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A bound on the scrambling index of a primitive matrix using Boolean rank

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The scrambling index of an $n \times n$ primitive matrix A is the smallest positive integer k such that $A^k(A^t)^k = J$, where A^t denotes the transpose of A and J denotes the $n \times n$ all ones matrix. For an $m \times n$ Boolean matrix M, its *Boolean rank* $b(M)$ is the smallest positive integer b such that $M = AB$ for some $m \times b$ Boolean matrix A and $b \times n$ Boolean matrix B. In this paper, we give an upper bound on the scrambling index of an $n \times n$ primitive matrix M in terms of its Boolean rank $b(M)$. Furthermore we characterize all primitive matrices that achieve the upper bound.

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1. Introduction

For terminology and notation used here we follow [3]. A matrix A is called *nonnegative* if all its elements are nonnegative, and denoted by $A \geqslant 0$. A matrix A is called *positive* if all its elements are positive, and denoted by $A > 0$. For an $m \times n$ matrix A, we will denote its (i, j)-entry by A_{ij}, its ith row by $A_{i\cdot}$, and its jth column by $A_{\cdot j}$. For $m \times n$ matrices A and B, we say that B is dominated by A if $B_{ij} \leqslant A_{ij}$ for each i and j, and denote this by $B \leqslant A$. We denote the $m \times n$ all ones matrix by $J_{m,n}$ (and by J_n if $m = n$), the $m \times n$ all zeros matrix by $O_{m,n}$, the all ones n-vector by j_n, the $n \times n$ identity matrix by

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I_n, and its ith column by $e_i(n)$. The subscripts m and n will be omitted whenever their values are clear from the context.

Let $D=(V,E)$ denote a *digraph* (directed graph) with vertex set $V=V(D)$, arc set $E=E(D)$ and order n. Loops are permitted but multiple arcs are not. A $u\to v$ *walk* in a digraph D is a sequence of vertices $u,u_1,\ldots,u_t,v\in V(D)$ and a sequence of arcs $(u,u_1),(u_1,u_2),\ldots,(u_t,v)\in E(D)$, where the vertices and arcs are not necessarily distinct. We shall use the notation $u\to v$ and $u\not\to v$ to denote, respectively, that there is an arc from vertex u to vertex v and that there is no such an arc. Similarly, $u\xrightarrow{k}v$ and $u\overset{k}{\not\to}v$ denote, respectively, that there is a directed walk of length k from vertex u to vertex v, and that there is no such a walk.

For an $n\times n$ nonnegative matrix $A=(a_{ij})$, its digraph, denoted by $D(A)$, is the digraph with vertex set $V(D(A))=\{1,2,\ldots,n\}$, and (i,j) is an arc of $D(A)$ if and only if $a_{ij}\neq 0$. Then, for a positive integer $r\geqslant 1$, the (i,j)th entry of the matrix A^r is positive if and only if $i\xrightarrow{r}j$ in the digraph $D(A)$. Since most of the time we are only interested in the existence of such walks, not the number of different directed walks from vertex i to vertex j, we interpret A as a Boolean $(0,1)$-matrix, unless stated otherwise. A *Boolean* $(0,1)$*-matrix* is a matrix with only 0's and 1's as its entries. Using *Boolean arithmetic*, $(1+1=1,\ 0+0=0,\ 1+0=1)$, we have that AB and $A+B$ are Boolean $(0,1)$-matrices if A and B are.

A digraph D is called *primitive* if for some positive integer t there is a walk of length exactly t from each vertex u to each vertex v. If D is primitive the smallest such t is called the *exponent* of D, denoted by $\exp(D)$. Equivalently, a square nonnegative matrix A of order n is called *primitive* if there exists a positive integer r such that $A^r>0$. The minimum such r is called the *exponent* of A, and denoted by $\exp(A)$. Clearly $\exp(A)=\exp(D(A))$. There are numerous results on the exponent of primitive matrices [3]. In 1950, Wielandt [7] stated that $\exp(A)\leqslant(n-1)^2+1$ and that equality is attained by W_n, where

$$W_2=\begin{bmatrix}1&1\\1&0\end{bmatrix}\quad\text{and}\quad W_n=\begin{bmatrix}0&1&0&\cdots&0&0\\0&0&1&0&\cdots&0\\\vdots&\vdots&\ddots&\ddots&\cdots&\vdots\\0&0&\cdots&0&1&0\\1&0&\cdots&\cdots&0&1\\1&0&\cdots&\cdots&0&0\end{bmatrix}\text{ when } n\geqslant 3.$$

Several authors (see, for example, [3, p. 81]) later proved that $\exp(A)=(n-1)^2+1$ if and only if $PAP^t=W_n$ for some permutation matrix P.

