# Positive Semidefinite Zero Forcing and Applications

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## **1** Overview

Mathematical structures consisting of nodes and connections between them, called graphs, can be used to model real-world networks and situations, such as the spread of a disease over time. Graph infection, also called zero forcing because of its algebraic properties, is such a model that also has connections to quantum physics. This Research in Teams strived to better understand zero forcing for a particular type of network that all graphs can be related to. Results can be applied to general graph infection and help provide answers to related questions in linear algebra and the control of quantum systems. In particular, we were interested in the relationship between zero forcing and the possible zero/nonzero patterns of unitary matrices.

### 2 Mathematical Background

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. The neighborhood of a vertex v in a graph G, denoted by N(v), is the set of vertices adjacent to v. Consider a bipartite graph  $G = (M \cup N, E)$ . We will say that a subset S of either M or N has Property A if for all  $v \in S$ , there exists  $w \neq v \in S$  such that  $N(v) \cap N(w) \neq \emptyset$ . A bipartite graph  $G = (M \cup N, E)$  is called *strongly quadrangular* if S having Property A implies that

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

when S is a subset of either M or N.

Suppose that the vertices of a graph G are colored either white or black. The positive semidefinite colorchange 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.

The adjacency graph of a real symmetric positive semidefinite *n*-by-*n* matrix *H* has vertex set  $\{1, ..., n\}$  and edge set  $\{ij : i \neq j, a_{ij} \neq 0\}$ . Note that the diagonal entries of the matrix do not affect the graph. Given

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a graph G on n vertices, let  $\mathcal{P}(G)$  be the set of positive semidefinite matrices whose graph is isomorphic to G. The real positive semidefinite minimum rank of G,  $mr_+(G)$ , is the smallest possible rank among matrices in  $\mathcal{P}(G)$ . Setting  $M_+(G) = n - mr_+(G)$  gives the corresponding maximum nullity of G. The connection with zero forcing is that  $Z_+(G) \ge M_+(G)$  for all graphs G.

A matrix U is real orthogonal if  $UU^T = U^T U = I$ , where  $U^T$  is the transpose of T and I is the appropriate-size identity matrix. A zero/nonzero pattern is a matrix with entries from  $\{0, *\}$ . The support of a matrix is the zero/nonzero pattern obtained by replacing all nonzero entries with "\*". The bipartite graph B(P) of a zero/nonzero pattern P is obtained from P by letting the rows and columns be the vertices and placing an edge between row i and column j if and only if the ij entry of U is \*.

An *n*-by-*n* matrix A is *fully indecomposable* if it does not have a p by q zero submatrix with p + q = n. An orthogonal matrix is fully indecomposable if and only if its bipartite graph is connected [1].

A Givens rotation is an orthogonal matrix of the form

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

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

#### 3 Known Results

We assume all graphs are connected. For a bipartite graph  $G = (M \cup N, E)$ ,  $M_+(G) \leq Z_+(G) \min\{|M|, |N|\}$ . Given an *n*-by-*n* zero/nonzero pattern *P*, *P* is the support of a real orthogonal matrix if and only if  $M_+(B(P)) = n$  [2]. It was conjectured that *P* is the support of a real orthogonal matrix if and only if B(P) is strongly quadrangular [5], but examples have been found of patterns that are strongly quadrangular but do not support a real orthogonal matrix [3].

**Theorem 1** ([1]). 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 whose supports do not intersect. There exists a Givens rotation G such that the zero/nonzero pattern of GA(AG) has the support 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.

**Theorem 2** ([6]). A zero/nonzero pattern of degree at most four supports an orthogonal matrix if and only if *it is strongly quadrangular.* 

**Theorem 3** ([4]). *There are three strongly quadrangular* 5-by-5 *patterns that do not support orthogonal matrices:* 

0	0	*	*	*	0	0	*	*	*	0	0	*	*	*
0	0	*	*	*	0	0	*	*	*	0	0	*	*	*
*	*	0	*	*	*	*	0	*	*	*	*	0	*	*
*	*	*	*	*	*	*	*	0	*	*	*	*	0	*
*	*	*	*	*	*	*	*	*	*	*	*	*	*	0

**Theorem 4** ([6]). *Let P* (or its transpose) be a zero/nonzero pattern equivalent to a pattern with the following form:

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

where  $k \ge 1$ , J is the matrix of all \*s, and

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

Further suppose that the rows of X have disjoint support and every column of Y has support disjoint from every column of Z. Then P does not support an orthogonal matrix. Further, these patterns are strongly quadrangular.

#### 4 New Results

Throughout, let  $G = (V = M \cup N, E)$  be a bipartite graph with |M| = |N| = n. Our first result motivates what follows:

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

Since it was originally conjectured that a pattern would support a unitary matrix if and only if it was strongly quadrangular, this result shows that  $Z_+$  gives a stronger criterion than strong quadrangularity. As a result, we wonder whether the following is true:

**Conjecture.** An *m*-by-*m* zero/nonzero pattern *P* is the support of a real orthogonal matrix if and only if  $Z_+(B(P)) = m$ .

If a pattern P does support a unitary matrix, then  $Z_+(B(P)) = m$ , so a pattern for which  $Z_+(B(P)) < m$  automatically satisfies the conjecture.

We showed that the published examples where an *m*-by-*m* pattern *P* is strongly quadrangular but *P* is not the support of a real orthogonal matrix have  $Z_+(B(P)) < m$ .

**Theorem 6.** Suppose P is a pattern from either Theorem 3 or Theorem 4. Then  $Z_+(B(P)) = m$ .

In particular, the conjecture is true for all 5-by-5 or smaller patterns:

**Theorem 7.** For  $m \le 5$ , an m-by-m zero/nonzero pattern P is the support of a real orthogonal matrix if and only if  $Z_+(B(P)) = m$ .

We next considered pattern reduction techniques that can aid in the search for a possible counterexample to the conjecture.

**Theorem 8.** If P is a pattern that contains a row (or column) with exactly two nonzero entries, let P' be the pattern obtained by deleting that row (column) and one of the necessarily identical columns (rows) corresponding to the two nonzero entries. Then P supports a unitary if and only if P' does and  $Z_+(B(P)) = m$  if and only if  $Z_+(B(P')) = m - 1$ .

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

**Theorem 9.** Let P' be the pattern obtained from a pattern P by replacing two rows (or two columns) with the union of those rows (columns). If P supports a unitary then P' does and if  $Z_+(B(P)) = m$  then  $Z_+(B(P')) = m$ .

This work considerably narrowed the computations required to check the conjecture for 6-by-6 and 7-by-7 patterns. For example, in the 6-by-6 case, the reductions provided by the above results leave 147 exceptional 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 we will have established the conjecture above for 6-by-6 matrices.

#### References

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