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On the singularity of graphs: Zero forcing parameters

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Περίληψη

Η αλγεβρική πολλαπλότητα της ιδιοτιμής μηδέν στο φάσμα ενός γραφή- ματος ονομάζεται πολλαπλότητα μηδενός του γραφήματος και συμβολίζεται με $\eta(G)$. Σε αυτή την εργασία ε- ξετάζουμε γραφήματα με μέγιστη πολλαπλότητα μηδενός $M(G)$, χρησιμοποιώντας τον αριθμό επιβολής μηδέν, $Z(G)$, μια παράμετρο που αποτελεί άνω φράγμα για την πολλαπλότητα μηδε- νός ενός γραφήματος. Προσδιορίζουμε συγκεκριμένα γραφήματα για τα οποία ισχύει η ισότητα $M(G) = Z(G)$. Επιπλέον, δίνουμε κάποιες εναλλακτικές αποδείξεις που αφορούν τη μέγιστη πολλαπλότητα μηδενός ενός γραφήματος.

Abstract

The algebraic multiplicity of the eigenvalue zero in a graph's spectrum is called the nullity of the graph and is denoted by $\eta(G)$. This paper considers graphs with maximum nullity, $M(G)$, using as a tool the zero forcing number, $Z(G)$, a parameter that upper bounds the nullity of the graph. We identify certain graphs for which the equality $M(G) = Z(G)$ holds. Furthermore, we provide some alternative proofs concerning the maximum nullity of graphs.

Keywords. maximum nullity, zero forcing number, Tutte-Coxeter graph, Gray graph, null spread, zero spread, core graph.

1. Introduction

Let $G = (V, E)$ be a finite, undirected graph with nonempty vertex set V and edge set E. The *adjacency matrix*, $A(G)$ or $A = (a_{ij})$, of a graph G on n vertices is $a_{ij} = 1$, if ij is an edge in G and 0 otherwise. For an undirected graph the adjacency matrix is symmetric. A graph, G, is said to be *singular* (resp. *non-singular*), if the adjacency matrix, $A(G)$, is a singular (resp. *non-singular*) matrix; that is 0 is an eigenvalue of G. The *nullity* of G, $\eta(G)$, is the multiplicity of the zero eigenvalue of A. It follows that there exist linearly independent vectors, x, such that $Ax = 0$; the dimension of the nullspace, $ker(A) = \{x \in \mathbb{R}^n : Ax = 0\}$, is therefore the nullity of G.

Recently, the nullity of a graph has received a lot of attention as it has a number of direct applications in organic chemistry, where it has been shown that for the graphs corresponding to conjugated hydrocarbons, $\eta(G) = 0$, is a necessary condition for the above molecules to be stable [7]. The characterization of all graphs G with $\eta(G) > 0$ posed by Collatz et al. [3] is still an open problem. In Section 2 of this paper, we identify some graphs with maximum nullity with the use of the zero forcing number, a parameter that upper bounds the nullity of a graph, introduced in [1]. In Section 3, we study the relation between the non-zero part of a kernel eigenvector of a graph (core graph) and the zero forcing number as well as its vertex spread [4]. We conclude this paper with some alternative proofs concerning the maximum nullity of graphs using the above parameters.

2. Singular graphs for which $M(G) = Z(G)$

The problem of determining the maximum nullity of a simple graph has received much attention in the last years [5] and for several families of graphs, such as trees, this problem has been solved. By Proposition 2.4, it is obvious that the zero forcing number, $Z(G)$, is a useful tool in the maximum nullity problem, as it gives an upper bound to the maximum nullity of a graph. In this section, we identify certain singular graphs with maximum nullity, that is graphs for which $M(G) = Z(G)$.

We will be using the following definitions.

