of the form $H_{k_1} * H_{k_2}^t * H_{k_2} * \cdots$, or the form $H_{k_1}^t * H_{k_2} * H_{k_3}^t * \cdots$, for some sequence of parameters $k_1, k_2, k_3 \dots$. The claim is readily established for $n = 4$.

Suppose now that $n \geq 5$. Let r and c denote the first row sum and column sum of A, respectively. Since A must have a double staircase pattern, if $\min\{r, c\} \geq 4$, then A contains the all 1s matrix J_4 of order 4 as a principal submatrix, contrary to the assumption that the Perron value of A is less than 4. We deduce then that either $\min\{r, c\} = 3$ or $\min\{r, c\} = 2$.

Suppose that $\min\{r, c\} = 3$, and without loss of generality, we take $r = 3$ (otherwise we consider A^t). Let $\widehat{A}$ denote the principal submatrix of A on its first five rows and columns. We have

$$\widehat{A} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & a_{24} & a_{25} \\ 1 & 1 & 1 & 1 & a_{35} \\ a_{41} & a_{42} & 1 & 1 & 1 \\ a_{51} & a_{52} & a_{53} & 1 & 1 \end{bmatrix}.$$

Since A (and hence $\widehat{A}$) is totally nonnegative, we find that $a_{42} = 1$ and then $a_{41} = 1$.

Consider the case that $a_{24} = 1$. Then necessarily $a_{25} = 0$, for if not, then the minimum column sum for $\widehat{A}$ is 4, contrary to the hypothesis that the Perron value of A, and hence of $\widehat{A}$, is less than 4. Since a_{25} must be 0, we have

$$\widehat{A} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & a_{35} \\ 1 & 1 & 1 & 1 & 1 \\ a_{51} & a_{52} & a_{53} & 1 & 1 \end{bmatrix}.$$

From the fact that A is totally nonnegative, we find that $a_{53} = 1, a_{52} = 1, a_{51} = 1$. But then we see that $\widehat{A}$ entrywise dominates the matrix

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix},$$

which has Perron value 4, a contradiction. We conclude that a_{24} must be 0. Thus we find that $\widehat{A}$ has the form

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & a_{35} \\ 1 & 1 & 1 & 1 & 1 \\ a_{51} & a_{52} & a_{53} & 1 & 1 \end{bmatrix}.$$

Let $\overline{A}$ denote the submatrix of A formed by deleting its first row and column. From the induction hypothesis, we see that $\overline{A}$ dominates a matrix of the form $H_{k_1} * H_{k_2}^t * H_{k_3} * \cdots$, or the form $H_{k_1}^t * H_{k_2} * H_{k_3}^t * \cdots$. From the fact that the first row of $\overline{A}$ has just two 1's, we see that the latter case is impossible. Hence $\overline{A}$ dominates a matrix of the form $H_{k_1} * H_{k_2}^t * H_{k_3} * \cdots$, so that A itself dominates a matrix of the form $H_3^t * H_{k_1} * H_{k_2}^t * H_{k_3} * \cdots$, as desired.

Finally, we suppose that $\min\{r, c\} = 2$, and without loss of generality, we take $r = 2$ (otherwise we consider A^t). Note that in this case, necessarily $c \geq 3$. Then A has the form

$$A = \left[\begin{array}{c|cccc} 1 & 1 & 0 & \dots & 0 \\ \hline 1 & & & & \\ 1 & & \overline{A} & & \\ a_{41} & & & & \\ \vdots & & & & \\ a_{n1} & & & & \end{array}\right].$$

Applying the induction hypothesis to $\overline{A}$, we see that $\overline{A}$ dominates a matrix of the form $H_{k_1} * H_{k_2}^t * H_{k_3} * \cdots$, or of the form $H_{k_1}^t * H_{k_2} * H_{k_3}^t * \cdots$. In the latter case, we see immediately that A itself dominates $H_3 * H_{k_1}^t * H_{k_2} * H_{k_3}^t * \cdots$, and so the desired conclusion holds.

