

A FURTHER LOOK INTO COMBINATORIAL ORTHOGONALITY*

SIMONE SEVERINI[†] AND FERENC SZÖLLŐSI[‡]

Abstract. Strongly quadrangular matrices have been introduced in the study of the combinatorial properties of unitary matrices. It is known that if a $(0, 1)$ -matrix supports a unitary then it is strongly quadrangular. However, the converse is not necessarily true. In this paper, strongly quadrangular matrices up to degree 5 are fully classified. It is proven that the smallest strongly quadrangular matrices which do not support unitaries have exactly degree 5. Further, two submatrices not allowing a $(0, 1)$ -matrix to support unitaries are isolated.

Key words. Strong quadrangularity, Combinatorial matrix theory, Combinatorial orthogonality, Orthogonal matrices.

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1. Introduction. Orthogonality is a common concept which generalizes perpendicularity in Euclidean geometry. It appears in different mathematical contexts, like linear algebra, functional analysis, combinatorics, etc. The necessary ingredient for introducing orthogonality is a notion that allow to measure the angle between two objects. For example, in sufficiently rich vector spaces, this consists of the usual inner product $\langle \cdot, \cdot \rangle$. Specifically, two vectors $u = (u_1, \dots, u_n)$ and $v = (v_1, \dots, v_n)$, from a vector space over a generic field \mathbb{F} , are said to be *orthogonal*, if $\langle u, v \rangle = 0$. It is immediately clear that u and v are orthogonal only if there is a special relation between their entries, and that this relation does not only involve the magnitude and the signs, but also the position of the zeros, if there are any.

At a basic level, dealing with orthogonality from the combinatorial point of view means, among other things, to study patterns of zeros in arrangements of vectors, some of which are orthogonal to each other. A natural, somehow extremal scenario, is when the vectors form a square matrix. Indeed, a matrix M with entries on \mathbb{F} is said to be *orthogonal* if $\langle M_i, M_j \rangle = 0$, for every two different rows and columns, M_i and M_j . In this setting one can state the following natural problem: characterize the zero pattern of orthogonal matrices. This is a typical problem in combinatorial

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[†]Institute for Quantum Computing and Department of Combinatorics and Optimization, University of Waterloo, N2L 3G1 Waterloo, Canada (simoseve@gmail.com).

[‡]Budapest University of Technology and Economics (BUTE), Institute of Mathematics, Department of Analysis, Egy J. u. 1, H-1111 Budapest, Hungary (szoferi@math.bme.hu).

matrix theory, the field of matrix theory concerning intrinsic properties of matrices viewed as arrays of numbers rather than algebraic objects in themselves (see [4]).

The term “zero pattern” is not followed by a neat mathematical definition. By zero pattern, we intuitively mean the position of the zeros seen as forming a whole. A more concrete definition may be introduced in the language of graph theory. Let $D = (V, E)$ be a directed graph, without multiple edges, but possibly with self-loops (see [2] for this standard graph theoretic terminology). Let $A(D)$ be the adjacency matrix of D . We say that a matrix M with entries on \mathbb{F} is *supported* by D (or, equivalently, by $A(D)$), if we obtain $A(D)$ when replacing with ones the nonzero entries of M . In other words, D supports M , if $A(D)$ and M have the same zero pattern. If this is the case, then D is said to be the *digraph* of M . Equivalently, $A(D)$ is said to be the *support* of M .

Studying the zero pattern of a family of matrices with certain properties is equivalent to characterizing the class of digraphs of the matrices. When the field is \mathbb{R} or \mathbb{C} , an orthogonal matrix is also said to be *real orthogonal* or *unitary*, respectively. These are practically ubiquitous matrices, with roles spanning from coding theory to signal processing, and from industrial screening experiments to the quantum mechanics of closed systems, etc. Historically, the problem of characterizing zero patterns of orthogonal matrices was first formulated by Fiedler [10, 11], and it is contextually related to the more general problem of characterizing ortho-stochastic matrices.