The *scrambling index* of a primitive digraph D is the smallest positive integer k such that for each pair of vertices u and v, there exists some vertex $w=w(u,v)$ (dependent on u and v) such that $u\xrightarrow{k}w$ and $v\xrightarrow{k}w$ in D. The scrambling index of D is denoted by $k(D)$. For $u,v\in V(D)$ $(u\neq v)$, we define the *local scrambling index of u and v* as

$$k_{u,v}(D)=\min\{k:\ u\xrightarrow{k}w \text{ and } v\xrightarrow{k}w \text{ for some } w\in V(D)\}.$$

Then

$$k(D)=\max_{u,v\in V(D)}\{k_{u,v}(D)\}.$$

An analogous definition for scrambling index can be given for nonnegative matrices. The *scrambling index* of a primitive matrix A, denoted by $k(A)$, is the smallest positive integer k such that any two rows of A^k have at least one positive element in a coincident position. The scrambling index of a primitive matrix A can also be equivalently defined as the smallest positive integer k such that $A^k(A^t)^k=J$, where A^t denotes the transpose of A. If A is the adjacency matrix of a primitive digraph D, then $k(D)=k(A)$. As a result, throughout the paper, where no confusion occurs, we use the digraph D and the adjacency matrix $A(D)$ interchangeably.

In [1,2], Akelbek and Kirkland obtained an upper bound on the scrambling index of a primitive digraph D in terms of the order and girth of D, and gave a characterization of the primitive digraphs with the largest scrambling index.

Theorem 1.1 [1]. *Let D be a primitive digraph with n vertices and girth s. Then*

$$k(D) \leqslant n - s + \begin{cases} \left(\frac{s-1}{2}\right) n, & \text{when } s \text{ is odd,} \\ \left(\frac{n-1}{2}\right) s, & \text{when } s \text{ is even.} \end{cases}$$

When $s = n - 1$, an upper bound on $k(D)$ in terms of the order of a primitive digraph D can be achieved [1]. We state the theorem in terms of primitive matrices below.

Theorem 1.2 [1]. *Let A be a primitive matrix of order* $n \geqslant 2$. *Then*

$$k(A) \leqslant \left\lceil \frac{(n-1)^2 + 1}{2} \right\rceil. \tag{1}$$

Equality holds in (1) *if and only if there is a permutation matrix P such that* PAP^t *is equal to* W_2 *or* J_2 *when* $n = 2$ *and* W_n *when* $n \geqslant 3$.

The digraph $D(W_n)$ is called the Wielandt graph and denoted by $D_{n-1,n}$. It is a digraph with a Hamilton cycle $1 \to 2 \to \cdots \to n \to 1$ together with an arc from vertex $n-1$ to vertex 1. For simplicity, let $h_n = \left\lceil \frac{(n-1)^2+1}{2} \right\rceil$. The next proposition gives some information about the Wielandt graph $D_{n-1,n}$.

Proposition 1.3 [1]. *For* $D_{n-1,n}$, *where* $n \geqslant 3$,

(a) $k_{n,\lfloor \frac{n}{2} \rfloor}(D_{n-1,n}) = h_n$, *and for all other pairs of vertices u and v of* $D_{n-1,n}$, $k_{u,v}(D_{n-1,n}) < h_n$.
(b) *There are directed walks from vertices n and* $\left\lfloor \frac{n}{2} \right\rfloor$ *to vertex* 1 *of length* h_n, *that is* $n \xrightarrow{h_n} 1$ *and* $\left\lfloor \frac{n}{2} \right\rfloor \xrightarrow{h_n} 1$.

For an $m \times n$ Boolean matrix M, we define its *Boolean rank* $b(M)$ to be the smallest positive integer b such that for some $m \times b$ Boolean matrix A and $b \times n$ Boolean matrix B, $M = AB$. The Boolean rank of the zero matrix is defined to be zero. $M = AB$ is called a *Boolean rank factorization* of M.

In [4], Gregory et al. obtained an upper bound on the exponent of a primitive Boolean matrix in terms of Boolean rank.

Proposition 1.4 [4]. *Suppose that* $n \geqslant 2$ *and that M is an* $n \times n$ *primitive Boolean matrix with* $b(M) = b$. *Then*

$$\exp(M) \leqslant (b-1)^2 + 2. \tag{2}$$

In [4], Gregory et al. also gave a characterization of the matrices for which equality holds in (2). In [5], Liu et al. gave a characterization of primitive matrices M with Boolean rank b such that $\exp(M) = (b-1)^2 + 1$.

In this paper, we give an upper bound on the scrambling index of a primitive matrix M using Boolean rank $b = b(M)$, and characterize all Boolean primitive matrices that achieve the upper bound.

2. Main results

We start with a basic result.

