On Zero Forcing and the Inverse Eigenvalue Problem for Graphs

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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 $V(G) = \{v_1, v_2, \ldots, v_n\}$ 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 $E(G) = \{\{1, 7\}, \{2, 7\}, \{3, 7\}, \{4, 7\}, \{5, 7\}, \{6, 7\}\}$.

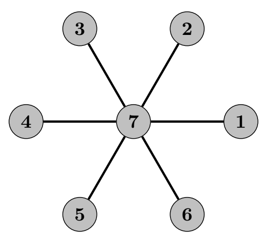

Figure 1: A star graph of order 7.

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

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

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 σ such that there is a matrix $A \in \mathcal{S}(G)$ with spectrum σ. 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 σ 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 $\lambda_1 \leq \lambda_2 \leq \cdots \lambda_n$, there is a matrix $A \in \mathcal{S}(K_n)$ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ 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 σ corresponds to the eigenvalues of a matrix $A \in \mathcal{S}(P_n)$ if and only if the entries of σ are distinct [5].

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 λ 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 refereed 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 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 [3], 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.

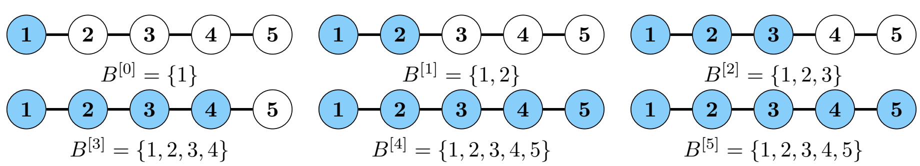

Figure 2: A zero forcing set for a path graph of order 5.

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.

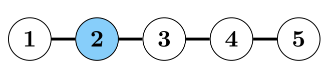

Figure 3: A non zero forcing set for a path graph of order 5.

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 $\alpha \subseteq \{1, 2, \ldots, n\}$ 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. □

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 $Z(G) \geq M(G)$. □

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 $G - B$ denote the resulting graph after the blue vertices (and adjacent edges) have been removed, and let $W_1, \ldots, W_k$ 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 $i \in \{1, \ldots, k\}$, 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 $A \in \mathcal{S}(G)$ 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 $W_1, \ldots, W_k$ denote the vertex sets of the connected components of $G \setminus B$. For every $i \in \{1, \ldots, k\}$, 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 $A_1, \ldots, A_k$ corresponds to the vertex sets $W_1, \ldots, W_k$, respectively, D corresponds to the vertex set B, and C_i corresponds to the edges between W_i and B, for all $i \in \{1, \ldots, k\}$.

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

The column inclusion property for Hermitian positive semidefinite matrices [7], guarantees that each column in C_i is the span of the columns in A_i, for all $i \in \{1, \ldots, k\}$. Therefore, for each $i \in \{1, \ldots, k\}$, 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 $i \in \{1, \ldots, k\}$. 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 $\mathbf{x} \in$ 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 $M_+(G) \leq Z_+(G)$. □

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 Historical Background of the Minimum Rank

Parter appears to be the first to study the spectral properties of matrices with a given graph; in 1960, he published his investigation of sign symmetric matrices with multiple eigenvalues whose underlying graph is a tree [9].

Recall that a *forest* is an acyclic graph, i.e., a graph with no cycles, and a *tree* is a connected forest. Moreover, given a tree T and a vertex $v \in V(T)$, a *branch* of T at v is a connected component of $T - v$. If $A \in S(T)$, then each branch of T at v determines a principal submatrix of A, namely $A[W]$, where W is the vertex set of the branch. The following result is due to Parter [9].

Theorem 3.1. *Let T be a tree and let $A \in \mathcal{S}(T)$. Then,* nullity $(A) \geq 2$ *if and only if there exists a vertex $v \in V(T)$ and at least three branches $T[W_i]$ of T at v such that the principal submatrix $A[W_i]$ is singular.*

The following result is due to Fiedler [4]

Theorem 3.2. *Let T be a tree and let $A \in \mathcal{S}(T)$ with* nullity $(A) \geq 2$. *Then, there exists an $i \in \{1, 2, \ldots, n\}$ such that every null vector $\boldsymbol{x} = [x_i]$ has $x_i = 0$.*

An index $i \in \{1, 2, \ldots, n\}$ with the property that every eigenvector of A corresponding to an eigenvalue λ has its ith coordinate zero is known as a *Fiedler index* of A corresponding to λ.

