

# On Zero Forcing and the Inverse Eigenvalue Problem for Graphs

Thomas R. Cameron

January 19, 2021

## Abstract

This note is intended to introduce the connection between the inverse eigenvalue problem of a graph and the zero forcing number of a graph.

## 1 Introduction

Let  $\mathbb{G}$  denote the collection of all simple graphs (no loops nor multi-edges) of order  $n$ . With each graph  $G \in \mathbb{G}$ , there is a vertex set  $V(G) = \{v_1, v_2, \dots, v_n\}$  and an edge set  $E(G)$ , where  $\{v_i, v_j\} \in E(G)$  if and only if  $i \neq j$  and  $v_i$  and  $v_j$  are adjacent vertices. For example, let  $G$  be the star graph of order 7 shown in Figure 1. Then,  $V(G) = \{1, 2, 3, 4, 5, 6, 7\}$  and  $E(G) = \{\{1, 7\}, \{2, 7\}, \{3, 7\}, \{4, 7\}, \{5, 7\}, \{6, 7\}\}$ .

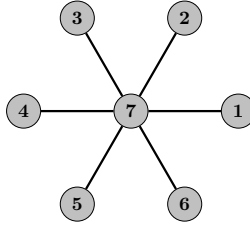


Figure 1: A star graph of order 7.

Every  $n \times n$  symmetric matrix  $A = [a_{ij}]_{i,j=1}^n$  is associated with a graph  $G \in \mathbb{G}$ , where  $a_{ij} \neq 0$  if and only if  $\{v_i, v_j\} \in E(G)$ . Given a graph  $G \in \mathbb{G}$ , the set of all  $n \times n$  symmetric matrices associated with  $G$  is denoted by

$$\mathcal{S}(G) = \{A = [a_{ij}]_{i,j=1}^n : a_{ij} = a_{ji} \ \forall i \neq j, \ a_{ij} \neq 0 \Leftrightarrow \{v_i, v_j\} \in E(G)\}.$$

For example, the star graph  $G$  shown in Figure 1 is associated with symmetric matrices of the form

$$A = \begin{bmatrix} \alpha_1 & 0 & \cdots & 0 & \beta_1 \\ 0 & \alpha_2 & \cdots & 0 & \beta_2 \\ \vdots & & \ddots & & \vdots \\ 0 & & & \alpha_6 & \beta_6 \\ \beta_1 & \beta_2 & \cdots & \beta_6 & \alpha_7 \end{bmatrix}.$$

The inverse eigenvalue problem of a graph can be stated as follows: Given a graph  $G \in \mathbb{G}$ , what are all possible length  $n$  multi-sets  $\sigma$  such that there is a matrix  $A \in \mathcal{S}(G)$  with spectrum  $\sigma$ . This important question is obviously difficult to answer in general; however, there are a few observations we can make.

- The empty graph of order  $n$ , denoted  $E_n$ , has no edges. Therefore,  $\mathcal{S}(E_n)$  is the set of all  $n \times n$  diagonal matrices. Since the eigenvalues of a diagonal matrix are equal to its diagonal entries, it follows that every length  $n$  multi-set  $\sigma$  corresponds to the eigenvalues of a matrix  $A \in \mathcal{S}(E_n)$ . It turns out, that the empty graph is the only graph with this property.
- Let  $K_n$  denote a complete graph of order  $n$ . Then,  $\mathcal{S}(K_n)$  is made up of symmetric matrices where all off-diagonal entries are non-zero. Furthermore, for any  $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ , there is a matrix  $A \in \mathcal{S}(K_n)$  with eigenvalues  $\lambda_1, \lambda_2, \dots, \lambda_n$  if and only if  $\lambda_1 < \lambda_n$  [1].

- Let  $P_n$  denote a path graph of order  $n$ . Then,  $\mathcal{S}(P_n)$  corresponds to tri-diagonal matrices with non-zero entries in the upper and lower diagonals. Furthermore, any length  $n$  multi-set  $\sigma$  corresponds to the eigenvalues of a matrix  $A \in \mathcal{S}(P_n)$  if and only if the entries of  $\sigma$  are distinct [3].

Due to the difficulty of the inverse eigenvalue problem of a graph, there is a focus on solving related but seemingly easier problems. For instance, one may want to find the maximum multiplicity of a graph  $G \in \mathbb{G}$ , denoted  $M(G)$ , which is defined as the largest integer  $k$  such that there is a matrix  $A \in \mathcal{S}(G)$  with an eigenvalue of multiplicity  $k$ . Note  $M(E_n) = n$ ,  $M(K_n) = (n - 1)$ , and  $M(P_n) = 1$ .