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Definition 2.1 Let the set of symmetric matrices over $\mathbb{R}$ be denoted by $\mathcal{S}_n(\mathbb{R})$. For such a matrix, the graph of A, $\mathcal{G}(A)$, is the graph with vertices $\{1,...,n\}$ and edges $\{\{i,j\} : a_{ij} \neq 0, 1 \leq i < j \leq n\}$. The maximum nullity of G is,

$$M(G) = max\,\{nullA : A \in \mathcal{S}(G)\},$$

where $\mathcal{S}(G)$, is the set of symmetric matrices, of G over $\mathbb{R}$, defined as

$$\mathcal{S}(G) = \{A \in \ \mathcal{S}_n(\mathbb{R}) : \mathcal{G}(A) = G\}.$$

Definition 2.2 Let, G, be a graph with each vertex colored either black or white.
Color change rule: If u is a black vertex of G and exactly one neighbor v of u is white, then change the color of v to black. We say u forces v and write $u \to v$.
Given a coloring of G, the *derived coloring* is the result of applying the color-change rule, until there are no more possible changes.
A *zero forcing set*, for a graph G, is a subset of vertices Z, such that, if initially the vertices in Z are colored black and the remaining vertices are colored white, the derived coloring of G is all black.
We define the *zero forcing number* of a graph G as the minimum $|Z|$, over all zero forcing sets $Z \subseteq V(G)$ and we denote it by $Z(G)$.
An *optimal zero forcing set* is a zero forcing set having the minimum number of elements.

For a given zero forcing set, a *chronological list of forces* is a list of forces in the order in which they are performed. An *optimal chronological list of forces* is a chronological list of forces of an optimal zero forcing set. A *forcing chain* (for a particular chronological list of forces) is a sequence of vertices $(u_1, u_2, ..., u_k)$, such that, for $\{i = 1, ..., k\}, u_i \longrightarrow u_{i+1}$ (u_i forces u_{i+1} to be colored black). A *maximal forcing chain* is a forcing chain that is not a proper subsequence of another zero forcing chain.

Definition 2.3 Let G be a graph, let Z be a zero forcing set, and let F be a chronological list of forces of Z. The *chain set* of F is the set of maximal forcing chains of F. An *optimal chain set* is a chain set from a chronological list of forces of an optimal zero forcing set.

Proposition 2.1 *[1] Let G be a graph, and let $Z \subseteq V$ be a zero forcing set. Then $M(G) \leq Z(G)$.*

We next present two examples of singular graphs that attain maximum nullity, by using the zero forcing number $Z(G)$. The *Tutte-Coxeter graph* (sometimes called Tutte's cage) is the (3, 8)-cage and is of order 30. It is vertex-transitive and 5-arc transitive. The Gray graph is a 3-regular graph on 54 vertices. It has been shown that the Gray graph is the unique smallest trivalent semi-symmetric graph.

Proposition 2.2 *For the Tutte-Coxeter graph $M(G) = Z(G)$.*

Proof. The characteristic polynomial of the graph is x^{10}(x-3)$(x-2)^9(x+2)^9$(x+3). It has a nullity of ten, and as shown, in Firure 1, $Z = \{1, 2, 3, 4, 5, 6, 11, 16, 29, 30\}$ is a zero forcing set for the Tutte-Coxeter graph. A list of forces, that occur chronologically, is described below.

$$1 \longrightarrow 10 \longrightarrow 9,\ 5 \longrightarrow 12 \longrightarrow 13, 2 \longrightarrow 15 \longrightarrow 14 \longrightarrow 27,$$

$$6 \longrightarrow 7 \longrightarrow 8 \longrightarrow 21,\ 3 \longrightarrow 20 \longrightarrow 19,\ 11 \longrightarrow 18 \longrightarrow 17 \longrightarrow 24,$$

$$4 \longrightarrow 25 \longrightarrow 26,\ 29 \longrightarrow 28,\ 30 \longrightarrow 23 \longrightarrow 22.$$