In [4], Fiedler also showed that one can often determine the location of an eigenvalue λ of $A \in \mathcal{S}(T)$ among the ordering of its eigenvalues from an eigenvector of A corresponding to λ.

Theorem 3.3. *Let T be a tree, $A \in \mathcal{S}(A)$, and $\boldsymbol{y} = [y_i]$ be an eigenvector corresponding to an eigenvalue λ. Let p be the number of edges $ij \in E(T)$ such that $a_{ij}y_iy_j < 0$, q the number of edges $ij \in E(T)$ such that $a_{ij}y_iy_j > 0$, and r the number of coordinates of $\boldsymbol{y}$ that are zero. If there does not exist an index i such that $y_i = 0$ and $y_j = 0$ for all j adjacent to i in T, then there are $p + r$ eigenvalues of A greater than λ and $q + r$ eigenvalues of A less than λ (counting multiplicity).*

For example, consider the tree graph shown in Figure 4. The adjacency matrix of this graph is

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

and has spectrum $\sigma(A) = \{-2, 2, -1, 1, 0, 0\}$. To illustrate Theorem 3.1, note that there are three branches of the vertex 2, namely $\{1\}$, $\{3\}$, and $\{4, 5, 6\}$, with corresponding principal submatrix of A that is singular. A similar argument can be made for the branches of the vertex 5. Moreover, the null (A) is spanned by the following basis vectors

$$\begin{bmatrix} 0 & 0 & 0 & -1 & 0 & 1 \end{bmatrix}^T$$
$$\begin{bmatrix} -1 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}^T$$

Hence, every null vector of A has a zero in the index 2 and 5, which illustrates Theorem 3.2. Finally, note the following eigenvalue-eigenvector pairs for the matrix A:

$$\begin{aligned} \lambda = -2, \quad \mathbf{v} &= \begin{bmatrix} -1 & 2 & -1 & 1 & -2 & 1 \end{bmatrix}^T, \\ \lambda = 2, \quad \mathbf{v} &= \begin{bmatrix} 1 & 2 & 1 & 1 & 2 & 1 \end{bmatrix}^T, \\ \lambda = -1, \quad \mathbf{v} &= \begin{bmatrix} 1 & -1 & 1 & 1 & -1 & 1 \end{bmatrix}^T, \\ \lambda = 1, \quad \mathbf{v} &= \begin{bmatrix} -1 & -1 & -1 & 1 & 1 & 1 \end{bmatrix}^T. \end{aligned}$$

Note that Theorem 3.3 holds for each of the eigenvalue-eigenvector pairs since none of the eigenvectors do not have any zero elements. For instance, every entry of the eigenvector associated with $\lambda = 2$ is positive. Hence, there are 5 (total number of edges) eigenvalues of A less than 2 (counting multiplicity). For the eigenvector associated with $\lambda = -1$, we have $p = 4$ (corresponding to edges $\{1, 2\}$, $\{2, 3\}$, $\{4, 5\}$, $\{5, 6\}$) and $q = 1$ (corresponding to the edge $\{2, 5\}$). Hence, there are 4 eigenvalues of A greater than -1 and 1 eigenvalue less than -1. A similar statement can be made for the eigenvectors associated with all other eigenvalues of A.

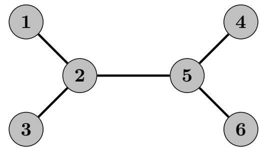

Figure 4: A tree graph of order 6.

In 1984, Wiener strengthened the result in Theorem 3.1 [10]. This stronger result, stated in Theorem 3.4, is now referred to as the Parter-Wiener theorem.

Theorem 3.4. *Let T be a tree and $A \in \mathcal{S}(T)$ with* $\text{nullity}\,(A) \geq 2$. *Then, there is a vertex $i \in V(T)$ such that* $\text{nullity}\,(A(i)) = \text{nullity}\,(A) + 1$, *and the principal submatrices of A corresponding to at least three branches of T at i are singular.*

Note that $A(i)$ is the principal submatrix of A obtained by deleting row and column i from the matrix A. Moreover, the vertex i for which $\text{nullity}\,((A - \lambda I)(i)) = \text{nullity}\,(A - \lambda I) + 1$ is known as a Parter-Wiener vertex for A corresponding to the eigenvalue λ. For example, the adjacency matrix of the tree graph in Figure 4 has Parter-Wiener vertices 2 and 5 corresponding to the eigenvalue 0. Over the subsequent years, the Parter-Wiener theorem has been further developed and produced many beautiful results, e.g., see Chapter 2 of [6].