The multiplicity of an eigenvalue  $\lambda$  of the symmetric matrix  $A$  is equal to the nullity of  $\lambda I - A$ , i.e., the dimension of the null space of  $\lambda I - A$ . Note that for any  $A \in \mathcal{S}(G)$ , it follows that  $\lambda I - A \in \mathcal{S}(G)$ . Therefore,

$$M(G) = \max \{ \text{nullity}(A) : A \in \mathcal{S}(G) \}.$$

For this reason, the maximum multiplicity of a graph is often referred to as the max nullity of the graph.

In a similar manner, the minimum rank of  $G$ , denoted  $mr(G)$ , is defined by

$$mr(G) = \min \{ \text{rank}(A) : A \in \mathcal{S}(G) \}.$$

Recall that the  $\text{rank}(A)$  is the dimension of the column space of  $A$ . By the rank-nullity theorem, we have

$$mr(G) + M(G) = n.$$

In 2006, at the AIMS Workshop on “Spectra of families of matrices described by graphs, digraphs, and sign pattern”, a novel connection between the maximum nullity of a graph and its zero forcing number was presented. Zero forcing was introduced independently by Burgarth and Giovannetti in the control of quantum systems [2], where it was called graph infection. For our purposes, zero forcing is a coloring game on a graph, where an initial set of vertices are colored blue and all other vertices are colored white. Then, the blue vertices force neighboring white vertices blue using a color change rule. There are many color changing rules, but the standard rule is that a blue vertex  $b$  can force a white vertex  $w$  blue if  $w$  is the only white neighbor of  $b$ . We will reference this rule as the Z-color change rule to distinguish it from the other variants.

Given a graph  $G \in \mathbb{G}$ , let  $B \subseteq V(G)$  denote the initial set of blue vertices; this is called the initial coloring of  $G$ . Then, denote by  $B^{[t]}$  the blue vertices after  $t$  applications of the Z-color change rule, where  $B^{[0]} = B$ . Because the graph is finite, there exists a  $t^* \geq 0$  for which  $B^{[t^*]} = B^{[t^*+k]}$ , for all  $k \in \mathbb{N}$ , i.e., no more changes are possible from applying the Z-color change rule. We reference  $B^{[t^*]}$  as the final coloring of  $B$ . If  $B^{[t^*]} = V(G)$ , i.e., the final coloring is all of the vertices of  $G$ , then we say that  $B$  is a zero forcing set of  $G$ . The zero forcing number of  $G$  is defined as the cardinality of the smallest zero forcing set of  $G$ :

$$Z(G) = \min \left\{ |B| : B^{[t^*]} = V(G) \right\}.$$

For example, consider the application of the Z-color change rule to a path graph on 5 vertices shown in Figure 2. It is clear that  $B^{[4]}$  is the final coloring of  $B$  since  $B^{[5]} = B^{[4]}$ . Furthermore, since  $B^{[4]}$  encompasses all vertices in the graph, it follows that  $B = \{1\}$  is a zero forcing set and, hence, the zero forcing number of this path graph is equal to 1.

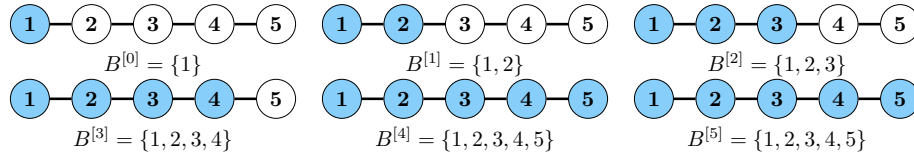


Figure 2: A zero forcing set for a path graph of order 5.

One can easily generalize the above example and conclude that the zero forcing number of all path graphs is equal to 1, i.e.,  $Z(P_n) = 1$ . Note that not every initial coloring of 1 vertex is a zero forcing set of  $P_n$ . Indeed, consider the initial coloring of a path graph on 5 vertices shown in Figure 3.

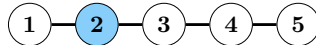


Figure 3: A non zero forcing set for a path graph of order 5.

We are now ready to present the connection between the zero forcing number and the maximum nullity of a graph. First we require the following lemma.

**Lemma 1.1.** *Suppose that  $\alpha \subseteq \{1, 2, \dots, n\}$  with  $|\alpha| < k$  and  $U$  is a subspace of  $\mathbb{R}^n$  of dimension  $k$ . Then,  $U$  contains a non-zero vector of  $\mathbf{v}$  with  $\mathbf{v}[\alpha] = 0$ .*

*Proof.* Note that if  $U$  and  $V$  are subspaces of  $\mathbb{R}^n$  whose dimensions satisfy

$$\dim V > n - \dim U,$$

then  $U$  and  $V$  must have a non-trivial intersection, i.e., there is a non-zero vector in  $U \cap V$ . Now, define

$$V = \{\mathbf{v} \in \mathbb{R}^n : \mathbf{v}[\alpha] = 0\},$$

and note that  $\dim V = n - |\alpha| > n - k = \dim U$ . Hence, there exists a non-zero vector  $\mathbf{v} \in U \cap V$ , and the result follows.  $\square$