Since, $|Z|$=10 and $M(G) \leq Z(G)$, Z is an optimal zero forcing set. □

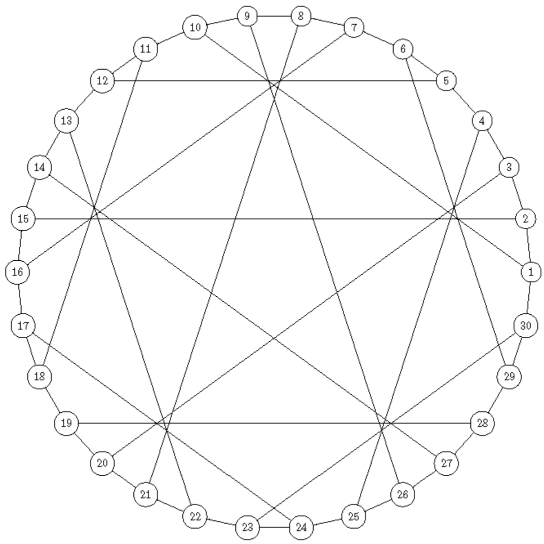

Figure 1: The Tutte-Coxeter graph

Proposition 2.3 *For the Gray graph $M(G) = Z(G)$.*

Proof. The characteristic polynomial of the Gray graph is x^{16}(x-3)(x+3)$(x^2-6)^6(x^2-3)^{12}$ and the graph has a nullity of sixteen. A zero forcing set for the Gray graph is

$$Z = \{1, 2, 3, 4, 7, 14, 23, 27, 28, 31, 34, 45, 48, 52, 53, 54\}.$$

A chronological list of forces is described below:

$$2 \longrightarrow 15 \longrightarrow 16 \longrightarrow 17, 3 \longrightarrow 44 \longrightarrow 43,$$
$$53 \longrightarrow 46 \longrightarrow 47 \longrightarrow 40, 45 \longrightarrow 32 \longrightarrow 33 \longrightarrow 20,$$
$$14 \longrightarrow 13, 27 \longrightarrow 26, 54 \longrightarrow 25 \longrightarrow 24 \longrightarrow 49 \longrightarrow 50.$$

Thus, $M(Z) = Z(G) = 16$. □

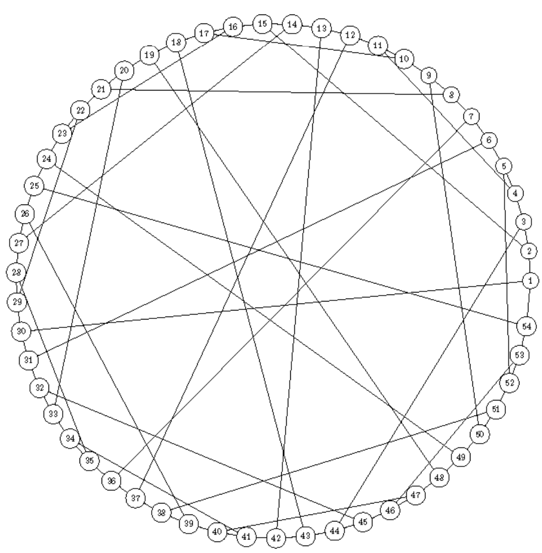

Figure 2: The Gray graph

3. Core graphs

One of the most important parts of a graph G is a graph's core, the subgraph of G, that is related to the non-zero part of the eigenvectors of G. In this section, we use the concept of vertex spread, another zero forcing parameter, that was introduced in [4], in order to examine core graphs, as well as the core of a graph. The importance of $M(G) = Z(G)$ is yet again obvious.

The *null spread* and the *zero spread* of a vertex u, defined in [4], are respectively:

Definition 3.1 Let $G = (V, E)$ be a graph, and $u \in V$. Then, $G - u$ is the induced subgraph of G, that is obtained on deleting u. We give the following definitions: The *null spread* and the *zero spread* of a vertex u, are respectively:

— $n_u(G) = M(G) - M(G - u)$

— $z_u(G) = Z(G) - Z(G - u)$.

Observation 3.1 According to the interlacing theorem, the nullity of a graph can change, at most by one, on deleting a vertex. Thus,

$$-1 \leq n_u(G) \leq 1.$$

Theorem 3.2 *[4] Let G be a graph and let u be a vertex of G. Then,*

$$-1 \leq z_u(G) \leq 1.$$

The proposition below, is the direct result of Proposition 2.4.

