Note on positive semidefinite maximum nullity and positive semidefinite zero forcing number of partial 2-trees

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Abstract

The maximum positive semidefinite nullity of a multigraph G is the largest possible nullity over all real positive semidefinite matrices whose ijth entry (for $i \neq j$) is nonzero whenever $\{i, j\}$ is a single edge in G and is zero if i and j are not adjacent. The definition of the positive semidefinite zero forcing number for simple graphs in [1] is extended to multigraphs; as for simple graphs, this parameter bounds the maximum nullity from above. The tree cover number $\mathrm{T}(G)$ is the minimum number of vertex disjoint induced simple trees that cover all of the vertices of G. The result in [2] that $\mathrm{M}_+(G) = \mathrm{T}(G)$ for an outerplanar multigraph G is extended to show that $\mathrm{Z}_+(G) = \mathrm{M}_+(G) = \mathrm{T}(G)$ for a multigraph G of tree-width at most 2.

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1 Introduction

The standard minimum rank (maximum nullity) problem for a simple graph G is to determine the smallest possible rank (largest possible nullity) over all real symmetric matrices described by the graph ($A = [a_{ij}]$ is described by G if for $i \neq j$, a_{ij} is nonzero whenever $\{i, j\}$ is an edge in G and is zero otherwise). The minimum rank problem and maximum nullity problem are equivalent. More generally, one can consider the minimum rank or maximum nullity of matrices that are described by a graph and that satisfy additional conditions, yielding variants on the standard problem, such as the problem of determining the minimum positive semidefinite rank (maximum positive semidefinite nullity) of a graph. The positive semidefinite zero forcing number, introduced in [1], can be determined by software [5], and assists in the computation of positive semidefinite maximum nullity, just as the zero forcing number helps determine maximum nullity.

Although our main interest is in simple graphs, van der Holst and others have used multigraphs as a tool to describe the effect of matrix operations on the nonzero structure that is described by a simple graph, and we follow that approach here. In Section 2 we introduce the positive semidefinite zero forcing number for a multigraph and show that it is an upper bound for maximum positive semidefinite nullity. We also provide precise definitions of terms we will use, including graph

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terminology and orthogonal representations. In Section 3 we prove that for a multigraph (or simple graph) of tree-width at most two, the positive semidefinite zero forcing number is equal to the maximum positive semidefinite nullity. We also observe that the proof of Theorem 3.4 in [2] establishes that maximum positive semidefinite nullity is equal to tree cover number for a graph of tree-width at most two, extending that result from outerplanar graphs.

2 Multigraphs

Every graph discussed is undirected, finite (meaning both the vertex set and edge set are finite), and has nonempty vertex set. In a *simple graph* $G = (V, E)$, the edge set E is a set of two-element subsets of vertices. In a *general graph* $G = (V, E)$, the edge set E is a multiset of two-element submultisets of vertices. A *multigraph* $G = (V, E)$ is a general graph in which E is a multiset of two-element subsets of vertices. That is, in a multigraph multiple copies of an edge $\{v, w\}$ are permitted, but a loop $\{v, v\}$ is not. In a multigraph, a *multiple edge*, denoted by $v \approx w$, is an edge that appears more than once in E; a *single edge*, denoted by $v \sim w$, is an edge that appears exactly once in E. The vertices v and w are *adjacent* if $v \sim w$ or $v \approx w$.

In a multigraph, w is a *neighbor* of v if v and w are adjacent; the set of neighbors of v is denoted by $N(v)$. The *degree* of vertex v in G is $d_G(v) = |N(v)|$ (note this may be less than the number of edges incident with v). For a multigraph $G = (V, E)$ and $W \subseteq V$, the *induced submultigraph* $G[W]$ is the multigraph with vertex set W and edge set consisting of those edges in E having both vertices in W. The subgraph induced by $V \setminus W$ is usually denoted by $G - W$, or in the case $W = \{v\}$, by $G - v$. The *contraction* of edge e between u and v, denoted by G/e, is obtained by identifying the vertices u and v, deleting any loops that arise in the process.

Van der Holst [7, 8] and others, e.g., [2, 3], use a multiple edge in a multigraph to indicate a completely free entry when describing symmetric matrices. More precisely, if G is a multigraph of order n, then $\mathcal{S}_+(G)$ is the set of all positive semidefinite $n \times n$ real matrices $A = [a_{ij}]$ satisfying

1. $a_{ij} = 0$ if $i \neq j$ and i and j are not adjacent,
2. $a_{ij} \neq 0$ if $i \neq j$ and $i \sim j$, and
3. $a_{ij} \in \mathbb{R}$ if $i = j$, or $i \neq j$ and $i \approx j$.