**Theorem 1.2.** *Let  $G \in \mathbb{G}$ . Then,  $M(G) \leq Z(G)$ .*

*Proof.* Let  $B \subseteq V(G)$  be a zero forcing set of  $G$ , and let  $A \in \mathcal{S}(G)$ . If  $|B| < \text{nullity}(A)$ , then Lemma 1.1 implies that there exists a non-zero vector  $\mathbf{x} \in \text{null}(A)$  such that  $\mathbf{x}_i = 0$  for all  $i \in B$ . However, if a vector  $\mathbf{x} \in \text{null}(A)$  satisfies  $\mathbf{x}_i = 0$  for all  $i \in B$ , then it follows that  $\mathbf{x} = \mathbf{0}$ .

Indeed, let  $j \in V(G) \setminus B$  be any vertex that is forced by some  $i \in B$ ; at least one such vertex must exist since  $B$  is a zero forcing set. Then, the equation  $A\mathbf{x} = \mathbf{0}$  implies that  $a_{ij}\mathbf{x}_j = 0$ , which gives  $\mathbf{x}_j = 0$  since  $a_{ij} \neq 0$ . If necessary, we can repeat the above argument on the zero forcing set  $B \cup \{j\}$ , and perhaps again, until all vertices in  $V(G)$  are accounted for at which point it follows that  $\mathbf{x} = \mathbf{0}$ .

This contradiction with Lemma 1.1 implies that  $|B| \geq \text{nullity}(A)$ . Since  $B$  and  $A$  are arbitrary, it follows that  $Z(G) \geq M(G)$ .  $\square$

Theorem 1.2 can be used to determine the maximum nullity of a graph via its zero forcing number. For instance, we know that the path graph satisfies  $Z(P_n) = 1$ . Therefore, Theorem 1.2 implies that  $M(P_n) \leq 1$ . Since there is always a singular matrix in  $\mathcal{S}(G)$ , for any graph  $G$ , it follows that  $M(P_n) = 1$ .

As a more interesting example, consider the star graph in Figure 1. Note that  $B = \{1, 2, 3, 4, 5\}$  is a zero-forcing set of minimal size. This observation can easily be generalized and we conclude that the zero forcing number of the star graph  $K_{1,n-1}$  of order  $n$  satisfies  $Z(K_{1,n-1}) = n - 2$ . Therefore, the maximum nullity and minimum rank satisfy

$$M(K_{1,n-1}) \leq n - 2 \text{ and } mr(K_{1,n-1}) \geq 2,$$

respectively. Furthermore, the adjacency matrix of the star graph  $K_{1,n-1}$ :

$$A = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 0 & 1 \\ \vdots & & \ddots & & \vdots \\ 0 & & & 0 & 1 \\ 1 & 1 & \cdots & 1 & 0 \end{bmatrix}.$$

is a  $n \times n$  matrix in  $\mathcal{S}(K_{1,n-1})$  that satisfies  $\text{rank}(A) = 2$ . Therefore,  $M(K_{1,n-1}) = n - 2$  and  $mr(K_{1,n-2}) = 2$ .

## 2 Positive Semidefinite Zero Forcing

As mentioned in Section 1, there are many color change rules that can be used in the coloring game of zero forcing. The so-called standard zero forcing rule provides an upper bound on the maximum nullity of a graph via Theorem 1.2. The positive semidefinite zero forcing rule provides an upper bound on the maximum positive semidefinite nullity:

$$M_+(G) = \max \{\text{nullity}(A) : A \in \mathcal{S}(G), \forall \lambda \in \sigma(A), \lambda \geq 0\}.$$

Note that the additional condition on the eigenvalues of  $A$ , i.e.,  $\lambda \geq 0$  for all  $\lambda \in \sigma(A)$ , implies that  $A$  must be positive semidefinite.

Given a graph  $G \in \mathbb{G}$ , let  $B \subseteq V(G)$  denote the initial coloring of  $G$ . Let  $G \setminus B$  denote the resulting graph after the blue vertices (and adjacent edges) have been removed, and let  $W_1, \dots, W_k$  denote the vertex sets of the connected components of  $G - B$ . If  $b \in B$  and  $w \in W_i$  is the only white neighbor of  $b$  in  $G[W_i \cup B]$ , for some  $i \in \{1, \dots, k\}$ , then the positive semidefinite zero forcing rule says that  $b$  can force  $w$  blue.