Proposition 3.1 *Let G be a graph, such that, $M(G) = Z(G)$, and let u be a vertex of G. Then,*
i. $n_u(G) \geq z_u(G)$.
ii. If $z_u(G) = 1$, then $n_u(G) = 1$.
iii. If $n_u(G) = -1$, then $z_u(G) = -1$.

Let us consider a graph G, of nullity one, with a kernel eigenvector $x = [x_1, x_2, ..., x_m, 0, ..., 0]^T$, where $x_i \neq 0, i = 1, 2, ..., m$. The subgraph F of G, induced by the first m vertices corresponding to the first m entries, is called the *core* of G [8]. The set of the remaining vertices, corresponding to the zero entries of the kernel eigenvector, is called the *periphery*.

Definition 3.2 Let x be a kernel eigenvector of a singular graph, on at least two vertices. If x has only non-zero entries, then G is referred to as a *core graph*.

Example 3.1 In Figure 3 and Figure 4, the core vertices are colored black. In Figure 3, the white vertex belongs to the periphery of the graph.

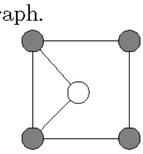

Figure 3: The core of a singular graph of nullity one

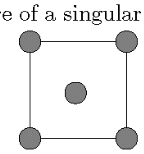

Figure 4: An example of a core graph

Theorem 3.3 *Let $G = (V, E)$ be a singular graph, on at least two vertices. Then G is a core graph, if and only if, $n_u(G) = 1, \forall u \in V$.*

Proof. Let G be a core graph of nullity $M(G)$, and $M(G)$ kernel eigenvectors. Let A' be the adjacency matrix of $G - u$, $u \in V$, where A can be written as

$$A = \begin{pmatrix} 0 & u \\ u^T & A' \end{pmatrix}.$$

Since u is a core vertex, we can insist that only one of the graph's kernel eigenvectors is not orthogonal to the unit vector $e_1 = (1, 0, ..., 0)^T$. The remaining, orthogonal to e_1 eigenvectors, $x_{M(G)-1}$, restricted to $G - u$, are kernel eigenvectors of $G - u$. Furthermore, if $G - u$ had more than $M(G) - 1$ kernel eigenvectors, the nullity of G would be more than $M(G)$. Thus, $M(G - u) = M(G) - 1$ and $n_u(G) = 1$. Let $n_u(G)$=1, $\forall u \in V$. Since, the nullity decreases on deleting the vertex u, it means there needs to be at least one kernel eigenvector not orthogonal to the unit vector e_u. Thus, u, $\forall u \in V$ is a core vertex. □

Theorem 3.4 *Let $G = (V, E)$ be a singular graph, such that, $M(G) = Z(G)$. If $z_u(G) = 1$, $\forall u \in V$, then G is a core graph.*

Proof. Let $z_u(G) = 1$, $\forall u \in V$. By Proposition 3.4, $n_u(G) = 1$, $\forall u \in V$, and thus by Theorem 3.7, G is a core graph. □

Proposition 3.2 *Let G be a graph, and $u \in V$ a vertex, such that, $M(G-u) = Z(G-u)$. If $z_u(G) \leq 0$, then u is not a core vertex.*

Proof. Let u be a core vertex of G. Then, on deleting u, the nullity decreases by one, as shown in Theorem 3.7. Since, $z_u(G) \leq 0$, it follows that $Z(G) \leq M(G) - 1$, a contradiction, since by Proposition 2.4, $M(G) \leq Z(G)$. □

4. Graphs with maximum nullity

We have defined the graphs of maximum nullity, as those for which:

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

Lemma 4.1 *Let G be a graph on n vertices. Then $Z(G) = n$, if and only if, G is a null graph.*

Proof. If G is a null graph, it is trivial. Let $Z(G) = n$. Then, we are not able to perform any color change, meaning that each vertex is an isolated vertex. □

Lemma 4.2 *Let G be a connected graph on n vertices. Then $Z(G) = n - 1$, if and only if, G is a complete graph.*