Lemma 2.1. *Suppose that A and B are* $n \times m$ *and* $m \times n$ *Boolean matrices respectively, and that neither has a zero line. Then*

(a) *AB is primitive if and only if BA is primitive.*
(b) *If AB and BA are primitive, then*

$$|k(AB) - k(BA)| \leqslant 1. \tag{3}$$

Proof. Part (a) was proved by Shao [6]. We only need to show part (b). Since AB and BA are primitive matrices, A and B have no zero rows. Then $AA^t \geqslant I_n$ and $BJ_nB^t = J_m$. Suppose $k(AB) = k$. By the definition of scrambling index

$$(AB)^k((AB)^t)^k = J_n.$$

Then

$$\begin{aligned}(BA)^{k+1}((BA)^t)^{k+1} &= B(AB)^k AA^t((AB)^t)^k B^t \geqslant B(AB)^k I_n((AB)^t)^k B^t \\ &= B(AB)^k((AB)^t)^k B^t = BJ_nB^t = J_m.\end{aligned}$$

Thus $k(BA) \leqslant k + 1 = k(AB) + 1$. The result follows by exchanging the roles of A and B. □

Proposition 2.2 [5]. *Let M be an $n \times n$ primitive Boolean matrix, and $M = AB$ be a Boolean rank factorization of M. Then neither A nor B has a zero line.*

Theorem 2.3. *Let M be an $n \times n$ $(n \geqslant 2)$ primitive matrix with Boolean rank $b(M) = b$. Then*

$$k(M) \leqslant \left\lceil \frac{(b-1)^2+1}{2} \right\rceil + 1. \tag{4}$$

Proof. Let $M = AB$ be a Boolean rank factorization of M, where A and B are $n \times b$ and $b \times n$ Boolean matrices respectively. Then by Lemma 2.2 neither A nor B has a zero line. By Lemma 2.1, we have

$$k(M) = k(AB) \leqslant k(BA) + 1.$$

Since BA is primitive and BA is a $b \times b$ matrix, by Theorem 1.2,

$$k(BA) \leqslant \left\lceil \frac{(b-1)^2+1}{2} \right\rceil,$$

from which Theorem 2.3 follows. □

From (1) we see that no matrix of full Boolean rank n can attain the upper bound in (4). Further, since the only $n \times n$ primitive Boolean matrix with Boolean rank 1 is J_n, no matrix of Boolean rank 1 can attain the upper bound in (4). Thus we may assume that $2 \leqslant b \leqslant n - 1$.

For simplicity, let

$$h = \left\lceil \frac{(b-1)^2+1}{2} \right\rceil.$$

Recall from Theorem 1.2 that $k(W_b) = h$. We first make some observations about W_b. Recall that $D = D(W_b)$ is the Wielandt graph $D_{b-1,b}$ with b vertices.

Lemma 2.4. *If $b \geqslant 3$, then the zero entries of $(W_b)^{h-1}\,(W_b^t)^{h-1}$ occur only in the $\left(b, \left\lfloor \frac{b}{2} \right\rfloor\right)$ and $\left(\left\lfloor \frac{b}{2} \right\rfloor, b\right)$ positions.*

Proof. By Proposition 1.3 we know that $k_{b,\left\lfloor \frac{b}{2} \right\rfloor}(D_{b-1,b}) = h$, and for all other pairs of vertices u and v, $k_{u,v}(D_{b-1,b}) < h$. Therefore in W_b^{h-1} every pair of rows intersect with each other except rows b and $\left\lfloor \frac{b}{2} \right\rfloor$. Thus the only zero entries of $(W_b)^{h-1}\,(W_b^t)^{h-1}$ are in the $\left(b, \left\lfloor \frac{b}{2} \right\rfloor\right)$ and $\left(\left\lfloor \frac{b}{2} \right\rfloor, b\right)$ positions. □

For an $n \times n$ $(n \geqslant 2)$ matrix A, let $A(\{i_1, i_2\}, \{j_1, j_2\})$ be the submatrix of A that lies in the rows i_1 and i_2 and the columns j_1 and j_2.

Lemma 2.5. *For $b \geqslant 3$, $W_b^{h-1}\left(\left\{\left\lfloor \frac{b}{2}\right\rfloor, b\right\}, \{b-1, b\}\right)$ is either* $\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$ *or* $\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$.