The positive semidefinite maximum nullity of a multigraph G is

$$\mathrm{M}_+(G) = \max\{\operatorname{null} A \,|\, A \in \mathcal{S}_+(G)\}.$$

Multigraphs are useful even when the focus is on simple graphs; see, for example, [3].

Maximum positive semidefinite nullity over complex (Hermitian) positive semidefinite matrices described by G, denoted $\mathrm{M}_+^{\mathbb{C}}(G)$, has also been defined and studied, e.g., [7, 3, 6, 9]. Although in general maximum complex positive semidefinite nullity can be strictly greater than maximum real positive semidefinite nullity [1], it is a consequence of Theorem 3.2 below that maximum complex positive semidefinite nullity is equal to maximum real positive semidefinite nullity for multigraphs of tree-width at most 2 (see also [2] for more discussion of this issue). Following the approach taken in [2], we focus on real matrices, but note in some cases where the results apply to complex matrices.

2.1 The positive semidefinite zero forcing number

In a simple graph $G = (V, E)$ where the vertices in a set $S \subseteq V$ are colored black and the remaining vertices are colored white, the *positive semidefinite color change rule* is: If $W_1, \ldots, W_k$ are the sets of vertices of the k components of $G - S$ (note that it is possible that $k = 1$), $w \in W_i$, $u \in S$, and w is the only white neighbor of u in $G[W_i \cup S]$, then change the color of w to black; in this case, we say u *forces* w and write $u \to w$. A *positive semidefinite zero forcing set* is a set of black vertices B such that repeated application of the color change rule changes all the vertices of G to black. The *positive semidefinite zero forcing number of a graph* G, denoted $\mathrm{Z}_+(G)$, is the minimum of $|B|$ over all positive semidefinite zero forcing sets $B \subseteq V$. It is shown in [1] that for every simple graph G, $\mathrm{M}_+(G) \le \mathrm{Z}_+(G)$.

The definition of $\mathcal{S}_+(G)$ for a multigraph G suggests the following definition of the positive semidefinite zero forcing number of a multigraph.

Definition 2.1. The *positive semidefinite zero forcing number of a multigraph* $G = (V, E)$, denoted by $\mathrm{Z}_+(G)$, is the minimum of $|B|$ over all positive semidefinite zero forcing sets $B \subseteq V$ using the *positive semidefinite color change rule for multigraphs*: Let S be the set consisting of all the black vertices. Let $W_1, \ldots, W_k$ be the sets of vertices of the k components of $G - S$ (note that it is possible that $k = 1$). Let $w \in W_i$. If $u \in S$, w is the only white neighbor of u in $G[W_i \cup S]$, and w is joined to u by a single edge, then change the color of w to black.

The proof of the following theorem is very similar to the proof of Theorem 3.5 in [1].

Theorem 2.2. *If G is a multigraph, then* $\mathrm{M}_+(G) \le \mathrm{Z}_+(G)$.

As in [1], Theorem 2.2 remains true if $\mathrm{M}_+(G)$ is replaced by $\mathrm{M}_+^{\mathbb{C}}(G)$, where $\mathrm{M}_+^{\mathbb{C}}(G)$ is the maximum nullity over complex Hermitian positive semidefinite matrices described by G.

2.2 Orthogonal representations

Let $G = (V, E)$ be a multigraph of order n. We say that $\vec{V} = \{\vec{v}_1, \ldots, \vec{v}_n\} \subset \mathbb{R}^d$ is an *orthogonal representation* of G if $\langle \vec{v}_i, \vec{v}_j \rangle = 0$ whenever i and j are not adjacent and $\langle \vec{v}_i, \vec{v}_j \rangle \ne 0$ whenever $i \sim j$. Note that there is no restriction on $\langle \vec{v}_i, \vec{v}_j \rangle$ when $i \approx j$. Then letting $C = [\vec{v}_1 \ldots \vec{v}_n]$, the Gram matrix of $\vec{V}$ is $C^T C = [a_{ij}]$ where $a_{ij} = \vec{v}_i^{\,T} \vec{v}_j = \langle \vec{v}_j, \vec{v}_i \rangle$. It is easy to see that $C^T C \in \mathcal{S}_+(G)$ with $\operatorname{rank} C^T C = \operatorname{rank} C \le d$. Furthermore, for each $A \in \mathcal{S}_+(G)$, $A = C^T C$ for some matrix $C \in \mathbb{R}^{d \times n}$ where $d = \operatorname{rank} C = \operatorname{rank} A$. The columns of C form an orthogonal representation of G since if $A = [a_{ij}]$, $a_{ij} = \vec{c}_i^{\,T} \vec{c}_j = \langle \vec{c}_j, \vec{c}_i \rangle$ where $\vec{c}_i$ represents the ith column of C. Orthogonal representations can also be used for complex (Hermitian) positive semidefinite matrices, replacing the transpose by the Hermitian adjoint.

