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THE POSSIBLE NUMBERS OF ZEROS IN AN ORTHOGONAL MATRIX*

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Abstract. It is shown that for $n \geq 2$ there is an $n \times n$ indecomposable orthogonal matrix with exactly k entries equal to zero if and only if $0 \leq k \leq (n-2)^2$.

Key words. orthogonal matrix, indecomposable matrix, zero-nonzero pattern

AMS subject classifications. 15A57, 05C50

1. Introduction. By a *pattern* we simply mean the arrangement of zero and nonzero entries in a matrix. An $n \times n$ pattern P is called *orthogonal* if there is a (real) orthogonal matrix U whose pattern is P. By $\#(U)$ or $\#(P)$ we mean the number of zero entries in the matrix U or pattern P. An $n \times n$ pattern (or matrix) P is called *indecomposable* if it has no $r \times q$ zero submatrix, $r + q = n$; equivalently, there do not exist permutation matrices Q_1 and Q_2 such that

$$Q_1 P Q_2 = \begin{bmatrix} P_{11} & O \\ P_{21} & P_{22} \end{bmatrix},$$

in which P_{11} and P_{22} are square and nonempty (or, equivalently the bipartite graph of P is connected). If P were an orthogonal pattern and there were such reducing blocks, then an elementary calculation shows that $P_{21} = O$ also. Since an $n \times n$ orthogonal matrix U is invertible, $\#(U) \leq n(n-1)$ (which is sharp because the identity is orthogonal), but to be indecomposable, U must have more nonzero entries. In [BBS], it was observed that the maximum number of zero entries in an $n \times n$ indecomposable orthogonal matrix, $n \geq 2$, is $(n-2)^2$, in response to a query made by [F].

What, then, about smaller numbers of zeros? It should be noted that if any single entry is changed to a nonzero in any indecomposable orthogonal pattern P that realizes $(n-2)^2$ zeros, $n \geq 5$, the resulting pattern is no longer orthogonal. Nonetheless, $(n-2)^2 - 1$ zeros can occur in an $n \times n$ indecomposable orthogonal matrix. It is our purpose here to show that there is an $n \times n$ indecomposable orthogonal matrix

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U such that $\#(U) = k$ if and only if $0 \le k \le (n-2)^2$, thereby greatly strengthening earlier observations. The same is true for complex unitary matrices.

2. Numbers of Zeros from 0 to $\frac{1}{2}(n-2)(n-1)$. Let P be an $n \times n$ indecomposable orthogonal matrix with columns $p_1, \dots, p_n$, and let

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

be a 2×2 orthogonal matrix with no zero entries. Then it is easy to show that the matrix

$$D_i(P) = \begin{bmatrix} p_1 & \cdots & p_{i-1} & ap_i & bp_i & p_{i+1} & \cdots & p_n \\ 0 & \cdots & 0 & c & d & 0 & \cdots & 0 \end{bmatrix}$$

is an $(n+1) \times (n+1)$ indecomposable orthogonal matrix. This idea comes from the notions of matrix weaving and woven matrices which can be found in [C].

It should be clear at this point that the above notion may as well be applied to orthogonal patterns. Thus we obtain the following lemma.

LEMMA 2.1. *If P is an $n \times n$ indecomposable orthogonal pattern, then $D_i(P)$ is an $(n+1) \times (n+1)$ indecomposable orthogonal pattern.*

Since for each θ, $0 < \theta < \frac{\pi}{2}$,

$$B(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

is an orthogonal matrix, it is clear that there are full (i.e. indecomposable) 2×2 orthogonal matrices and that there are ones arbitrarily close to the identity matrix I_2. It follows that for any $B(\theta)$ with a sufficiently small θ and for any vector $v \in \mathbb{R}^2$ with no zero components, the row vector $v^T B(\theta)$ has no zero components.

We denote by $K_{n,i}$ the $n \times n$ pattern whose only zero entries are the first i entries of the last row.

LEMMA 2.2. *For $n \ge 2$, each $K_{n,i}$, $i = 0, \dots, n-2$, is an indecomposable orthogonal pattern.*

Proof. First we show that if $K_{n,i}$ is an orthogonal pattern for $n \ge 2$ and some integer i satisfying $1 \le i \le n-2$, then $K_{n,i-1}$ is also an orthogonal pattern. For $n \ge 2$, suppose there exists an $n \times n$ orthogonal matrix $A = (a_{pq})$ and an integer i satisfying $1 \le i \le n-2$ so that A has pattern $K_{n,i}$. Define $R_j(\theta)$ to be the $n \times n$ orthogonal matrix with entries equal to the identity matrix except that

$$R_j(\theta)[\{j, j+1\}] = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

where the notation $A[\alpha]$ denotes the principal submatrix of A whose rows and columns are indexed by the set α.