Proof. By Proposition 1.3, we know that $k_{\lfloor \frac{b}{2}\rfloor, b}(D_{b-1,b}) = h$ and $\left\lfloor \frac{b}{2}\right\rfloor \xrightarrow{h} 1$ and $b \xrightarrow{h} 1$. From the digraph $D_{b-1,b}$, we know that the directed walks of length h from vertices $\left\lfloor \frac{b}{2}\right\rfloor$ and b to vertex 1 are either

$$\left\lfloor \frac{b}{2}\right\rfloor \xrightarrow{h-1} b-1 \xrightarrow{1} 1 \quad \text{and} \quad b \xrightarrow{h-1} b \xrightarrow{1} 1,$$

or

$$\left\lfloor \frac{b}{2}\right\rfloor \xrightarrow{h-1} b \xrightarrow{1} 1 \quad \text{and} \quad b \xrightarrow{h-1} b-1 \xrightarrow{1} 1.$$

For the first case, if $\left\lfloor \frac{b}{2}\right\rfloor \xrightarrow{h-1} b-1$ and $b \xrightarrow{h-1} b$, then $b \overset{h-1}{\nrightarrow} b-1$ and $\left\lfloor \frac{b}{2}\right\rfloor \overset{h-1}{\nrightarrow} b$. Otherwise it contradicts $k_{\lfloor \frac{b}{2}\rfloor, b}(D_{b-1,b}) = h$. Similarly, for the second case if $\left\lfloor \frac{b}{2}\right\rfloor \xrightarrow{h-1} b$ and $b \xrightarrow{h-1} b-1$, then $b \overset{h-1}{\nrightarrow} b$ and $\left\lfloor \frac{b}{2}\right\rfloor \overset{h-1}{\nrightarrow} b-1$. The result follows by applying these to the matrix W_b^{h-1}. $\square$

Theorem 2.6. *Suppose M is an $n \times n$ Boolean matrix with $3 \leqslant b = b(M) \leqslant n-1$. Then M is primitive and $k(M) = h+1$ if and only if M has a Boolean rank factorization $M = AB$, where A and B have the following properties:*

(i) $BA = W_b$,
(ii) *some row of A is $e^t_{\lfloor \frac{b}{2}\rfloor}(b)$, some row of A is $e^t_b(b)$, and*
(iii) *no column of B is $e_{b-1}(b) + e_b(b)$.*

Proof. First suppose M is primitive with $k(M) = h+1$, and $M = \widetilde{A}\widetilde{B}$ is a Boolean rank factorization of M. By Lemma 2.1, $\widetilde{B}\widetilde{A}$ is primitive and $k(\widetilde{B}\widetilde{A}) \geqslant h$. But $\widetilde{B}\widetilde{A}$ is a $b \times b$ matrix. By Theorem 1.2, $k(\widetilde{B}\widetilde{A}) \leqslant h$. Therefore $k(\widetilde{B}\widetilde{A}) = h$. Also by Theorem 1.2, there is a permutation matrix P such that $P\widetilde{B}\widetilde{A}P^t = W_b$. Let $B = P\widetilde{B}$ and $A = \widetilde{A}P^t$. Then $AB = \widetilde{A}P^tP\widetilde{B} = \widetilde{A}\widetilde{B} = M$. Thus A and B satisfy condition (i).

Since M is primitive, we have $\sum_{i=1}^{b} A_{.i} = j_n = \sum_{i=1}^{b} B^t_{i.}$. Since $k(M) = h+1$, the matrix M^h must have two rows that do not intersect. Without loss of generality, suppose rows p and q of M^h do not intersect. Then entries in the (p,q) and (q,p) positions of $M^h(M^t)^h$ are zero. Since matrix B has no zero row, we have $BB^t \geqslant I_b$. Thus

$$\begin{aligned}
&M^h(M^t)^h\\
&= (AB)^h((AB)^t)^h = A(BA)^{h-1}BB^t((BA)^t)^{h-1}A^t\\
&= A(W_b)^{h-1}BB^t\left(W_b^t\right)^{h-1}A^t\\
&\geqslant A(W_b)^{h-1}I_b\left(W_b^t\right)^{h-1}A^t = A(W_b)^{h-1}\left(W_b^t\right)^{h-1}A^t\\
&= AZA^t\\
&= \left[\left. J_{n,\lfloor \frac{b}{2}\rfloor-1}\ \right|\ \sum_{i=1}^{b-1} A_{.i}\ \left|\ J_{n,b-\lfloor \frac{b}{2}\rfloor-1}\ \right|\ \sum_{\substack{i=1\\ i\neq \lfloor \frac{b}{2}\rfloor}}^{b} A_{.i}\right]A^t\\
&= j_n\left(\sum_{i=1}^{\lfloor \frac{b}{2}\rfloor-1} A_{.i}\right)^t + \left(\sum_{i=1}^{b-1} A_{.i}\right)\left(A_{.\lfloor \frac{b}{2}\rfloor}\right)^t + j_n\left(\sum_{i=\lfloor \frac{b}{2}\rfloor+1}^{b-1} A_{.i}\right)^t + \left(\sum_{\substack{i=1\\ i\neq \lfloor \frac{b}{2}\rfloor}}^{b} A_{.i}\right)(A_{.b})^t,
\end{aligned}$$