Even if not explicitly, the same problem can also be found in some foundational issues of quantum theory (see [14]). Just recently, this was motivated by some other questions concerning unitary quantum evolution on graphs [1, 17]. Like many other situations involving orthogonality, characterizing the zero pattern of orthogonal matrices is not a simple problem. In some way, a justification comes from the difficulty that we encounter when trying to classify weighing, real and complex Hadamard matrices [16, 20, 21], and the related combinatorial designs [12] (see [13], for a more recent survey). One major obstacle is in the global features of orthogonality. Loosely speaking, it is in fact evident that the essence of orthogonality can not be isolated by looking at forbidden submatrices only, but the property is subtler because it asks for relations between the submatrices.

A first simple condition for orthogonality was proposed by Beasley, Brualdi and Shader in 1991 [3]. As a tool, the authors introduced combinatorial orthogonality. A $(0,1)$ -matrix is a matrix with entries in the set $\{0, 1\}$. A $(0,1)$ -matrix M is said to be *combinatorially orthogonal*, or, equivalently, *quadrangular*, if $\langle M_i, M_j \rangle \neq 1$, for every two different rows and columns, M_i and M_j . It is immediate to observe that the adjacency matrix of the digraph of an orthogonal matrix needs to be combinatorially orthogonal. However, as it was already pointed out in [3], this condition is not sufficient to characterize the zero pattern of orthogonal matrices. For the next

ten years, the few sporadic papers on this subject did focus on quantitative results, mainly about the possible number of zeros [5, 6, 8, 7]. In [18] the problem was re-considered with the idea of pursuing a systematic study of the qualitative side. The first step consisted of defining an easy generalization of combinatorial orthogonality. This led to the notion of strong quadrangularity. Let M be a $(0,1)$ -matrix of degree n , and let S be a set of rows of M , forming an $|S| \times n$ matrix. Suppose that for every $u \in S$ there exists a row $v \in S$ such that $\langle u, v \rangle \neq 0$. Thus, if the number of columns in S containing at least two ones is at least $|S|$ then M is said to be *row-strongly-quadrangular*. If both M and its transpose are row-strongly quadrangular then M is said to be *strongly quadrangular* (for short, SQ). Even if strong quadrangularity helps in exactly characterizing some classes of digraphs of orthogonal matrices [18], the condition is not necessary and sufficient. A counterexample involving a tournament matrix of order 15 was exhibited by Lundgren et al. [15].

Let us denote by \mathcal{U}_n the set of all $(0,1)$ -matrices whose digraph supports unitaries. Recall that an $n \times n$ matrix M is said to be *indecomposable* if it has no $r \times (n-r)$ zero submatrix. The goal of the paper is to investigate SQ matrices of small degree and find certain forbidden substructures which prevent a $(0,1)$ -matrix to support unitary matrices.

One of the tools used through the paper is a construction due to Diță [9], which is a generalization of the Kronecker product. Although the original construction was defined for complex Hadamard matrices, it can be easily extended to any unitary of composite degree.

LEMMA 1.1 (Diță's construction). *Let U_1, U_2, \dots, U_k be unitaries of degree n , and let $[H]_{ij} = h_{ij}$ be a unitary of degree k . Then the following matrix Q of degree kn is also unitary.*

$$Q = \begin{bmatrix} h_{11}U_1 & h_{12}U_2 & \dots & h_{1k}U_k \\ h_{21}U_1 & h_{22}U_2 & \dots & h_{2k}U_k \\ \vdots & \vdots & \ddots & \vdots \\ h_{k1}U_1 & h_{k2}U_2 & \dots & h_{kk}U_k \end{bmatrix}.$$

COROLLARY 1.2. *If $M_1, M_2, \dots, M_k \in \mathcal{U}_n$ then also the following matrix $K \in \mathcal{U}_{kn}$:*

$$K = \begin{bmatrix} M_1 & M_2 & \dots & M_k \\ M_1 & M_2 & \dots & M_k \\ \vdots & \vdots & \ddots & \vdots \\ M_1 & M_2 & \dots & M_k \end{bmatrix}.$$

Proof. Choose $H = \frac{1}{\sqrt{k}}F_k$, where F_k is the matrix of the Fourier transform over \mathbb{Z}_k , the abelian group of the integers modulo k . \square

It is clear why Diťa's construction is useful for our purposes. For example, the following matrix

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

is in \mathcal{U}_4 , since we can choose $U_1 = I_2, U_2 = \frac{1}{\sqrt{2}}F_2$ and then apply the construction.