Nylen appears to be the first to study the minimum rank of a graph, which appeared in his 1996 paper [8]. In that paper, Nylen made the following observations.

Proposition 3.5. *Let $G \in \mathbb{G}$ have order $n \geq 1$. Then,*

a. *If $A \in \mathcal{S}(G)$ and $v \in V(G)$, then the principal submatrix $A(v)$ corresponds to the induced subgraph $G - v$.*

b. *If G is disconnected with connected components $G_1, G_2, \ldots, G_k$, then*

$$mr(G) = \sum_{i=1}^{k} mr(G_i).$$

c. *If G has k connected components, then*

$$mr(G) \leq n - k.$$

d. *For each vertex $v \in V(G)$, we have*

$$mr(G) - 2 \leq mr(G - v) \leq mr(G).$$

e. *For each edge $e \in E(G)$, we have*

$$mr(G) - 1 \leq mr(G - e) \leq mr(G) + 1.$$

In addition, Nylen proved the following more substantial result.

Theorem 3.6. *Let $G \in \mathbb{G}$ and $A \in \mathcal{S}(G)$ with* $\text{rank}\,(A) = mr(G)$. *Then, for any vertex $i \in V(G)$, either* $\text{rank}\,(A(i)) = mr(G) - 2$ *or* $\text{rank}\,(A(i)) = mr(G)$.

The rest of Nylen's paper focuses on trees; in particular, he proved the following result, which provides an algorithm for computing the minimum rank of a tree. Note that a *high-degree* vertex of a graph is a vertex with degree at least 3; a *Nylen path* in a forest F is a path with at most one high-degree vertex, and whose initial and terminal vertices each have degree 1.

Theorem 3.7. *Let P be a Nylen path of the forest F. Then,*

a. *If P has a high-degree vertex v, then $mr(F) = mr(F - i) + 2$.*

b. *If P does not have a high-degree vertex, then $mr(F) = |V(P)| - 1 + mr(F - V(P))$.*

4 Colin de Verdiére Type Parameters

5 Computational Approaches to Zero Forcing Number

5.1 Integer Program

In this section, we review the integer program model introduced by Brimkov et al. [2] to compute the zero forcing number of a graph $G \in \mathbb{G}$. This integer program is shown in (1a)–(1e), and we reference this program by ZIP (G). Note that every edge in $E(G)$ is replaced by two directed edges with opposite direction. A binary variable s_v indicates whether vertex v is in the zero forcing set; an integer variable x_v ranging in $\{0, \ldots, T\}$ indicates at which timestep vertex v is forced, where T is the maximum difference between the forcing times of two vertices; finally, a binary variable y_e for each directed edge $e = (u, v)$ indicates whether u forces v. The notation $\delta^-(v)$ refers to the set of edges pointing towards the node v, $N(u)$ denotes the open neighborhood of u, i.e., all vertices $v \in V(G)$ that are adjacent to u, and $N[u]$ denotes the closed neighborhood of u, i.e., $N[u] = N(u) \cup \{u\}$.

$$\text{minimize} \quad \sum_{v \in V} s_v \tag{1a}$$

$$\text{subject to} \quad s_v + \sum_{e \in \delta^-(v)} y_e = 1, \quad \forall v \in V, \tag{1b}$$

$$x_u - x_v + (T+1)y_e \leq T, \quad \forall e = (u,v) \in E, \tag{1c}$$

$$x_w - x_v + (T+1)y_e \leq T, \quad \forall e = (u,v) \in E,\ \forall w \in N(u) \setminus \{v\}, \tag{1d}$$

$$s \in \{0,1\}^n,\ x \in \{0, \ldots, T\}^n,\ y \in \{0,1\}^m \tag{1e}$$

The triple (s, x, y), where $s \in \{0,1\}^n,\ x \in \{0, \ldots, T\}^n,\ y \in \{0,1\}^m$, is a *feasible solution* of ZIP (G) provided that s, x, y satisfy (1b)–(1e). If, in addition, s is minimal with respect to the objective function 1a, then we say that (s, x, y) is an *optimal solution* of ZIP (G). The corresponding minimal value of the objective function 1a is the optimal value of ZIP (G).

