GRAPHS OF UNITARY MATRICES AND POSITIVE SEMIDEFINITE ZERO FORCING

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The possible zero/nonzero patterns of unitary matrices are of interest in quantum evolution and the study of quantum systems on graphs. In particular, a quantum random walk can be defined on a directed graph if and only if that graph is associated with a unitary matrix pattern. We propose positive semidefinite zero forcing as a way to determine whether there exists a unitary matrix with a given zero/nonzero pattern. We show that zero forcing is a better criterion than strong quadrangularity of the pattern and prove that an n-by-n pattern supports a unitary matrix if and only if its positive semidefinite zero forcing number equals n for $n \leq 5$.

Keywords: unitary matrices, zero/nonzero patterns, positive semidefinite zero forcing, strong quadrangularity.

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The zero/nonzero patterns of unitary matrices are of interest both in quantum physics and mathematics. For example, the quantum analog of a random walk, useful in quantum computation [2, 3], can only be defined on directed graph if that graph is the directed graph of a unitary pattern. As another example, the "no-go lemma" [10, 11, 16] asserts that a pattern whose directed graph is an n-path is not the pattern of a unitary matrix and, as a result, there does not exist a nontrivial homogeneous local one-dimensional quantum cellular automaton. These patterns also appear in work on the foundations of quantum mechanics [14] and in the study of quantum systems [18].

Related research includes conditions on the possible number of zeros in an n-by-n unitary matrix [7], as well as studying similar questions for sign patterns [22]. Zero forcing was defined to help study minimum rank problems [1], and is of interest in the control of quantum systems [4]. For further information, we highly recommend the detailed survey of quantum applications of patterns of unitary matrices in a recent article of Severini and Szöllősi [19] and the discussion in Severini's first article on this topic [20].

In this article, we address the question of whether, given a zero/nonzero pattern, there exists a unitary matrix with that pattern. While we specifically consider unitary matrices, similar questions can be asked for real orthogonal and rational orthogonal matrices. Hall and Severini recently showed that in general a pattern that supports a unitary matrix need not support a real or rational orthogonal matrix [12]. However, 5-by-5 and smaller unitary patterns do support both real and rational orthogonal matrices [8]. In this paper, all of our results work equally well if "unitary" is replaced by "real orthogonal" or "rational orthogonal". It would be interesting to know if other types of zero forcing could be used to detect unitary patterns that do not support a real orthogonal matrix.

1. Matrices and graphs

A graph $G = (V, E)$ consists of a set V of vertices and a set E of unordered pairs of vertices called edges. We assume all graphs to be simple in that there are no multiple edges or loops (edges from a vertex to itself). a bipartite graph is a graph whose vertex set can be partitioned into two sets $V = M \cup N$ where no edge has both vertices in M or both vertices in N. a directed graph (digraph) is a graph with directed edges (ordered pairs of vertices). The neighborhood of a vertex v in a graph G, denoted by $N(v)$, is the set of vertices adjacent to v.

a (zero/nonzero) pattern is a matrix with entries from $\{0, 1\}$. The pattern of a complex matrix is the matrix obtained by replacing all nonzero entries with "1". The size of an m-by-n matrix or pattern is $\max\{m, n\}$. The support of a matrix or pattern is the set of the locations of its nonzero entries.

A complex matrix U is unitary if $UU^* = U^*U = I$, where I is the identity matrix. a pattern is unitary if it is the pattern of a unitary matrix. We will say that two patterns are equivalent if one can be obtained from the other by permutation of rows and columns and/or matrix transpose. Thus, if P and Q are equivalent patterns, P is unitary if and only if Q is, and we will often consider single representatives of the equivalence classes in what follows. a pattern (or matrix) P generates a bipartite graph $B(P)$ by taking the rows as one partite set, the columns as the other, and placing an edge between row i and column j if and only if the i, j entry is nonzero.