where $Z = (W_b)^{h-1}\left(W_b^t\right)^{h-1}$ is the $b \times b$ matrix which has zero entries only in the $\left(\left\lfloor \frac{b}{2}\right\rfloor, b\right)$ and $\left(b, \left\lfloor \frac{b}{2}\right\rfloor\right)$ positions. Since AZA^t is dominated by $M^h(M^t)^h$ and $M^h(M^t)^h$ has zero entries in the (p,q) and (q,p) positions, the entries in the (p,q) and (q,p) positions of AZA^t are also zero. Thus

$$\sum_{i=1}^{\left\lfloor \frac{b}{2}\right\rfloor-1} A_{qi} + \left(\sum_{i=1}^{b-1} A_{pi}\right) A_{q\left\lfloor \frac{b}{2}\right\rfloor} + \sum_{i=\left\lfloor \frac{b}{2}\right\rfloor+1}^{b-1} A_{qi} + \left(\sum_{\substack{i=1\\ i\neq\left\lfloor \frac{b}{2}\right\rfloor}}^{b} A_{pi}\right) A_{qb} = 0 \tag{5}$$

and

$$\sum_{i=1}^{\left\lfloor \frac{b}{2}\right\rfloor-1} A_{pi} + \left(\sum_{i=1}^{b-1} A_{qi}\right) A_{p\left\lfloor \frac{b}{2}\right\rfloor} + \sum_{i=\left\lfloor \frac{b}{2}\right\rfloor+1}^{b-1} A_{pi} + \left(\sum_{\substack{i=1\\ i\neq\left\lfloor \frac{b}{2}\right\rfloor}}^{b} A_{qi}\right) A_{pb} = 0. \tag{6}$$

Then $A_{qi} = 0$ and $A_{pi} = 0$ for $i = 1, \ldots, b-1$ and $i \neq \left\lfloor \frac{b}{2}\right\rfloor$. Substituting these back in (5) and (6), we have

$$A_{q\left\lfloor \frac{b}{2}\right\rfloor} A_{p\left\lfloor \frac{b}{2}\right\rfloor} + A_{qb}A_{pb} = 0. \tag{7}$$

Thus rows $A_{p.}$ and $A_{q.}$ are disjoint. Since A has no zero rows, each of these rows has precisely one nonzero entry. Therefore some row of A is $e^t_{\left\lfloor \frac{b}{2}\right\rfloor}(b)$ and some row of A is $e^t_b(b)$. This concludes (ii).

We claim B cannot have a column which is equal to $u = e_{b-1}(b) + e_b(b)$. Otherwise, suppose some column of B is u. Since B has no zero row, by Proposition 2.2, $BB^t \geqslant I_b + uu^t$. Thus

$$\begin{aligned}
M^h(M^t)^h &= (AB)^h((AB)^t)^h = A(BA)^{h-1}BB^t((BA)^t)^{h-1}A^t\\
&= A(W_b)^{h-1}BB^t\left(W_b^t\right)^{h-1}A^t\\
&\geqslant A(W_b)^{h-1}\left(I_b + uu^t\right)\left(W_b^t\right)^{h-1}A^t\\
&= A\left[(W_b)^{h-1}\left(W_b^t\right)^{h-1} + \left(W_b^{h-1}u\right)\left(W_b^{h-1}u\right)^t\right]A^t.
\end{aligned}$$

By Lemma 2.4, $W_b^{h-1}\left(\left\{\left\lfloor \frac{b}{2}\right\rfloor, b\right\}, \{b-1, b\}\right)$ is either $\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$ or $\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$. Then $W_b^{h-1}u \geqslant e_{\left\lfloor \frac{b}{2}\right\rfloor}(b) + e_b(b)$. By Lemma 2.4, the zero entries of $W_b^{h-1}\left(W_b^t\right)^{h-1}$ are in the $\left(b, \left\lfloor \frac{b}{2}\right\rfloor\right)$ and $\left(\left\lfloor \frac{b}{2}\right\rfloor, b\right)$ positions. Therefore $W_b^{h-1}\left(W_b^t\right)^{h-1} + \left(W_b^{h-1}u\right)\left(W_b^{h-1}u\right)^t = J_b$. Since A has no zero lines, we have $M^h(M^t)^h = AJ_bA^t = J_n$, which is a contradiction to $k(M) = h+1$. This proves (iii).