Let $\vec{V}$ be an orthogonal representation of $G = (V, E)$ with $\vec{v} \in \vec{V}$ representing $v \in V$. We define the orthogonal removal of $\vec{v}$ from $\vec{V}$ by $\vec{V} \ominus \vec{v} = \{\vec{u}'\}_{\vec{u} \ne \vec{v}}$ where

$$\vec{u}' = \vec{u} - \frac{\langle \vec{u}, \vec{v} \rangle}{\langle \vec{v}, \vec{v} \rangle} \vec{v}.$$

By considering $\vec{V}$ expressed in an orthogonal basis for $\mathbb{F}^d$ with $\vec{v}$ as one of the basis vectors, it is easy to see that $\operatorname{rank}(\vec{V} \ominus v) = \operatorname{rank} \vec{V} - 1$.

Define the orthogonal removal of v from G by starting with $G - v$ and, for every distinct $u, w \in N(v)$, letting u and w be connected by $|E(G[\{u, v, w\}])| - 1$ edges in the new graph (where $E(H)$ represents the edges of a multigraph H.) We denote this new graph by $G \ominus v$. To justify this double use of the symbol $\ominus$, we have the following observation, noted in [6]:

Observation 2.3. *Let $G = (V, E)$ be a multigraph of order at least 2. If $\vec{V}$ is an orthogonal representation of G with $\vec{v} \in \vec{V}$ representing $v \in V$, then $\vec{V} \ominus \vec{v}$ is an orthogonal representation for $G \ominus v$.*

2.3 Tree-width

For a positive integer k, a *simple k-tree* is constructed inductively by starting with a complete simple graph on $k+1$ vertices and singly connecting each new vertex to the vertices of an existing clique on k vertices. A *partial simple k-tree* is a subgraph of a simple k-tree. The *tree-width* $\operatorname{tw}(G)$ of a simple graph G is the least positive integer k such that G is a partial simple k-tree.

The *underlying simple graph* of a multigraph is obtained by replacing each multiple edge by a single edge. We apply terms for simple graphs to multigraphs by means of the underlying simple graph. For example, a multigraph is a (partial) k-tree if its underlying simple graph is a simple (partial) k-tree.

The proof of Theorem 3.4 in [2] uses certain properties of outerplanar graphs. These properties remain true for partial 2-trees and are stated in the following four lemmas that will be used in the proof of Theorem 3.2 below. Lemmas 2.4, 2.5, and 2.6 are well known for simple graphs and their extension to multigraphs is clear.

Lemma 2.4. *If the multigraph $G = (V, E)$ is a partial k-tree, then there exists a vertex $v \in V$ such that $d_G(v) \leq k$.*

Lemma 2.5. *If the multigraph $G = (V, E)$ is a partial k-tree and $v \in V$, then $G - v$ is a partial k-tree.*

Lemma 2.6. *If the multigraph $G = (V, E)$ is a partial k-tree and $e \in E$, then G/e is a partial k-tree.*

Lemma 2.7. *Suppose the multigraph $G = (V, E)$ is a partial 2-tree, $v \in V$ and $d_G(v) \leq 2$. Then $G \ominus v$ is a partial 2-tree.*

Proof. If $d_G(v) = 1$, $G \ominus v = G - v$. So assume $d_G(v) = 2$ and $N(v) = \{u, w\}$. If $u \sim w$ in G, then $G \ominus v$ is obtained from the partial 2-tree $G - v$ by adding extra edges to edge $\{u, w\}$, so $G \ominus v$ is a partial 2-tree. If u and w are not adjacent, then $G \ominus v$ can be obtained from G by an edge contraction and possibly adding extra multiple edges, so $G \ominus v$ is a partial 2-tree. ☐

2.4 Tree cover number

First introduced in [2], the *tree cover number* of a multigraph G, denoted $\mathrm{T}(G)$, is the minimum number of vertex disjoint induced simple trees that cover the vertices of G. If T is a simple tree, then $\mathrm{M}_+(T) = 1$ [8], so for simple trees M_+ and T are equal. Recently Barioli et al [2] established the equality of T and M_+ for outerplanar multigraphs, and the proof remains valid for multigraphs of tree-width at most 2 (see Theorem 3.2 below).