An n-by-n matrix (or pattern) A is *fully indecomposable* if it does not have a p-by-q zero submatrix with $p + q = n$. a pattern is fully indecomposable if and only if its bipartite graph is connected [6]. Whether or not a pattern that is not fully indecomposable is unitary can be determined by studying the same question for its fully indecomposable subpatterns, so we will assume that all graphs are connected and only consider matrices and patterns that are fully indecomposable.

A bipartite graph $G = (M \cup N, E)$ is called *strongly quadrangular* if for each subset S of either M or N that has the property that, for all $v \in S$, there exists $w \neq v \in S$ such that $N(v) \cap N(w) \neq \emptyset$,

$$\left| \bigcup_{v,w \in S; v \neq w} N(v) \cap N(w) \right| \geq |S|.$$

We will say the pattern P is strongly quadrangular if and only if $B(P)$ is.

It was conjectured that a pattern P is unitary if and only if it is strongly quadrangular [20]. In fact, we have the following result.

THEOREM 1 ([19, Proposition 2.4]). *A pattern P of size at most four is unitary if and only if it is strongly quadrangular.*

However, examples were found of patterns that are strongly quadrangular but are not unitary [15]. For example, we have the following theorem:

THEOREM 2 ([8, Proposition 2.1]). *Up to equivalence, there are three strongly quadrangular 5-by-5 patterns that are not unitary:*

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

2. Minimum rank and zero forcing

A complex Hermitian positive semidefinite n-by-n matrix (or symmetric pattern) $A = [a_{ij}]$ defines a graph $G(A)$ that has vertex set $\{1, \ldots, n\}$ and edge set $\{ij : i \neq j, a_{ij} \neq 0\}$. Note that the diagonal entries of the matrix do not impact the graph. Given a graph G on n vertices, let $\mathcal{P}(G)$ be the set of positive semidefinite matrices whose graph is isomorphic to G. The *minimum semidefinite rank* of G, $\operatorname{msr}(G)$, is the smallest possible rank among matrices in $\mathcal{P}(G)$. Setting $M_+(G) = n - \operatorname{msr}(G)$ gives the corresponding *maximum nullity* of G. As it turns out, minimum rank and maximum nullity are intimately related to unitary patterns.

THEOREM 3 ([13, Proposition 3.1]). *An n-by-n pattern P is unitary if and only if $M_+(B(P)) = n$.*

Suppose that the vertices of a graph G are colored either white or black. The positive semidefinite color-change rule is the following: If there exists a black vertex v that has exactly one white neighbor u in a connected component of the graph obtained from G by removing all of the black vertices, then change the color of u to black. a *(positive semidefinite) zero forcing set* for a graph G is a subset of vertices Z such that given a coloring of the vertices of G where all the vertices of Z are black, repeated application of the color-change rule can result in all of the vertices being colored black. The (positive semidefinite) zero forcing number $Z_+(G)$ is the size of a smallest zero forcing set. Because row and column permutations and the transpose of a pattern P correspond to graph isomorphisms of $B(P)$, if P and Q are equivalent patterns then $Z_+(B(P)) = Z_+(B(Q))$.

Zero forcing is of interest here since $Z_+(G) \geq M_+(G)$ for all graphs G [9]. In particular, for a bipartite graph $G = (M \cup N, E)$, $M_+(G) \leq Z_+(G) \leq \min\{|M|, |N|\}$, since removing either M or N leaves only isolated vertices, and so both M and N are zero forcing sets for G. Thus, using Theorem 3, one has the following theorem.

THEOREM 4. *If $Z_+(B(P)) < n$ for an n-by-n pattern P, then P is not unitary.*

3. The converse

One may also hope the converse to Theorem 4 is true, so that an m-by-m pattern P is unitary if and only if $Z_+(B(P)) = m$. We will see however, that this is unfortunately not the case in general.