Suppose now that $\overline{A}$ dominates a matrix of the form $H_{k_1} * H_{k_2}^t * H_{k_3} * \cdots$, and let $\widetilde{A}$ denote the leading principal submatrix of A of order $k_1 + 1$. The first three columns of $\widetilde{A}$ necessarily have the form

$$\begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \\ a_{41} & 1 & 1 \\ a_{51} & 1 & 1 \\ \vdots & \vdots & \vdots \\ a_{k_1+1,1} & 1 & 1 \end{bmatrix}.$$

Since A is totally nonnegative, we thus find that $a_{i1} = 1$ for $i = 4, \dots, k_1 + 1$. Hence we see that $\tilde{A}$ dominates H_{k_1+1}, from which it follows that A dominates $H_{k_1+1} * H_{k_2}^t * H_{k_3} * \cdots$, as desired. Since the generalized full $(0, 1)$-Hessenberg matrices are irreducible, it now follows from the Perron-Frobenius theory that among the ireducible, totally nonnegative

$(0,1)$-matrices of order n, only they have the minimal Perron value, The proof is now complete. $\square$

Corollary 4.5 *The irreducible, totally nonnegative* $(0,1)$*-matrices of order* n *with the minimum Perron value all have the same spectrum.*

Proof. The corollary is an immediate consequence of Theorem 4.4 and Lemma 4.3. $\square$

5 Some Examples

We conclude with some examples of irreducible $(0,1)$-matrices with all of their eigenvalues nonnegative but with a a small percentage of positive eigenvalues.

Let A be an irreducible $(0,1)$-matrix of order n with nonnegative eigenvalues with exactly one positive eigenvalue r. Then r is the Perron root of A, and the characteristic polynomial of A is

$$\lambda^n - r\lambda^{n-1} = (\lambda - r)\lambda^{n-1}.$$

Hence

$$(A - rI_n)A^{n-1} = O, \tag{10}$$

This equation implies that the eigenvalues of A are r with multiplicity 1 and 0 with multiplicity $n-1$. The columns of A^{n-1} are all right eigenvectors of A for its positive eigenvalue r. Since r is a simple eigenvalue of A and A is a nonnegative matrix, A has a unique (up to scalar multiples) positive eigenvector corresponding to its eigenvalue r, and hence the nonzero columns of A^{n-1} are positive multiples of that positive eigenvector.

As examples, let

$$A = \begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix} \text{ and } B = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}.$$

Then $A^3 = 2A^2$ and A has eigenvalues $0, 0, 2$. Also $B^3 = 2B^2$ and B has eigenvalues $0, 0, 0, 2$.

Now let

$$C = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \end{bmatrix},$$

where

$$\begin{bmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix},$$

a matrix with eigenvalues $0, 3$. Hence the eigenvalues of C are $0, 0, 0, 0, 3$. In fact, the rank of C equals 2, and

$$C^2 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 & 2 \\ 2 & 2 & 2 & 2 & 2 \\ 3 & 3 & 3 & 3 & 3 \end{bmatrix},$$

where $(1, 1, 2, 2, 3)^t$ is a positive eigenvector of C for its eigenvalue 3. None of the matrices A, B, and C is totally nonnegative.

Finally, let H'_n be the matrix obtained from the (0,1)- Hessenberg matrix H_n by replacing the 1 in position $(n, 1)$ with 0. For instance,

$$H'_4 = \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}.$$

The eigenvalues of H_4 are $0, 0, 2 \pm \sqrt{2}$ and are nonnegative, but H'_4 is not totally nonnegative. The eigenvalues of H'_5 are $0, 0, 1, 2 \pm \sqrt{3}$. The eigenvalues of H'_6 are $0, 0, 0, 1, 1, 4$. The eigenvalues of H'_7 are $0, 0, 0, 1.3194 \pm 0.49781i, 0.1185, 4.2426$. Thus for $n = 4, 5, 6$, H'_n is a matrix with nonnegative eigenvalues but not totally nonnegative; H'_7 does not have all eigenvalues nonnegative.

We plan to further investigate irreducible $(0, 1)$-matrices with nonnegative eigenvalues in a subsequent paper.

References

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