Proof. The sufficiency is clear. Let $Z(G) = n - 1$, and let us suppose that some vertex, u, of G is of degree less than $n - 1$, say k. If we choose u and all, except one, of its neighbours to be colored black, then we can perform exactly one color change and the black vertices of the graph are now $k + 1$. Let w be one of the k black vertices. Then, w can have at most $n - k - 1$ white neighbours. If we choose all, except one, of its neighbours (and the rest of the non adjacent to w vertices) to be colored black, then we can perform exactly one color change, and now the derived coloring is, all the graph vertices black. The set, consisting of the $k + (n - k - 2) = n - 2$ black vertices is a zero forcing set for G. Since $Z(G) = n - 1$ is the minimum forcing number, we derive a contradiction. □

Theorem 4.1 *A graph is of nullity n iff it is a null graph.*

Proof. Clearly, if G is a null graph, its nullity is its order. Let $M(G) = n$, then $Z(G) \geq M(G) = n$, so by Lemma 4.1, G is a null graph. □

Theorem 4.2 *There are no connected graphs of nullity $n - 1$.*

Proof. Let G be a graph, of nullity $n - 1$. Then, $Z(G) \geq M(G)$. If, $Z(G) = n - 1$, and G is connected, then by Lemma 4.2, G is a complete graph. It is well known that the complete graph has 2 distinct eigenvalues $n - 1$ and 1 with multiplicities 1 and $n - 1$, respectively. If $Z(G) = n$, then it is a null graph with nullity n. Thus, there are no connected graphs of nullity $n - 1$.

□

We complete this section by deriving some simple results on the nullity of certain extremal graphs.

Lemma 4.3 *[2] Suppose that G is a simple graph on at least n vertices and G has no isolated vertex. Then, $\eta(G) = n - 2$, if and only if, G is isomorphic to a complete bipartite graph K_{n_1,n_2}, where $n_1 + n_2 = n$, $n_1, n_2 > 0$.*

Corollary 4.1 *Let G be a simple connected graph on n vertices. Then, $M(G) = Z(G) = n - 2$, if and only if G is isomorphic to a complete bipartite graph K_{n_1,n_2}.*

Proof. The zero forcing number of K_{n_1,n_2} is $Z(K_{n_1,n_2}) = n - 2$, since if u is a black vertex of the first set of vertices in order to perform a color change only one vertex v of the second set of vertices must be white. As the same applies for v, $Z(K_{n_1,n_2}) = n - 2$. By Lemma 4.5, the proof is trivial.

Lemma 4.4 *[2] Suppose that G is a simple graph on at least n vertices and G has no isolated vertex. Then, $\eta(G) = n-3$, if and only if, G is isomorphic to a complete tripartite graph K_{n_1,n_2,n_3}, where $n_1 + n_2 + n_3 = n$, $n_1, n_2, n_3 > 0$.*

Corollary 4.2 *There are no connected graphs with $M(G) = Z(G) = n - 3$.*

Proof.
By Lemma 4.7 the complete tripartite graph is the only connected graph with $M(K_{n_1,n_2,n_3}) = n-3$. As it can be easily shown, the zero forcing number of the complete tripartite is $Z(K_{n_1,n_2,n_3}) = n - 2 > M(K_{n_1,n_2,n_3})$ (Figure 5).

□

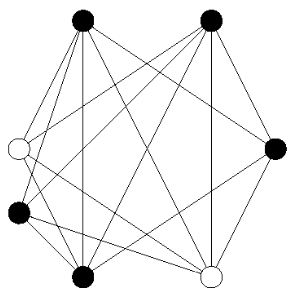

Figure 5: A zero forcing set for the complete tripartite $K_{2,2,3}$

5. Conclusion

This paper demonstrates the importance of the zero forcing parameters in relation to the graph's nullity. A singular graph achieves maximum nullity, when it reaches its zero forcing number and in this parer, we provide some examples of individual graphs, for which $M(G) = Z(G)$. A graph's core can, also, be examined by its vertex spread, in the case, where $M(G) = Z(G)$ holds. In the last section of this paper, we present some alternative proofs concerning the maximum nullity of graphs.

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