Finally, suppose that $M = AB$ is a Boolean rank factorization of M and A and B satisfy (i), (ii) and (iii). By Proposition 2.2 and Lemma 2.1(a), neither A nor B has a zero line and the matrix M is primitive since W_b is. By Theorem 2.3, $k(M) \leqslant h+1$. Since $BA = W_b$ and A has no zero row, each column of B is dominated by a column of W_b. Thus each column of B is in the set $S_1 = \{e_1(b), e_2(b), \ldots, e_b(b), u\}$, where $u = e_{b-1}(b) + e_b(b)$. But by (iii), no column of B is u. Hence each column of B is in the set $S_1' = \{e_1(b), e_2(b), \ldots, e_b(b)\}$. Therefore $BB^t \leqslant I_b$. Also since matrix B has no zero row, $BB^t \geqslant I_b$. Hence $BB^t = I_b$. Thus

$$\begin{aligned}
M^h(M^t)^h &= (AB)^h((AB)^t)^h = A(BA)^{h-1}BB^t((BA)^t)^{h-1}A^t\\
&= A(W_b)^{h-1}I_b\left(W_b^t\right)^{h-1}A^t\\
&= A(W_b)^{h-1}\left(W_b^t\right)^{h-1}A^t\\
&= AZA^t,
\end{aligned}$$

Table 1
($b \geqslant 3$).

$$M_1 = \left[\begin{array}{cccccc|c} 0 & J & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & J & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & J & 0 & J \\ 0 & 0 & \cdots & 0 & 0 & J & 0 \\ J & 0 & \cdots & 0 & 0 & 0 & 0 \\ \hline J & 0 & \cdots & 0 & 0 & 0 & 0 \end{array}\right] \qquad M_2 = \left[\begin{array}{cccccc|c} 0 & J & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & J & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & J & 0 & J \\ 0 & 0 & \cdots & 0 & 0 & J & 0 \\ J & 0 & \cdots & 0 & 0 & 0 & 0 \\ \hline J & 0 & \cdots & 0 & 0 & J & 0 \end{array}\right]$$

$$M_3 = \left[\begin{array}{cccccc|cc} 0 & J & 0 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & J & 0 & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & J & 0 & J & J \\ 0 & 0 & \cdots & 0 & 0 & J & 0 & 0 \\ J & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ \hline J & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ J & 0 & \cdots & 0 & 0 & J & 0 & 0 \end{array}\right]$$

where, by Lemma 2.4, $Z = (W_b)^{h-1}\,(W_b^t)^{h-1}$ is the $b \times b$ matrix which has zero entries only in the $\left(\left\lfloor \frac{b}{2} \right\rfloor, b\right)$ and $\left(b, \left\lfloor \frac{b}{2} \right\rfloor\right)$ positions. By (ii) some row of A is $e^t_{\lfloor \frac{b}{2} \rfloor}(b)$ and some row of A is $e^t_b(b)$. Without loss of generality, suppose row p of A is $e^t_{\lfloor \frac{b}{2} \rfloor}(b)$ and row q of A is $e^t_b(b)$. Then

$$(M^h (M^t)^h)_{pq} = e^t_p(b) A Z A^t e_q(b) = Z_{\lfloor \frac{b}{2} \rfloor b} = 0.$$

Hence $k(M) > h$. Therefore $k(M) = h + 1$. □

Next we will reinterpret conditions (i)–(iii) of Theorem 2.6 to show that if $k(M) = h + 1$, then M is one of the three basic types of matrices in Theorem 2.7.

Theorem 2.7. *Suppose M is an $n \times n$ Boolean matrix with $b(M) = b$, where $3 \leqslant b \leqslant n - 1$. Then M is primitive with $k(M) = h + 1$ if and only if there is a permutation matrix P such that PMP^t has one of the forms in Table* 1.

In Table 1 the rows and columns of M_1, M_2 and M_3 are partitioned conformally, so that each diagonal block is square, and the top left hand submatrix common to each has b blocks in its partitioning.

Proof. Suppose M is primitive, $b \geqslant 3$, and $k(M) = h + 1$. Then by Theorem 2.6(i), M has a Boolean rank factorization $M = AB$ such that $BA = W_b$. As shown in the proof of Theorem 2.6, we know that each column of B is in the set $S'_1 = \{e_1(b), e_2(b), \ldots, e_b(b)\}$. Since B has no zero column, each row of A is dominated by a row of W_b. Therefore each row of A is in the set $S_2 = \{e^t_1(b), e^t_2(b), \ldots, e^t_b(b), v^t\}$, where $v = e_1(b) + e_b(b)$.

Next, we note that for each $1 \leqslant i \leqslant b$, the outer product $B_{.i}A_{i.}$ is dominated by W_b. Since each $B_{.i}$ and $A_{i.}$ must be in S'_1 and S_2 respectively and $(B_{.i}, A_{i.})$ must be one of the following pairs: (e_i, e^t_{i+1}), $1 \leqslant i \leqslant b - 1$, (e_{b-1}, e^t_1), (e_b, e_1), or (e_{b-1}, v^t), where $e_i = e_i(b)$ for any $i \in \{1, 2, \ldots, b\}$. Thus, for each i, $1 \leqslant i \leqslant b - 2$, $\left(e_i, e^t_{i+1}\right) = (B_{.k_i}, A_{k_i.})$ for some k_i. This also holds for $i = b - 1$ because, by (ii), some row of A must equal e^t_b. Some outer product $B_{.j}A_{j.}$ has a 1 in the $(b, 1)$ position, hence $(B_{.k_b}, A_{k_b.}) = (e_b, e^t_1)$ for some k_b. Finally some outer product $B_{.j}A_{j.}$ must have a 1 in the $(b - 1, 1)$ position, hence for some k_{b+1}, $(B_{.k_{b+1}}, A_{k_{b+1}.})$ is one of (e_{b-1}, e^t_1) or (e_{b-1}, v^t). It follows from the above argument that there is an $n \times n$ permutation matrix Q such that