2. SQ matrices of small degree. The purpose of this section is twofold. On the one hand, we would like to give a detailed list of SQ matrices of small degree. This is done in the perspective of further investigation. On the other hand, we directly enumerate indecomposable, SQ matrices up to degree 5. The method that we adopt in this enumeration is a three-step procedure. First, we simply construct *all* $(0, 1)$ -matrices of degree $n \leq 5$. Second, we exclude from this list matrices which are not SQ or contains a line (row or column) of zeros. Finally, we determine representative from equivalence classes of the remaining matrices. We also compute the order of their automorphism group. Recall that two matrices M_1 and M_2 are said to be *equivalent* if there are permutation matrices P and Q such that $PM_1Q = M_2$. As usual, the automorphism group of a $(0, 1)$ -matrix M is the set of ordered pairs (P, Q) of permutation matrices such that $PMQ = M$. Some heuristics helps to simplify our task.

LEMMA 2.1. *Two $(0, 1)$ -matrices having a different number of zeros are not equivalent.*

Of course, the converse statement is not necessarily true (see, *e.g.*, the two matrices of degree 4 with exactly four zeros below). Another natural heuristic consists of the number of ones in each row. For a given $(0, 1)$ -matrix $[M]_{i,j} = m_{ij}$, we define the multiset $\Lambda = \left\{ \sum_j m_{ij} : i = 1, \dots, n \right\}$. Thus the following observation is easy verify:

LEMMA 2.2. *Two $(0, 1)$ -matrices with different Λ 's are not equivalent.*

Again, the converse statement does not hold in general. Recall that a $(0, 1)$ -matrix is said to be *regular* if the elements of Λ are all equal. The following lemma is specifically useful for distinguishing regular matrices:

LEMMA 2.3. *Two $(0, 1)$ -matrices with nonisomorphic automorphism groups are not equivalent.*

It follows that two $(0, 1)$ -matrices with automorphism groups of different order are

not equivalent. Unfortunately, there are examples of nonequivalent matrices whose automorphism groups are isomorphic. In particular, it might happen that a matrix and its transpose are not equivalent. By combining together the above facts, with the help of a computer, one can fully classify matrices in \mathcal{U}_n for $n \leq 5$. By a careful analysis of the results, in Section 3 we are able to describe certain cases in which a matrix $M \notin \mathcal{U}_n$ even if it is SQ. The smallest such an example is of degree 5. Additionally, if $M \in \mathcal{U}_n$ for $n < 5$ then M is SQ and vice versa. We hereby present, up to equivalence, the list of all indecomposable, SQ matrices of degree $n \leq 5$. We need to fix some notational conventions: if a matrix is equivalent to a symmetric one we index it by S ; if a matrix is not equivalent to its transpose we index it by T . Regular matrices will be indexed by R . Finally, the order of the automorphism group of a matrix is written as a subscript. This information describes the number of equivalent matrices in a given class. In particular, $(n!)^2 = |\text{Aut}M| \cdot \#\{\text{Equivalent matrices to } M\}$.

2.1. n=1.

$$\left\{ \left[\begin{array}{c} 1 \\ 1 \end{array} \right]_1^{RS} \right\}$$

This matrix, and more generally, every all-one matrix J_n , clearly supports unitaries, since there is an $n \times n$ complex Hadamard matrix for any n [13, 21].