Let $G = (V = M \cup N, E)$ be a bipartite graph with $|M| = |N| = n$. We do have the following result:

THEOREM 5. *If $Z_+(G) = n$ then G is strongly quadrangular.*

Proof: Assume that G is not strongly quadrangular. Let (without loss of generality) $S \subseteq M$, define

$$T = \bigcup_{v,w \in S; v \neq w} N(v) \cap N(w) \subseteq N,$$

and suppose $|T| < |S|$. We claim that $Z = (M \setminus S) \cup T$ is a zero forcing set. From the definition of T, any two vertices of S cannot have a common neighbor outside of T. Thus every two vertices of S are in different connected components in $G \setminus Z$, so that any vertex of T may force any neighbor in S. Once the vertices of S are black, all of the vertices of M are black, and the remaining vertices of N can be forced by those of M. □

Thus, Z_+ gives a potentially stronger criterion than strong quadrangularity for determining if a pattern is unitary. To show that it is indeed stronger, we consider a family of patterns that are known to not be unitary but some of which are strongly quadrangular [19].

THEOREM 6. *Let P be a zero/nonzero pattern equivalent to a pattern with the following form:*

$$\begin{bmatrix} Q & J_{3\times 2} & * \\ X & Y & * \end{bmatrix},$$

where $k \geq 1$, J *is the matrix of all ones, and*

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

Further suppose the columns of Y *have disjoint supports and that every column of* X *has support disjoint from every column of* Y. *Then* P *is not unitary and has* $Z_+(B(P)) < n$.

Proof: Let r_i and c_j denote the vertices corresponding to row i and column j, respectively, in $B(P)$. We claim that $\{r_3, c_2, c_4, \ldots, c_n\}$ is a zero forcing set. Because of the support assumptions, aside from r_2, if c_2 is adjacent to any white vertices, then those vertices are adjacent neither to c_1 nor to c_3. Thus c_2 may force r_2. Since r_2 is not adjacent to c_1, it may force c_3. Again using the support assumptions, c_3 may force r_1, which may force c_1, and the remaining vertices follow as one partite set is black. □

The family in Theorem 6 contains two of the examples of Theorem 2 [19]. The remaining pattern,

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

has $Z_+ < 5$, as the vertices corresponding to rows four and five and columns four and five give a zero forcing set, as the reader may verify. In particular,

COROLLARY 1. *A square pattern* P *of size* $m \leq 5$ *is unitary if and only if* $Z_+(B(P)) = m$.

4. A counterexample

Severini and Szöllősi [19] define another family of patterns that are not unitary but some of which are strongly quadrangular: Let P be a zero/nonzero pattern equivalent to a pattern with the following form:

$$\begin{bmatrix} Q & J_{3\times k} & X \\ Y & Z & * \end{bmatrix}$$

where $k \geq 1$, J is the matrix of all ones, and Q is as in Theorem 6.

Further suppose that the rows of X have disjoint supports and every column of Y has support disjoint from every column of Z. Then P is not unitary.

All but one of the known examples of nonunitary strongly quadrangular patterns have been drawn either from this family or from the family of Theorem 6. The one exception was the first such example [15], and it provided the inspiration for the definition of the family above. As it turns out, and as the reader may verify, this family has strongly quadrangular 6-by-6 elements P all of which have $Z_+(B(P)) < 6$, but also contains the 7-by-7 pattern

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

which has $Z_+(B(Q)) = 7$.

We should remark that although there are infinitely many graphs G for which $M_+(G) < Z_+(G)$ [17], all previously known examples were built from the smallest known example, the Möbius Ladder graph on eight vertices. Thus the pattern Q provides a new example for which $M_+(G) < Z_+(G)$.

Also, for any graph G, one can repeatedly subdivide edges of G to get a bipartite graph B for which $M_+(G) = M_+(B)$ [13] and $Z_+(G) = Z_+(B)$. Thus, there are infinitely many bipartite graphs for which $M_+(G) < Z_+(G)$. However, we have been unable to produce a bipartite graph with equal-size partite sets and maximum possible Z_+ using edge subdivision of the known graphs with $M_+(G) < Z_+(G)$. Thus the pattern Q also provides the first example of a bipartite graph B on with equal-size partite sets for which $M_+(B) < Z_+(B) = |B|/2$.