$$BQ^t = [\overline{B}|\widetilde{B}] \quad \text{and} \quad QA = \begin{bmatrix} \overline{A} \\ \widetilde{A} \end{bmatrix},$$

where

$$\overline{B} = \left[e_1 j_{n_1}^t | e_2 j_{n_2}^t | \cdots | e_b j_{n_b}^t\right] \text{ and } \overline{A} = \begin{bmatrix} j_{n_1} e_2^t \\ \hline j_{n_2} e_3^t \\ \hline \cdots \\ \hline j_{n_{b-1}} e_b^t \\ \hline j_{n_b} e_1^t \end{bmatrix}$$

for some $n_1, \ldots, n_b \geqslant 1$, and where each $(\widetilde{B}_{.i}, \widetilde{A}_{i.})$ is one of (e_{b-1}, e_1^t) or (e_{b-1}, v^t). Thus $\widetilde{B}$ and $\widetilde{A}$ can be one of the following pairs of matrices:

$$\widetilde{B}_1 = e_{b-1} j_{m_1}^t, \quad \widetilde{A}_1 = j_{m_1} e_1^t \text{ for some } m_1 \geqslant 1;$$
$$\widetilde{B}_2 = e_{b-1} j_{m_2}^t, \quad \widetilde{A}_2 = j_{m_2} v^t \text{ for some } m_2 \geqslant 1;$$
$$\widetilde{B}_3 = \left[e_{b-1} j_{m_3}^t | e_{b-1} j_{p_3}^t\right], \quad \widetilde{A}_3 = \begin{bmatrix} j_{m_3} e_1^t \\ \hline j_{p_3} v^t \end{bmatrix} \text{ for some } m_3, p_3 \geqslant 1.$$

It is now readily verified that

$$\begin{bmatrix} \overline{A} \\ \widetilde{A}_i \end{bmatrix} [\overline{B}|\widetilde{B}_i] = M_i \text{ for } 1 \leqslant i \leqslant 3,$$

so that QMQ^t is one of the matrices in Table 1.

Finally, since the Boolean rank factorization

$$M_i = \begin{bmatrix} \overline{A} \\ \widetilde{A}_i \end{bmatrix} [\overline{B}|\widetilde{B}_i]$$

satisfies conditions (i)–(iii) of Theorem 2.6, each M_i is primitive and $k(M) = h + 1$. □

When $b(M) = 2$, we have the following result.

Theorem 2.8. *Suppose M is an $n \times n$ primitive Boolean matrix with $b(M) = b = 2$. Then $k(M) = 2$ if and only if M has a Boolean rank factorization $M = AB$, where A and B have the following properties*:

(i) *$BA = W_2$ or $BA = J_2$,*
(ii) *some row of A is $e_1^t(2)$, some row of A is $e_2^t(2)$, and*
(iii) *no column of B is $e_1(2) + e_2(2)$.*

Proof. First suppose M is primitive with $k(M) = 2$, and $M = \widetilde{A}\widetilde{B}$ is a Boolean rank factorization of M. By Lemma 2.1, $\widetilde{B}\widetilde{A}$ is primitive and $k(\widetilde{B}\widetilde{A}) \geqslant 1$. But $\widetilde{B}\widetilde{A}$ is a 2×2 matrix. By Theorem 1.2, $k(\widetilde{B}\widetilde{A}) \leqslant 1$. Therefore $k(\widetilde{B}\widetilde{A}) = 1$. Also by Theorem 1.2, there is a permutation matrix P such that $P\widetilde{B}\widetilde{A}P^t = W_2$ or $P\widetilde{B}\widetilde{A}P^t = J_2$. Let $B = P\widetilde{B}$ and $A = \widetilde{A}P^t$. Then $AB = \widetilde{A}P^tP\widetilde{B} = \widetilde{A}\widetilde{B} = M$. Thus A and B satisfy condition (i).

Proof of the conditions (ii) and (iii) are similar to the proof of Theorem 2.6. □

By a similar argument, we can reinterpret conditions (i)–(iii) of Theorem 2.8 to show that if M satisfies $k(M) = 2$, then M is one of the 21 basic types of matrices which we will show in the following.