2.2. n=2.

$$\left\{ \left[\begin{array}{cc} 1 & 1 \\ 1 & 1 \end{array} \right]_4^{RS} \right\}$$

2.3. n=3.

$$\left\{ \left[\begin{array}{ccc} 0 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{array} \right]_4^S, \left[\begin{array}{ccc} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{array} \right]_{36}^{RS} \right\}$$

2.4. n=4.

$$\left\{ \left[\begin{array}{cccc} 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{array} \right]_{36}^S, \left[\begin{array}{cccc} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{array} \right]_8^S, \left[\begin{array}{cccc} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 \end{array} \right]_6^S, \left[\begin{array}{cccc} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{array} \right]_{24}^{RS}, \right.$$

$$\left. \left[\begin{array}{cccc} 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{array} \right]_4^S, \left[\begin{array}{cccc} 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{array} \right]_{24}^T, \left[\begin{array}{cccc} 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{array} \right]_{16}^T, \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{array} \right]_{576}^{RS} \right\}$$

$$\begin{bmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}^T_{24}, \begin{bmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}^T_4, \begin{bmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}^T_4, \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}^T_{48},$$

$$\begin{bmatrix} 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}^T_{24}, \begin{bmatrix} 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}^T_8, \begin{bmatrix} 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}^T_{12}, \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}^T_{48},$$

$$\left. \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}^T_{24}, \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}^T_8, \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}^T_{16} \right\}$$

While constructing unitaries matching a given pattern up to degree 4 is a simple task, considering $n = 5$ brings up several difficulties. First of all, as one can see, there are many equivalence classes and presenting unitaries for each and every class is out of reach. Secondly, it turns out that there are at least two such matrices which do not support a unitary. We index these matrices by N . This statement will be formally proved in Section 3. Since the number of SQ matrices grows very fast, lacking of computational power, we did stop our counting at $n = 5$. However, we propose two further special cases which are arguably easier to handle.

2.5.1. Symmetric SQ matrices. It is evident that the main difficulty in classifying SQ matrices is *not* the actual construction of the matrices, but determining equivalence classes. This is a time-consuming procedure even for small degrees. The following lemma shows that classifying only *symmetric* SQ matrices is definitely an easier problem.

LEMMA 2.5. *If a $(0, 1)$ -matrix M is equivalent to a symmetric one, then there is a permutation matrix R , such that $RMR = M^T$.*

Proof. Suppose that M is equivalent to a symmetric matrix, denoted by S . Then there are permutation matrices P and Q , such that $PMQ = S = S^T$, so $PMQ = Q^T M^T P^T$, and hence $(QP)M(QP) = M^T$. This implies that $R = QP$ is a permutation matrix, as required. \square

Determining whether a $(0, 1)$ -matrix M is equivalent to a symmetric one therefore simply boils down to a two phase procedure: first, we check if there are permutations matrices for which $RMR = M^T$; second, we check if $Q^T R M Q$ is symmetric for a certain Q . If there exists such a pair of permutation matrices R and Q , then M is equivalent to a symmetric matrix. This procedure is clearly faster than simultaneously looking for P and Q such that PMQ is symmetric.

2.5.2. Regular SQ matrices. Here we focus on *regular* SQ matrices. We have classified these matrices up to degree 6. The results up to degree 5 can be found in the lists above. The list for degree 6 is included below. Let σ be the number of nonzero entries in each row of a regular matrix. There are regular SQ matrices of order 6 with $\sigma = 6, 5, 3, 2, 1$, since $J_6, J_6 - I_6, J_3 \oplus J_3, J_2 \oplus J_2 \oplus J_2, I_6$ are such examples, where I_n denotes the $n \times n$ identity matrix. It can be checked that in fact these are the only ones. However, the case $\sigma = 4$ turns out to be interesting, since one out of the four regular matrices does not support unitaries. This fact will be investigated later in Theorem 3.1 of Section 3.