5. Further results

We next consider patterns larger than 5-by-5 and more general techniques. In particular, is it true that a 6-by-6 pattern P is unitary if and only if $Z_+(B(P)) = 6$? As mentioned above, we have not so far found any counterexamples. Algorithms exist to compute Z_+ [5], and we can rule out many patterns as nonunitary. Unfortunately, to prove a pattern is unitary remains difficult. To help reduce the number of equivalence classes we must check, we recall some known techniques for constructing unitary matrices from known unitary matrices and show that these constructions behave as we would wish with respect to zero forcing.

THEOREM 7 ([13, Proposition 4.6]). *An n-by-n square pattern whose support contains the support of the n-by-n upper Hessenberg pattern*

$$\begin{bmatrix} 1 & 1 & 1 & \dots & 1 & 1 \\ 1 & 1 & 1 & \dots & 1 & 1 \\ 0 & 1 & 1 & \dots & 1 & 1 \\ 0 & 0 & 1 & \dots & 1 & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & 1 \end{bmatrix}$$

is unitary.

A Givens rotation is an orthogonal matrix of the form

$$P \begin{bmatrix} \cos\theta & -\sin\theta & \\ \sin\theta & \cos\theta & O^T \\ O & & I \end{bmatrix} P^T$$

for some permutation matrix P, $0 \le \theta < 2\pi$, and appropriately sized zero matrix O and identity matrix I.

THEOREM 8. *Suppose A is an n-by-n real orthogonal matrix with zero/nonzero pattern P. Let i and j be rows (or columns) of A. There exists a Givens rotation G such that the zero/nonzero pattern of GA (AG) has the supports of i and j replaced by the union of the supports of i and j. Further, if A is rational, then G can be chosen to be rational as well.*

Proof: Let G be a Givens rotation affecting rows i and j of A. If, for some k, either the i,k or j,k-entry of A is nonzero, then there are only finitely many values of $\theta \in [0, 2\pi)$ for which either of the corresponding entries of GA can be zero. It follows that for all but finitely many values of θ, the matrix GA has nonzero entries in row i and j wherever there was a nonzero entry in either row of A. The proof for columns is similar. □

Define the union of two patterns of the same size to be the pattern with zeros only where both patterns had zeros.

COROLLARY 2. *Let P' be the pattern obtained from an n-by-n pattern P by replacing two rows (or two columns) with the union of those rows (columns). If P is unitary then so is P'.*

THEOREM 9 ([21, Theorem 1.1]). *Let Q be an n-by-n orthogonal matrix of the* *form*

$$Q = \begin{bmatrix} U & 0 \\ V & W \end{bmatrix}$$

where U *is* k*-by-*$(k+l)$ *and* W *is* $(m+l)$*-by-*m *for some positive* k *and* m *and nonnegative* l *with* $k+l+m=n$. *Then the rank of* V *is* l.

THEOREM 10. *Suppose* P *is an* n*-by-*n *pattern of the form*

$$\begin{bmatrix} a & vw^T \\ 0 & B \end{bmatrix}$$

where A *is of size* $(k+1)$*-by-*k *and* B *is* $(n-k-1)$*-by-*$(n-k)$ *for some positive* k, *and* v *and* w *are column patterns. Then* P *is unitary if and only if both the patterns*

$$P_A = \begin{bmatrix} a & v \end{bmatrix} \text{ and } P_B = \begin{bmatrix} w^T \\ B \end{bmatrix}$$

are unitary. Moreover, $Z_+(B(P)) = n$ *implies* $Z_+(B(P_A)) = k+1$ *and* $Z_+(B(P_B)) = n-k$.