Theorem 5.1. *Let $G \in \mathbb{G}$. The optimal value of* ZIP (G) *is equal to the zero-forcing number of G.*

Proof. Let $B \subseteq V$ denote a zero-forcing set of G. Also, fix some chronological list of forces that results in a total coloring of G, and let $\mathcal{F}$ be the associated set of forcing chains. Since B is a zero forcing set, every vertex $v \in V(G)$ is either in B, i.e., $s_v = 1$, or is forced by some other vertex $u \in V(G)$, i.e., $y_e = 1$ where $e = (u, v)$. Thus, constraint (1b) must hold. Now, let x_v be the time step in which $v \in V(G)$ is forced. Since a vertex cannot force until all but one of its neighbors are forced, it follows that for every edge $e = (u, v)$ for which $y_e = 1$, u must be forced before v, i.e., $x_u < x_v$. Similarly, $x_w < x_v$ for all neighbors w of u. Thus, constraints (1c) and (1d) are satisfied. If $y_e = 0$, then constraints (1c) and (1d) hold since T is the maximum difference between the forcing times of two vertices. Therefore, constraints (1b)–(1e) are valid for any zero-forcing set B and associated set of forcing chains $\mathcal{F}$.

Conversely, let (s, x, y) be a feasible solution of ZIP (G). Define $B \subseteq V(G)$ to be the set of vertices for which $s_v = 1$. By constraint (1b), each vertex $v \in V(G)$ is either in B or is the head of exactly one edge $e = (u, v)$ such that $y_e = 1$. Consider any such edge; then, by constraints (1c) and (1d), there must be an integer $x_v \in \{0, \ldots, T\}$ such that $x_w + 1 \leq x_v$ for all $w \in N[u] \setminus \{v\}$. Therefore, the edges $e = (u, v)$ for which $y_e = 1$ define a chronological list of forces. Since every vertex $v \in V(G)$ is either in B or is the head of exactly one edge $e = (u, v)$ such that $y_e = 1$, it follows that B is a zero-forcing set. If, in addition, s is minimal with respect to the objective function (1a), i.e., (s, x, y) is an optimal solution of ZIP (G), then B is a minimal zero-forcing set and it follows that the objective value of ZIP (G) is the zero-forcing number of G. □

6 Propagation Time and Throttling Number

Given a color change rule and a graph G, the propagation time of $B \subseteq V(G)$, denoted $pt(G, B)$, is the smallest t such that $B^{[t]} = V(G)$ or ∞ if B is not a zero-forcing set. The propagation time of G is defined by

$$pt(G) = \min \{pt(G, B) \colon B \text{ is a minimal zero-forcing set}\}.$$

In Figure 5, we illustrate the standard propagation process and blue sets $B^{[i]}$ for a tree T and initial set $B = B^{[0]}$ such that $pt(T) = pt(G, B)$.

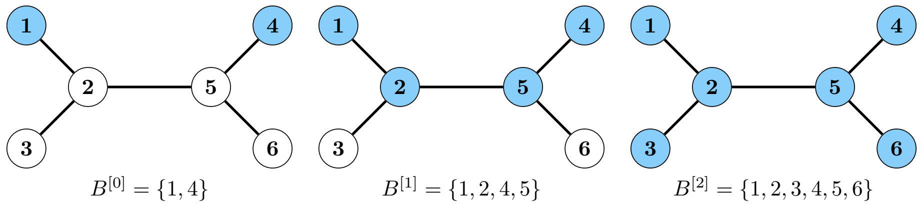

Figure 5: A zero forcing set for a tree graph of order 6.

Given a color change rule and a graph G, the throttling number of $B \subseteq V(G)$ is defined by

$$th(G, B) = |B| + pt(G, B).$$

Furthermore, the throttling number of G is defined by

$$th(G) = \min_{B \subseteq V(G)} th(G, B).$$

Note that throttling number is not necessarily attained for minimal zero-forcing sets. Indeed, consider the path graph of order n, denoted by P_n. Note that $Z(P_n) = 1$, and any of the two leafs in P_n will serve as a zero forcing set, e.g., see Figure 2. Since every other node will be forced, one at a time, it follows that $pt(P_n, B) = n - 1$, for any minimal zero-forcing set. Therefore,

$$th(P_n, B) = n$$

for any minimal zero-forcing set B. However, if we let the initial coloring B be made up of both leafs in P_n, then $pt(P_n, B) = \lceil (n-2)/2 \rceil$, and it follows that

$$th(P_n, B) = 2 + \lceil (n-2)/2 \rceil.$$

Therefore, $th(P_n) < n$ for all $n > 3$.