$$\left\{ \begin{array}{l} \left[\begin{array}{cccccc} 1 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 \end{array} \right]_{72}^{RS} \\ \left[\begin{array}{cccccc} 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \end{array} \right]_{384}^{RS} \end{array} \right\},$$

$$\left\{ \begin{array}{l} \left[\begin{array}{cccccc} 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 \end{array} \right]_{12}^{RS} \\ \left[\begin{array}{cccccc} 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 \end{array} \right]_{32}^{NRS} \end{array} \right\}$$

We conclude by summarizing our observations:

- The number of inequivalent indecomposable SQ matrices of degree $n = 1, 2, \dots, 5$ is 1, 1, 2, 10, 63, respectively. All known terms of this sequence match the number of triples of standard tableaux with the same shape of height less than or equal to three. This sequence is A129130 in [19].
- The number of inequivalent SQ matrices of orders $n = 1, 2, \dots, 5$ is 1, 2, 4, 15, 80, respectively.
- The number of inequivalent indecomposable symmetric SQ matrices of degree $n = 1, 2, \dots, 5$ is 1, 1, 2, 6, 23, respectively.
- The number of inequivalent symmetric SQ matrices of degree $n = 1, 2, \dots, 5$ is 1, 2, 4, 11, 44, respectively.
- The number of inequivalent indecomposable regular SQ matrices of orders $n = 1, 2, \dots, 6$ is 1, 1, 1, 2, 2, 4.
- The number of inequivalent regular SQ matrices of degree $n = 1, 2, \dots, 6$ is 1, 2, 2, 4, 3, 9, respectively.

3. Beyond strong quadrangularity. In [15], the authors exhibited the adjacency matrix of a tournament on 15 vertices, which, despite being SQ, it is not in

\mathcal{U}_{15} . The first result of this section is a refined version of that. Specifically, we have the following:

THEOREM 3.1. *Let M (or its transpose) be a $(0, 1)$ -matrix equivalent to a matrix in the following form, for $k \geq 1$:*

$$\begin{bmatrix} Q & J_{3 \times k} & X \\ Y & Z & * \end{bmatrix}, \text{ where } Q = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{bmatrix}.$$

Further, suppose that

1. the rows of X are mutually orthogonal,
2. every column of Y is orthogonal to every column of Z .

Then M does not support unitaries.

Proof. The idea of the proof is exactly the same as in [15]. Suppose on the contrary that there exists a unitary U whose support is M . Let R_i and C_i denote the i -th row and column of U respectively, for each $i = 1, \dots, n$ and let $[U]_{ij} = u_{i,j}$. Now observe, that $\langle C_1, C_j \rangle = u_{1,1}\bar{u}_{1,j} + u_{3,1}\bar{u}_{3,j} = 0$, where $j = 3, 4, \dots, k+2$. This implies $-\bar{u}_{1,1}/\bar{u}_{3,1} = u_{3,j}/u_{1,j}$, where $j = 3, 4, \dots, k+2$. So the vectors $[u_{1,3}, \dots, u_{1,k+2}]$ and $[u_{3,3}, \dots, u_{3,k+2}]$ are scalar multiples of each other. Similarly: $\langle C_2, C_j \rangle = u_{2,2}\bar{u}_{2,j} + u_{3,2}\bar{u}_{3,j} = 0$, where $j = 3, 4, \dots, k+2$. So, this implies $-\bar{u}_{2,2}/\bar{u}_{3,2} = u_{3,j}/u_{2,j}$, where $j = 3, 4, \dots, k+2$. So the vectors $[u_{2,3}, \dots, u_{2,k+2}]$ and $[u_{3,3}, \dots, u_{3,k+2}]$ are scalar multiples of each other. It follows that $\langle R_1, R_2 \rangle = \langle [u_{1,3}, \dots, u_{1,k+2}], [u_{2,3}, \dots, u_{2,k+2}] \rangle \neq 0$, a contradiction. \square

The next statement summarizes the main features of the matrices satisfying the conditions of Theorem 3.1.