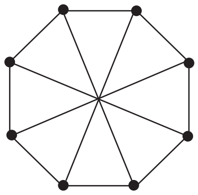

Figure 1: The Möbius ladder ML_8, also known as V_8

For the Möbius ladder $ML_8 = V_8$ shown in Figure 1, $\mathrm{Z}_+(ML_8) = 4 > \mathrm{M}_+(ML_8) = 3 > \mathrm{T}(ML_8) = 2$. The parameter values have been previously established: $\mathrm{T}(ML_8) = 2$ in [2] and

$\mathrm{M}_+(ML_8) = 3$ in [9]. Using the simple graph parameter ordered set number $OS(G)$, defined in [9], and the result that for a simple graph G, $OS(G) + \mathrm{Z}_+(G) = |G|$ [1], results in [9] imply $\mathrm{Z}_+(ML_8) = 4$ (this can also be established through the use of software [5]).

3 Graphs of tree-width at most 2

It is well known that if T is a (simple) tree, $\mathrm{M}_+(T) = \mathrm{Z}_+(T) = \mathrm{T}(T) = 1$. Since all three parameters sum over connected components, $\mathrm{M}_+(T) = \mathrm{Z}_+(T) = \mathrm{T}(T)$ for any (simple) forest (i.e., partial 1-tree). It is also easy to see that these parameters are equal for a multigraph tree or forest. We show that $\mathrm{M}_+(G) = \mathrm{Z}_+(G) = \mathrm{T}(G)$ for any multigraph G that is a partial 2-tree. Note that the proof of Theorem 3.4 in [2], although stated for outerplanar graphs, actually shows that $\mathrm{M}_+(G) = \mathrm{T}(G)$ for any partial 2-tree.

A vertex v of a multigraph G is *singly-isolated* if $v \approx w$ for all $w \in N(v)$. If v is singly-isolated in G then

$$\begin{aligned} \mathrm{T}(G - v) &= \mathrm{T}(G) - 1; \quad (1)\\ \mathrm{M}_+(G - v) &= \mathrm{M}_+(G) - 1; \quad (2)\\ \mathrm{Z}_+(G - v) &= \mathrm{Z}_+(G) - 1. \quad (3) \end{aligned}$$

Equations (1) and (2) appear in [2], and (3) is equally straightforward, because v must appear in any positive semidefinite zero forcing set for G and cannot perform a force.

It is shown in [2] that if G is a multigraph, v is not singly-isolated in G, and $d_G(v) \le 2$, then

$$\begin{aligned} \mathrm{T}(G \ominus v) &= \mathrm{T}(G); \quad (4)\\ \mathrm{M}_+(G \ominus v) &= \mathrm{M}_+(G). \quad (5) \end{aligned}$$

These results play a crucial role in the proof of the equality of tree cover number and maximum positive semidefinite nullity for outerplanar graphs [2, Theorem 3.4], and we prove a comparable result for positive semidefinite zero forcing number.

Proposition 3.1. *Let G be a multigraph. Let v be a vertex of G such that v is not singly-isolated and $d_G(v) \le 2$. Then*

$$\mathrm{Z}_+(G \ominus v) = \mathrm{Z}_+(G). \tag{6}$$

Proof. Since v is not singly-isolated, $d_G(v) \ge 1$. First assume $d_G(v) = 1$, and let $N(v) = \{u\}$. Since v is not singly-isolated, $v \sim u$. Then $G \ominus v = G - v$. Any positive semidefinite zero forcing set for $G - v$ is a positive semidefinite zero forcing set for G, so $\mathrm{Z}_+(G \ominus v) \ge \mathrm{Z}_+(G)$. A minimum positive semidefinite zero forcing set B for G cannot include both v and u. If $v \notin B$, then B is a positive semidefinite zero forcing set for $G - v$. If $v \in B$, then $B \setminus \{v\} \cup \{u\}$ is a positive semidefinite zero forcing set for $G - v$. Thus $\mathrm{Z}_+(G \ominus v) \le \mathrm{Z}_+(G)$.

Now assume $d_G(v) = 2$, and let $N(v) = \{u, w\}$. Since v is not singly-isolated, without loss of generality we assume that $v \sim u$.

