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# Strong structural controllability of networks: Comparison of bounds using distances and zero forcing\*



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#### ARTICLE INFO

# Article history: Received 9 April 2021 Received in revised form 25 May 2022 Accepted 22 June 2022 Available online 17 September 2022

Keywords: Control of networks Controllability Graph theory

#### ABSTRACT

We study the strong structural controllability (SSC) of networks, where the external control inputs are injected to only some nodes, namely the leaders. For such systems, one measure of controllability is the dimension of strong structurally controllable subspace (SSCS), which is equal to the smallest possible rank of controllability matrix under admissible coupling weights among the nodes In this paper, we compare two tight lower bounds on the dimension of SSCS: one based on the distances of followers to leaders, and the other based on the graph coloring process known as zero forcing. We first show that each of these two bounds can be arbitrarily better than the other in some special cases. We then show that the distance-based lower bound is usually better than the zero-forcing-based bound when the value of the latter is less than the dimensionality of the overall network state, n. On the other hand, we also show that any set of leaders that makes the distance-based bound equal to n necessarily makes the zero-forcing-based bound equal to n (the converse is not true). These results indicate that while the zero-forcing-based approach may be preferable when the focus is only on verifying complete SSC (dimension of SSCS is equal to n), the distance-based approach usually yields a closer bound on the dimension of SSCS when the bounds are both smaller than n. Furthermore, we also present a novel bound based on combining these two approaches, which is always at least as good as, and in some cases strictly greater than, the maximum of the two original bounds. Finally, we support our analysis with numerical results on various graphs.

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# 1. Introduction

Networks where each node's state is linearly influenced by its neighbors' states appear in numerous systems such as sensor networks, distributed robotics, power grids, social networks, and biological systems. Such systems are often modeled using their interaction graphs where the nodes represent the agents, and the weighted edges denote the couplings among agents. One major research question regarding such systems is whether a desired global behavior can be induced by injecting external inputs to only some agents, so-called leaders. This question has motivated numerous studies on relating *network controllability* to the structure of the interaction graph.

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Notions of network controllability can be broadly grouped into three categories based on how they treat the coupling weights among agents: (1) controllability under specific weights, (2) structural controllability under a set of admissible weights, (3) strong structural controllability under a set of admissible weights. The latter two approaches are motivated by the uncertainty in the coupling weights of networks in real life, i.e., the weights belong to some feasible set but their exact values are unknown. Such a network is structurally controllable if there exist admissible weights that make the system controllable. Furthermore, the network is strong structurally controllable if it is controllable under any admissible allocation of weights. In such cases, the admissible weights may be arbitrary non-zero values (e.g., Chapman & Mesbahi, 2013; Liu, Slotine, & Barabási, 2011; Monshizadeh, Camlibel, & Trentelman, 2015; Monshizadeh, Zhang, & Camlibel, 2014; Mousavi, Haeri, & Mesbahi, 2018; Trefois & Delvenne, 2015; Work et al., 2008) or may need to satisfy additional constraints (e.g., Li, Chen, Pequito, Pappas, & Preciado, 2020; Mousavi, Haeri, & Mesbahi, 2019; Van Waarde, Camlibel, & Trentelman, 2017; Yazıcıoğlu, Abbas, & Egerstedt, 2016). Studies on structural or

This paper was recommended for publication in revised form by Associate Editor Julien M. Hendrickx under the direction of Editor Christos G. Cassandras.

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strong structural controllability also have some extensions to networks with time-varying dynamics (e.g., Liu, Lin, & Chen, 2013; Mousavi, Haeri, & Mesbahi, 2020; Srighakollapu, Kalaimani, & Pasumarthy, 2021). Various graph-theoretic tools have been utilized to provide topology-based characterizations of network controllability. Examples include equitable partitions (e.g., Rahmani, Ji, Mesbahi, & Egerstedt, 2009), maximum matchings (e.g., Chapman & Mesbahi, 2013; Liu et al., 2011), centrality based measures (e.g., Liu, Slotine, & Barabási, 2012; Pan & Li, 2014), dominating sets (e.g., Nacher & Akutsu, 2014), distances (e.g., Van Waarde et al., 2017; Yazıcıoğlu et al., 2016; Zhang, Cao, & Camlibel, 2013), and zero forcing (e.g., Jia, Trentelman, Baar, & Camlibel, 2019: Monshizadeh et al., 2015, 2014: Mousavi et al., 2018: Trefois & Delvenne, 2015; Work et al., 2008). Studies on network controllability have several important applications such as selecting a minimal set of leaders (e.g., Clark, Alomair, Bushnell, & Poovendran, 2017; Pasqualetti, Zampieri, & Bullo, 2014; Summers, Cortesi, & Lygeros, 2015; Tzoumas, Rahimian, Pappas, & Jadbabaie, 2015) or designing/modifying the network topology to achieve/maintain a desired level of controllability (e.g., Abbas, Shabbir, Yazıcıoğlu, & Koutsoukos, 2021; de Badyn & Mesbahi, 2016; Yazıcıoğlu & Egerstedt, 2013).