Theorem 2.9. *Suppose M is an $n \times n$ Boolean matrix with $b(M) = b = 2$. Let $M = AB$ be a Boolean rank factorization. Then M is primitive with $k(M) = 2$ if and only if there is a permutation matrix P such that PMP^t has one of the forms in Table 2 if $BA = W_2$ or PMP^t has one of the forms in Table 3 if $BA = J_2$.*

Table 2
($b=2$).

$$\left[\begin{array}{cc|c} 0 & J & 0 \\ J & 0 & J \\ \hline J & 0 & J \end{array}\right], \quad \left[\begin{array}{cc|c} 0 & J & 0 \\ J & 0 & J \\ \hline J & J & J \end{array}\right], \quad \left[\begin{array}{cc|cc} 0 & J & 0 & 0 \\ J & 0 & J & J \\ \hline J & 0 & J & J \\ J & J & J & J \end{array}\right].$$

Table 3
($b=2$).

$$\begin{bmatrix} J & J & 0 & 0 \\ 0 & 0 & J & J \\ J & J & 0 & 0 \\ 0 & 0 & J & J \end{bmatrix}, \quad \left[\begin{array}{cccc|c} J & J & 0 & 0 & J \\ 0 & 0 & J & J & 0 \\ J & J & 0 & 0 & J \\ 0 & 0 & J & J & 0 \\ \hline J & J & J & J & J \end{array}\right], \quad \left[\begin{array}{cccc|c} J & J & 0 & 0 & 0 \\ 0 & 0 & J & J & J \\ J & J & 0 & 0 & 0 \\ 0 & 0 & J & J & J \\ \hline J & J & J & J & J \end{array}\right], \quad \left[\begin{array}{cccc|cc} J & J & 0 & 0 & J & 0 \\ 0 & 0 & J & J & 0 & J \\ J & J & 0 & 0 & J & 0 \\ 0 & 0 & J & J & 0 & J \\ \hline J & J & J & J & J & J \\ J & J & J & J & J & J \end{array}\right],$$

$$\begin{bmatrix} J & J & 0 \\ 0 & 0 & J \\ J & J & J \end{bmatrix}, \quad \left[\begin{array}{ccc|c} J & J & 0 & J \\ 0 & 0 & J & 0 \\ J & J & J & J \\ \hline J & J & J & J \end{array}\right], \quad \left[\begin{array}{ccc|c} J & J & 0 & 0 \\ 0 & 0 & J & J \\ J & J & J & J \\ \hline J & J & 0 & 0 \end{array}\right], \quad \left[\begin{array}{ccc|c} J & J & 0 & 0 \\ 0 & 0 & J & J \\ J & J & J & J \\ \hline 0 & 0 & J & J \end{array}\right],$$

$$\left[\begin{array}{ccc|cc} J & J & 0 & J & 0 \\ 0 & 0 & J & 0 & J \\ J & J & J & J & J \\ \hline J & J & J & J & J \\ J & J & 0 & J & 0 \end{array}\right], \quad \left[\begin{array}{ccc|cc} J & J & 0 & J & 0 \\ 0 & 0 & J & 0 & J \\ J & J & J & J & J \\ \hline J & J & J & J & J \\ 0 & 0 & J & 0 & J \end{array}\right],$$

$$\begin{bmatrix} J & J & J \\ J & 0 & 0 \\ 0 & J & J \end{bmatrix}, \quad \left[\begin{array}{ccc|c} J & J & J & J \\ J & 0 & 0 & J \\ 0 & J & J & 0 \\ \hline J & 0 & 0 & J \end{array}\right], \quad \left[\begin{array}{ccc|c} J & J & J & J \\ J & 0 & 0 & J \\ 0 & J & J & 0 \\ \hline 0 & J & J & 0 \end{array}\right], \quad \left[\begin{array}{ccc|c} J & J & J & J \\ J & 0 & 0 & 0 \\ 0 & J & J & J \\ \hline J & J & J & J \end{array}\right],$$

$$\left[\begin{array}{ccc|cc} J & J & J & J & J \\ J & 0 & 0 & J & 0 \\ 0 & J & J & 0 & J \\ \hline J & 0 & 0 & J & 0 \\ J & J & J & J & J \end{array}\right], \quad \left[\begin{array}{ccc|cc} J & J & J & J & J \\ J & 0 & 0 & J & 0 \\ 0 & J & J & 0 & J \\ \hline 0 & J & J & 0 & J \\ J & J & J & J & J \end{array}\right], \quad \begin{bmatrix} J & J & J & J \\ J & J & J & J \\ J & 0 & J & 0 \\ 0 & J & 0 & J \end{bmatrix}, \quad \begin{bmatrix} J & J & J & J \\ J & J & J & J \\ 0 & J & 0 & J \\ J & 0 & J & 0 \end{bmatrix}.$$

In Tables 2 and 3 the rows and columns of each matrix are partitioned conformally, so that each diagonal block is square.

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