As with the standard zero forcing rule, there exists a  $t^* \geq 0$  such that  $B^{[t^*]} = B^{[t^* + k]}$  for all  $k \in \mathbb{N}$ , and we say that  $B$  is a positive semidefinite zero forcing set if the final coloring satisfies  $B^{[t^*]} = V(G)$ . The positive semidefinite zero forcing number of  $G$  is defined as the cardinality of the smallest positive semidefinite zero forcing set of  $G$ :

$$Z_+(G) = \min \left\{ |B| : B^{[t^*]} = V(G) \right\}.$$

**Theorem 2.1.** *Let  $G \in \mathbb{G}$ . Then,  $M_+(G) \leq Z_+(G)$ .*

*Proof.* Let  $A \in S(G)$  be positive semidefinite with nullity  $(A) = M_+(G)$  and consider a non-zero vector  $\mathbf{x} \in A$ , which is guaranteed to exist since the max nullity is at least 1. Let  $B \subset V(G)$  denote the set of vertices such that  $\mathbf{x}_i = 0$ , and let  $W_1, \dots, W_k$  denote the vertex sets of the connected components of  $G \setminus B$ . For every  $i \in \{1, \dots, k\}$ , we claim that no  $w \in W_i$  can be the only neighbor of a  $b \in B$  in  $G[W_i \cup B]$ .

Indeed, note that we can write  $A$ , possibly after re-ordering the vertices of  $G$ , as follows

$$A = \begin{bmatrix} A_1 & 0 & \cdots & 0 & C_1 \\ 0 & A_2 & \cdots & 0 & C_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & A_k & C_k \\ C_1 & C_2 & \cdots & C_k & D \end{bmatrix},$$

where  $A_1, \dots, A_k$  corresponds to the vertex sets  $W_1, \dots, W_k$ , respectively,  $D$  corresponds to the vertex set  $B$ , and  $C_i$  corresponds to the edges between  $W_i$  and  $B$ , for all  $i \in \{1, \dots, k\}$ .

Now, consider the partition  $\mathbf{x} = [\mathbf{x}_1^T, \dots, \mathbf{x}_k^T, \mathbf{0}^T]^T$ , where  $\mathbf{x}_i$  has size equal to  $|W_i|$ , for all  $i \in \{1, \dots, k\}$ , and the zero vector  $\mathbf{0}$  has size equal to  $|B|$ . Note that all entries of  $\mathbf{x}_1, \dots, \mathbf{x}_k$  must be non-zero. Moreover, the equation  $A\mathbf{x} = \mathbf{0}$  implies that  $A_i\mathbf{x}_i = \mathbf{0}$  for all  $i \in \{1, \dots, k\}$ .

The column inclusion property for Hermitian positive semidefinite matrices [4], guarantees that each column in  $C_i$  is the span of the columns in  $A_i$ , for all  $i \in \{1, \dots, k\}$ . Therefore, for each  $i \in \{1, \dots, k\}$ , there exists a matrix  $Y_i$  such that  $C_i = A_i Y_i$ . Since  $A$  is symmetric, it follows that  $C_i = Y_i^T A_i$ ; hence,  $C_i \mathbf{x}_i = \mathbf{0}$  for all  $i \in \{1, \dots, k\}$ . But if  $w \in W_i$  were the only white neighbor of  $b \in B$  in  $G[W_i \cup B]$ , then  $C_i \mathbf{x}_i \neq \mathbf{0}$ , which is a contradiction.

This contradiction implies that  $B$  is not a positive semidefinite zero forcing set of  $G$ . Furthermore, it follows that there is no non-trivial  $\mathbf{x} \in \text{null}(A)$  with  $\mathbf{x}_i = 0$  for all  $i$  in a positive semidefinite zero forcing set of  $G$ . Therefore, by Lemma 1.1, we have  $M_+(G) \leq Z_+(G)$ .  $\square$

As an example of how Theorem 2.1 could be applied, consider the star graph  $K_{1,n-1}$ . Note that the “center” vertex constitutes a positive semidefinite zero forcing set of  $K_{1,n-1}$ . Therefore,

$$Z_+(K_{1,n-1}) = 1$$

and it follows that  $M_+(K_{1,n-1}) = 1$ .

Finally, note that every standard zero forcing set of a graph  $G \in \mathbb{G}$  constitutes a positive semidefinite zero forcing set; hence,  $Z_+(G) \leq Z(G)$ . Furthermore, it is also clear that  $M_+(G) \leq M(G)$ .

**Question 2.2.** *Is there a relationship between  $Z_+(G)$  and  $M(G)$ , i.e., does the following hold*

$$Z_+(G) \leq M(G)$$

*for all (or some) graphs  $G \in \mathbb{G}$ .*

### 3 Computation of Max Nullity and Zero-Forcing

### 4 Colin de Verdière Type Parameters

## References

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