We show first that $\mathrm{Z}_+(G \ominus v) \ge \mathrm{Z}_+(G)$ by showing that any positive semidefinite zero forcing set B for $G \ominus v$ is a positive semidefinite zero forcing set for G. If $u \not\to w$ and $w \not\to u$ in $G \ominus v$, then B is a positive semidefinite zero forcing set for G with the same sequence of forces and the additional force $u \to v$ at the end. If $u \to w$ (or $w \to u$) in $G \ominus v$, then $u \sim w$ in $G \ominus v$, so in G, u and w are not adjacent and $v \sim w$. Thus we can replace any force $u \to w$ (or $w \to u$) in $G \ominus v$ by the forces $u \to v \to w$ (or $w \to v \to u$) in G.

Finally we show that $\mathrm{Z}_+(G \ominus v) \le \mathrm{Z}_+(G)$. Let B be a minimum positive semidefinite zero forcing set for G. If $v \notin B$, then B is a positive semidefinite zero forcing set for $G \ominus v$ (in the case

u and w are not adjacent and $v \sim w$ in G, if the forces $u \to v \to w$ occur, replace by the force $u \to w$). Now assume $v \in B$. Then u and w cannot both be in B. If one of u, w is in B, let x denote that vertex. If neither u nor w is in B, let x denote the one of u, w that is forced first. Let y denote the one of u, w that is not x. Then $B \setminus \{v\} \cup \{y\}$ is a positive semidefinite zero forcing set for $G \ominus v$. □

Theorem 3.2. *Let multigraph G be a partial 2-tree. Then* $\mathrm{M}_+(G) = \mathrm{Z}_+(G) = \mathrm{T}(G)$.

Proof. We prove by induction on the order of G that $\mathrm{M}_+(G) = \mathrm{Z}_+(G) = \mathrm{T}(G)$. When $|G| = 1$, the result is clear. Assume that $\mathrm{M}_+(H) = \mathrm{Z}_+(H) = \mathrm{T}(H)$ for every partial 2-tree H of order less than n, and let $|G| = n$. Then G has a vertex v with $d_G(v) \leq 2$ by Lemma 2.4.

Suppose first that v is singly-isolated. Then $G - v$ is a partial 2-tree by Lemma 2.5 and

$$\mathrm{T}(G) = \mathrm{T}(G - v) + 1, \qquad \mathrm{M}_+(G) = \mathrm{M}_+(G - v) + 1, \qquad \mathrm{Z}_+(G) = \mathrm{Z}_+(G - v) + 1$$

by equations (1), (2), and (3). By the induction hypothesis, $\mathrm{M}_+(G - v) = \mathrm{Z}_+(G - v) = \mathrm{T}(G - v)$ so

$$\mathrm{M}_+(G) = \mathrm{Z}_+(G) = \mathrm{T}(G).$$

Now suppose that v is not singly-isolated. Then by applying equations (4), (5), and (6),

$$\mathrm{T}(G) = \mathrm{T}(G \ominus v), \qquad \mathrm{M}_+(G) = \mathrm{M}_+(G \ominus v), \qquad \mathrm{Z}_+(G) = \mathrm{Z}_+(G \ominus v).$$

By Lemma 2.7, $G \ominus v$ is a partial 2-tree, and thus by the induction hypothesis,

$$\mathrm{M}_+(G \ominus v) = \mathrm{Z}_+(G \ominus v) = \mathrm{T}(G \ominus v).$$

Thus

$$\mathrm{M}_+(G) = \mathrm{Z}_+(G) = \mathrm{T}(G).$$

□

Since any simple graph is a multigraph, and since for each of the parameters in Theorem 3.2 the value of the multigraph parameter on a simple graph is equal to the value of the analogous parameter defined for simple graphs, we have the same result for simple graphs.

Corollary 3.3. *If the simple graph G is a partial 2-tree, then* $\mathrm{M}_+(G) = \mathrm{Z}_+(G) = \mathrm{T}(G)$.

Every outerplanar simple graph is a partial 2-tree, because G is a partial 2-tree if and only if G does not have a K_4 minor [4, Fact 31, p. 112] and G is outerplanar if and only if G has neither a K_4 minor nor a $K_{2,3}$ minor [4, Fact 32, p. 112]. Thus Corollary 3.3 shows that if G is outerplanar, then $\mathrm{M}_+(G) = \mathrm{Z}_+(G)$ ($\mathrm{M}_+(G) = \mathrm{T}(G)$ was established in [2]).

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