PROPOSITION 3.2. *Under the conditions of Theorem 3.1, a SQ matrix of degree n satisfies the following properties:*

1. $k \geq 2$;
2. The first row of Y is $[1, 1]$;
3. The first row of Z is $[0, \dots, 0]$;
4. X has at least two columns;
5. $n \geq 6$.

Proof. Suppose that we have a matrix equivalent to M . Since its first two rows share a common 1, and X cannot have two rows who share a common 1, $k \geq 2$ follows. Similarly, the first and second column of M share a common 1, hence by quadrangularity, these share another 1, and up to equivalence, we can suppose that it is in the 4th row of M . Thus, the first row of Y can be chosen to be $[1, 1]$. By the second condition of Theorem 3.1, the first row of Z should be $[0, \dots, 0]$. Again,

since the 1st and 4th rows share a common 1, by quadrangularity, they should share another 1. However, we have already seen that the first row of Z is all 0. Thus, these rows must share this specific 1 in X . The same argument applies for the 2nd and 4th row of M , and since two rows of X cannot share a common 1, it must have at least two columns. It follows that $k \leq n - 4$ and therefore $n \geq 6$. \square

Next, we estimate the possible number of ones in matrices satisfying the conditions of Theorem 3.1.

LEMMA 3.3. *Suppose that a SQ matrix M of degree $n \geq 6$ satisfies the conditions of Theorem 3.1. Then, its possible number of ones is at most $n^2 - 3n + 6$, and hence, it has a least $3n - 6$ zeros.*

Proof. We simply count the number of ones in all blocks of M separately. First, the number of ones in Q is 4, and clearly, the number of 1s in J are $3k$. By the first condition of Theorem 3.1, the number of ones in X is at most $n - k - 2$. Now by Lemma 3.2 the first row of Z is $[0, \dots, 0]$ (up to equivalence), hence the number of ones in Y and Z together is at most $k(n - 4) + 2$, and finally the number of ones in the lower right submatrix is at most $(n - k - 2)(n - 3)$. Thus the possible number of ones is

$$4 + 3k + n - k - 2 + k(n - 4) + 2 + (n - k - 2)(n - 3) = n^2 - 4n + 10 + k \leq n^2 - 3n + 6. \square$$

We have the following:

COROLLARY 3.4. *The 6×6 matrix A below is SQ. However, by Theorem 3.1, $A \notin \mathcal{U}_6$.*

$$A = \left[\begin{array}{cc|cc|cc} 1 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ \hline 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 \end{array} \right]$$

Note that A is regular, therefore it is equivalent to the exceptional regular matrix of degree 6 appearing in Section 2.

The example above shows that there are indeed SQ matrices of degree 6, which cannot support unitaries. It is of particular interest to find out if there are such exceptional matrices already for degree 5. Lemma 3.2 explains that we cannot rely on Theorem 3.1, since this result does not say anything about matrices of order 5. By analyzing the list of Section 2, one can observe that such exceptional matrices do exist for degree 5. The reason for this phenomenon is summarized in the following:

THEOREM 3.5. *Let M (or its transpose) be a $(0, 1)$ -matrix equivalent to a matrix in the following form:*

$$\begin{bmatrix} Q & J_{3 \times 2} & * \\ X & Y & * \end{bmatrix}, \text{ where } Q = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{bmatrix}.$$

Further, suppose that

1. the columns of Y are mutually orthogonal,
2. every column of X is orthogonal to every column of Y .

Then M does not support unitaries.

Proof. Suppose on the contrary that we have a unitary U , whose support is M . Let us use the same notations as in the proof of Theorem 3.1. By orthogonality $\langle C_1, C_3 \rangle = u_{11}\bar{u}_{13} + u_{31}\bar{u}_{33} = 0$, $\langle C_1, C_4 \rangle = u_{11}\bar{u}_{14} + u_{31}\bar{u}_{34} = 0$, $\langle C_2, C_3 \rangle = u_{22}\bar{u}_{23} + u_{32}\bar{u}_{33} = 0$, $\langle C_2, C_4 \rangle = u_{22}\bar{u}_{24} + u_{32}\bar{u}_{34} = 0$, hence $u_{31} = -u_{11}\bar{u}_{13}/\bar{u}_{33}$, $u_{14} = -\bar{u}_{31}u_{34}/\bar{u}_{11}$, $u_{32} = -u_{22}\bar{u}_{23}/\bar{u}_{33}$, $u_{24} = -\bar{u}_{32}u_{34}/\bar{u}_{22}$. Thus