Now form the product $AR_i(\theta)$. Note that A and $AR_i(\theta)$ are entrywise equal except for columns i and $i+1$. These two columns of $AR_i(\theta)$ are

$$\begin{bmatrix} a_{1,i}\cos(\theta)+a_{1,i+1}\sin(\theta) \\ \vdots \\ a_{n-1,i}\cos(\theta)+a_{n-1,i+1}\sin(\theta) \\ a_{n,i+1}\sin(\theta) \end{bmatrix} \text{and} \begin{bmatrix} -a_{1,i}\sin(\theta)+a_{1,i+1}\cos(\theta) \\ \vdots \\ -a_{n-1,i}\sin(\theta)+a_{n-1,i+1}\cos(\theta) \\ a_{n,i+1}\cos(\theta) \end{bmatrix},$$

respectively. Since both A and $R_i(\theta)$ are orthogonal, the product $AR_i(\theta)$ is orthogonal. Now we only need to choose some θ sufficiently close to 0 so that we do not create any extra zero entries in $AR_i(\theta)$. Thus $AR_i(\theta)$ is an orthogonal matrix with pattern $K_{n,i-1}$.

Next we prove the lemma using the above result. We proceed by induction. Assume that for $n \geq 2$ there exists a full $n \times n$ orthogonal pattern P. Note that there is such a pattern for $n = 2$. By Lemma 2.1, $D_n(P)$ is also an orthogonal pattern. $D_n(P)$ has pattern $K_{n+1,(n+1)-2}$. By the above result, $K_{n+1,i}$, $i = 0,\ldots,(n+1)-2$, is also an orthogonal pattern. And $K_{n+1,0}$ is an $(n+1)\times(n+1)$ full orthogonal pattern, which completes the induction. Note that for i satisfying $0 \leq i \leq n-2$, $K_{n,i}$ is indecomposable as well. ◻

We now know that iterative application of the operator $D_j()$ to a $K_{n,i}$, $0 \leq i \leq n-2$, will produce indecomposable orthogonal patterns. Certain of these will be of particular interest.

For $2 \leq m \leq n$ and $0 \leq i \leq m-2$, we let

$$H_{n,m,i} = D_{n-1}(D_{n-2}(\cdots D_m(K_{m,i})\cdots)).$$

Then we obtain the following immediate corollary to Lemmas 2.1 and 2.2.

COROLLARY 2.3. *Each $H_{n,m,i}$, $2 \leq m \leq n$, $0 \leq i \leq m-2$ is an indecomposable orthogonal pattern.*

We note that since $H_{n,2,0}$ is the full $n \times n$ (upper) Hessenberg pattern, it follows that this pattern with $\#(H_{n,2,0}) = \frac{1}{2}(n-2)(n-1)$ is orthogonal. This is the sparsest pattern among the $H_{n,m,i}$ and its indecomposable orthogonality will also be used in the next section.

COROLLARY 2.4. *For each $k = 0,\ldots,\frac{1}{2}(n-2)(n-1)$, there is an $n \times n$ indecomposable orthogonal matrix with exactly k zero entries.*

Proof. We count the number of zeros in each $H_{n,m,i}$ where $2 \leq m \leq n$ and $0 \leq i \leq m-2$. $K_{m,i}$ has i zeros, $D_m(K_{m,i})$ has $i + ((m+1)-2)$ zeros and so on. So we have

$$\begin{aligned}\#(H_{n,m,i}) &= i + ((m+1)-2) + ((m+2)-2) + \cdots + ((m+(n-m))-2) \\ &= i + (m-1) + m + \cdots + (n-2) \\ &= i + \frac{1}{2}(n-2)(n-1) - \frac{1}{2}(m-2)(m-1).\end{aligned}$$

Now it is clear that we do indeed get all numbers of zeros between 0 and $\frac{1}{2}(n-2)(n-1)$ as we let m and i vary. ◻

3. Remaining Numbers of Zeros. From Corollary 2.3 we know that $H_{n,2,0}$, the $n \times n$ full upper Hessenberg pattern, is an indecomposable orthogonal pattern. Note that column i of $H_{n,2,0}$ has exactly $n-1-i$ zeros as long as $1 \leq i \leq n-1$. We will need this fact in the proof of the next lemma.