Proof: If P is unitary, that P_A and P_B are both unitary follows from Theorem 9. If

$$\begin{bmatrix} C & x \end{bmatrix} \text{ and } \begin{bmatrix} y^* \\ D \end{bmatrix}$$

are unitary matrices of the right dimensions, then C^*C, DD^*, $CC^* + xx^*$, and $D^*D + yy^*$ are identity matrices, $x^*x = yy^* = 1$, and $Dy = 0$, so that

$$\begin{bmatrix} C & xy^* \\ 0 & D \end{bmatrix} \begin{bmatrix} C & xy^* \\ 0 & D \end{bmatrix}^* = \begin{bmatrix} CC^* + xy^*yx^* & xy^*D^* \\ Dyx^* & D^*D + yy^* \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}.$$

For the zero forcing, subdivide the vertices of $B(P)$ as follows: Let R and C be the sets of vertices from the rows and columns. Let B_0 and B_* be the elements of C corresponding to zero and nonzero entries of w^T, respectively, and similarly define A_0 and A_* using R and v. Next, let $A_c = C \setminus (B_0 \cup B_*)$ and $B_r = R \setminus (A_0 \cup A_*)$. With this decomposition, notice that the vertices only are adjacent as indicated in the following diagram:

$$A_0 \leftrightarrow A_c \leftrightarrow A_* \leftrightarrow B_* \leftrightarrow B_c \leftrightarrow B_0.$$

Moreover, any two vertices of A_* have the same neighbors in B_* and vice versa.
Suppose without loss of generality that $Z_+(B(P_A)) < k+1$ and let Z_A be a zero forcing set of $B(P_A)$ of cardinality k. Choose a distinguished vertex $b \in B_*$. Then

the subgraph of $B(P)$ induced by $A_0 \cup A_* \cup A_c \cup \{b\}$ is isomorphic to $B(P_A)$. Use this isomorphism to color the vertices of $A_0 \cup A_* \cup A_c \cup \{b\}$ black or white according to Z_A. Next, color the vertices of $(B_* \setminus \{b\}) \cup B_0$ black. We claim the result, which has $k+n-k-1=n-1$ vertices, is a zero forcing set for $B(P)$. Since b is the only potentially white vertex of B_*, the copy of Z_A can force all of $A_0 \cup A_* \cup A_c \cup \{b\}$ as it would in $B(P_A)$, and the result is that every vertex of C is now black, which can force the remaining white vertices (B_c). □

In particular, Theorem 10 allows the following reduction: Given an n-by-n pattern P of the correct form and with $Z_+(B(P)) = n$, if the conjecture is true for all smaller matrices, then $Z_+(B(P_A)) = k+1$ and $Z_+(B(P_B)) = n-k$ imply that P_A and P_B are unitary, and thus P is unitary by Theorem 10.

The results of this section allow the following steps towards determining whether all 6-by-6 patterns P are unitary if and only if $Z_+(B(P)) = 6$: First, remove any patterns that have $Z_+ < 6$, as they are not unitary. Next, remove each pattern P' that can be obtained from a remaining pattern P as in Corollary 2, as, if the pattern P is not a counterexample, then neither will P' be—one can view this as letting Corollary 2 define a partial order on the patterns ($P < Q$ if Q can be obtained from P by taking the union of two rows or two columns) and then only having to consider the minimal patterns (those Q for which there does not exist a P with $P < Q$). Third, remove patterns that are equivalent to a pattern containing an upper Hessenberg pattern, as they are unitary and satisfy the conjecture, and any patterns that have the form of Theorem 10. Finally, take a representative from each remaining equivalence class.

This considerably narrows the computations required to check the 6-by-6 patterns, leaving 147 exceptional (equivalence classes of) patterns with $Z_+(B(P)) = 6$, and each of these patterns will need to be checked in order to determine if they admit a unitary matrix. If each pattern admits such a matrix, then a 6-by-6 pattern P is unitary if and only if $Z_+(B(P)) = 6$.

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