$$\begin{aligned} 0 = \langle C_3, C_4 \rangle &= u_{13}\bar{u}_{14} + u_{23}\bar{u}_{24} + u_{33}\bar{u}_{34} = -u_{13} \frac{u_{31}\bar{u}_{34}}{u_{11}} - u_{23} \frac{u_{32}\bar{u}_{34}}{u_{22}} + u_{33}\bar{u}_{34} = \\ &= \frac{\bar{u}_{34}}{\bar{u}_{33}} \left(|u_{13}|^2 + |u_{23}|^2 + |u_{33}|^2 \right) \neq 0, \end{aligned}$$

since the last expression in the brackets is strictly positive. This is a contradiction. \square

Now we present the dual of Proposition 3.2 and Lemma 3.3.

PROPOSITION 3.6. *Under the conditions of Theorem 3.5, a SQ matrix of degree n satisfies the following properties:*

1. The first row of X is $[1, 1]$;
2. The first row of Y is $[0, \dots, 0]$;
3. $n \geq 5$;

Proof. The first two properties are evident from the proof of Proposition 3.2. The third one follows from the fact that the only candidates of order 4 with these properties are not SQ. \square

LEMMA 3.7. *Suppose that a SQ matrix M of degree n satisfies the conditions of Theorem 3.5. Then, its possible number of ones is at most $n^2 - 2n + 4$, and hence, it has at least $2n - 4$ zeros.*

Proof. We count the number of ones in each block of M separately. First, the number of ones in Q is 4. Then the number of ones in $J_{3 \times 2}$ is 6. The first condition of

Theorem 3.5 and Proposition 3.6 imply that the number of ones in X and Y cannot be more than 2 in each row. Since there are $n - 3$ rows in X and Y , we conclude that the possible number of ones is at most $4 + 6 + 2(n - 3) + n(n - 4) = n^2 - 2n + 4$. \square

COROLLARY 3.8. *The following two symmetric, SQ matrices of degree 5 do not support unitaries:*

$$\left\{ \left[\begin{array}{ccc|ccc} 1 & 0 & & 1 & 1 & & 1 \\ 0 & 1 & & 1 & 1 & & 1 \\ 1 & 1 & & 1 & 1 & & 0 \\ \hline 1 & 1 & & 0 & 0 & & 1 \\ 1 & 1 & & 0 & 0 & & 1 \end{array} \right], \left[\begin{array}{ccc|ccc} 1 & 0 & & 1 & 1 & & 1 \\ 0 & 1 & & 1 & 1 & & 1 \\ 1 & 1 & & 1 & 1 & & 1 \\ \hline 1 & 1 & & 0 & 0 & & 1 \\ 1 & 1 & & 0 & 0 & & 1 \end{array} \right] \right\}.$$

These matrices are equivalent to the exceptional matrices of order 5 appearing in Section 2. We conclude this section with a SQ matrix of degree 10 which satisfies the conditions in both Theorem 3.1 and Theorem 3.5:

$$\left[\begin{array}{ccc|ccc|ccc} 1 & 0 & & 1 & 1 & & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & & 1 & 1 & & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & & 1 & 1 & & 0 & 0 & 0 & 0 & 1 & 1 \\ \hline 0 & 0 & & 1 & 0 & & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & & 0 & 1 & & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & & 0 & 0 & & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & & 0 & 0 & & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & & 0 & 0 & & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & & 0 & 0 & & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & & 0 & 0 & & 1 & 1 & 1 & 1 & 1 & 1 \end{array} \right].$$

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