LEMMA 3.1. *For $n \geq 2$, there exists an $n \times n$ indecomposable orthogonal matrix with k zeros, $k = \frac{1}{2}(n-2)(n-1), \ldots, (n-2)^2$.*

Proof. We proceed by induction. Suppose that there exists an $n \times n$ indecomposable orthogonal pattern P_k with exactly k zeros, $k = \frac{1}{2}(n-2)(n-1), \ldots, (n-2)^2$. Also suppose that P_k has a column, namely column $j(k)$, with exactly $n-2$ zeros. It is easily verified that these conditions hold for $n = 2$.

First note that we may take $P_{\frac{1}{2}(n-2)(n-1)}$ to be $H_{n,2,0}$. Form $D_i(H_{n,2,0})$, $i = 1, \ldots, n-1$. Now we count zeros. $H_{n,2,0}$ has $\frac{1}{2}(n-2)(n-1)$ zeros, we double a column with $n-1-i$ zeros and we add $n-1$ zeros along the bottom of the pattern.

$$\begin{aligned}
\#(D_i(H_{n,2,0})) &= (n-1-i) + (n-1) + \#(H_{n,2,0}) \\
&= -i + (n-1) + (n-1) + \frac{1}{2}(n-2)(n-1) \\
&= -i + (n-1) + \frac{1}{2}(n-1)(n) \\
&= -i + ((n+1)-2) + \frac{1}{2}((n+1)-2)((n+1)-1).
\end{aligned}$$

Since i ranges from 1 to $n-1$, $\#(D_i(H_{n,2,0}))$ ranges from $\frac{1}{2}((n+1)-2)((n+1)-1)$ to $((n+1)-3) + \frac{1}{2}((n+1)-2)((n+1)-1)$. Also note that the last row of $D_i(H_{n,2,0})$ has $(n+1)-2$ zeros so that $(D_i(H_{n,2,0}))^T$ is an indecomposable orthogonal pattern with a column that has exactly $(n+1)-2$ zeros, $i = 1, \ldots, n-1$.

Next, for each $k = \frac{1}{2}(n-2)(n-1)+1, \ldots, (n-2)^2$, form $D_{j(k)}(P_k)$. Again we count zeros. P_k has k zeros, we double a column with $n-2$ zeros and we add $n-1$ zeros along the bottom of the pattern.

$$\#(D_{j(k)}(P_k)) = k + (n-1) + (n-2).$$

Since k ranges from $\frac{1}{2}(n-2)(n-1)+1$ up to $(n-2)^2$, we have that $\#(D_{j(k)}(P_k))$ ranges from

$$\begin{aligned}
\frac{1}{2}(n-2)(n-1) + 1 + (n-1) + (n-2) &= \frac{1}{2}(n-1)(n) + (n-1) \\
&= \frac{1}{2}((n+1)-2)((n+1)-1) + ((n+1)-2)
\end{aligned}$$

up to

$$\begin{aligned}
(n-2)^2 + (n-1) + (n-2) &= (n^2 - 4n + 4) + (n-1) + (n-2) \\
&= n^2 - 2n + 1 \\
&= (n-1)^2 \\
&= ((n+1)-2)^2.
\end{aligned}$$

Note that since $D_{j(k)}(P_k)$ has a row with exactly $(n+1)-2$ zeros, $(D_{j(k)}(P_k))^T$ is an indecomposable orthogonal pattern that has a column with exactly $(n+1)-2$ zeros.

Combining the two ranges of constructed $(n+1)\times(n+1)$ indecomposable orthogonal patterns gives us matrices with numbers of zeros from $\frac{1}{2}((n+1)-2)((n+1)-1)$ up to $((n+1)-2)^2$. And since each of the transposes of these matrices has a column with exactly $(n+1)-2$ zeros, the induction is complete. □

THEOREM 3.2. *For $n \geq 2$, there is an $n \times n$ indecomposable orthogonal matrix with exactly k zeros if and only if* $0 \leq k \leq (n-2)^2$.

Proof. The theorem follows immediately from Corollary 2.4, Lemma 3.1 and the result of [BBS]. □

REMARK 3.3. It follows from Theorem 3.2 that for $n \geq 4$, there exists an $n \times n$ orthogonal matrix with exactly k zeros if and only if $0 \leq k \leq n(n-1)-4$ or $k = n(n-1)-2$ or $k = n(n-1)$.

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