In this paper, we focus on the strong structural controllability (SSC) of networks. More specifically, we consider the dimension of strong structurally controllable subspace (SSCS), i.e., the minimum possible rank of controllability matrix under admissible coupling weights among the nodes, as the measure of controllability. The exact computation of the dimension of SSCS is a challenging problem that involves finding the minimum rank of matrices with a given zero-nonzero or sign pattern, i.e., matrices whose specific entries are zero and the remaining non-zero entries can take any feasible value (e.g., Fallat & Hogben, 2007; Fazel, Hindi, & Boyd, 2004; Mousavi et al., 2019). Motivated by the intractability of exact computation, two graph-theoretic concepts have been utilized in the literature to yield a tight lower bound on this controllability measure: distances and zero forcing. While the zero-forcing-based bound is applicable to networks with arbitrary linear dynamics, the distance-based bound is applicable to an important subfamily which contains widely studied cases such as diffusively coupled networks (e.g., weighted Laplacian/adjacency dynamics) among others. In this paper, we focus on such systems where both lower bounds are applicable. In the distance-based approach, the lengths of the shortest paths from the leaders to the followers are used to obtain a lower bound on the dimension of SSCS. On the other hand, the zeroforcing-based approach is based on a graph coloring process (zero forcing process), where each node is initially colored black if it is a leader and colored white if it is a follower. Starting with this initial coloring, any white node becomes black if it is the only white out-neighbor of a black node. This color changing rule is applied until no further color changes are possible and the resulting number of black nodes yields a lower bound on the dimension of SSCS. In this paper, we first compare these two approaches. Our comparative results indicate that while the zero-forcing-based approach is better for verifying complete SSC (i.e., whether the controllability matrix has full rank under any admissible weighting of the edges), the distance-based approach is usually more informative when the leaders do not constitute a zero forcing set, i.e., the zero forcing process starting with only the leaders colored black do not make all the nodes black. We also propose a novel bound based on the combination of these two methods, which is always at least as good as, and in some cases greater than, the maximum of the two original bounds. Finally, we support our analysis with some numerical results. Some preliminary results of this paper were presented in (Yazıcıoğlu, Shabbir, Abbas, & Koutsoukos, 2020). The main contributions of this paper are as follows:

- (1) We first show that there exist networks where the distance-based bound and the zero-forcing-based bound can significantly outperform each other (Theorem 3), motivating the comparative analysis in this paper.
- (2) We characterize some generic cases where the distance-based bound is guaranteed to outperform the zero-forcing-based bound. In particular, the distance-based approach yields a better bound for networks where each leader has multiple followers as out-neighbors (Theorem 5) and for most networks with a single leader (Theorem 6).
- (3) We show that the zero-forcing-based approach is a better option when focusing only on complete SSC. In particular, we show that the distance-based bound can indicate complete SSC only if the zero-forcing-based bound also indicates complete SSC, i.e., the leader set is a zero forcing set (Theorem 7). We also show that the inverse is not true (e.g., see Fig. 5a).
- (4) We derive a novel lower bound on the dimension of SSCS by combining the distance-based and zero-forcing-based methods. We show that this new bound is always at least as good as (Theorem 8), and in some cases strictly greater than (e.g., see Fig. 6), the original bounds. We show that the combined bound outperforms the zero-forcing-based bound on any strongly connected graph unless the leader set is a zero forcing set (Theorem 11), equals the distance-based bound on most single-leader networks (Theorem 12), and outperforms the distance-based bound if the zero forcing process can infect multiple nodes with identical distances to the leaders (Theorem 13).
- (5) We compare the three bounds numerically for various randomly generated networks and leader sets.

The organization of this paper is as follows: Section 2 provides some preliminaries. Section 3 presents our results regarding the comparison of the distance-based and zero-forcing-based bounds. Section 4 provides a novel bound based on the combination of these two previous methods. Some numerical results are given in Section 5. Finally, Section 6 concludes the paper.

#### 2. Preliminaries

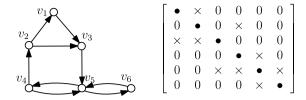
### 2.1. Graph basics

We consider a network represented by a simple directed graph G = (V, E) where the node set  $V = \{v_1, v_2, \ldots, v_n\}$  represent agents, and the edge set E represents interconnections between agents. An edge from a node  $v_i \in V$  to a node  $v_j \in V$  is denoted by  $e_{ij} = (v_i, v_j)$ . The out-neighborhood of node  $v_i$  is  $\mathcal{N}_i^{out} \triangleq \{v_j \in V : e_{ij} \in E\}$ . The in-neighborhood of node  $v_i$  is  $\mathcal{N}_i^{in} \triangleq \{v_j \in V : e_{ji} \in E\}$ . The distance  $d(v_i, v_j)$ , is the number of edges on the shortest path from  $v_i$  to  $v_j$ . Accordingly,  $d(v_i, v_i) = 0$  and  $d(v_i, v_j) = \infty$  if there is no path from  $v_i$  to  $v_j$ . The graph is strongly connected if there is a path from any node to any other node.

# 2.2. System model

For the sake of simplicity, let each agent  $v_i \in V$  have a scalar state  $x_i \in \mathbb{R}$ . The overall state of the system is x = 1

<sup>&</sup>lt;sup>1</sup> The model and our results can easily be extended to agents with higher-dimensional states, where the vector of states in each dimension k, say  $x^k = \begin{bmatrix} x_1^k & x_2^k & \cdots & x_n^k \end{bmatrix}^T \in \mathbb{R}^n$ , evolves under  $\dot{x}^k = Ax^k + Bu^k$  with  $u^k = [u_1^k, \dots, u_m^k]$ .



**Fig. 1.** A graph G=(V,E) and the corresponding structure satisfied by any  $A\in\mathcal{A}(G)$ . The entries marked as  $\times$  are non-zero and the entries on the diagonal can take any value.

 $\begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix}^T \in \mathbb{R}^n$ . The states evolve under the following dynamics:

$$\dot{x} = Ax + Bu. \tag{1}$$

Here, the matrix  $B \in \mathbb{R}^{n \times m}$  is the *input matrix*, where m is the number of leaders, i.e., the nodes to which an external control signal is applied. Let  $V_{\ell} = \{\ell_1, \ell_2, \dots, \ell_m\} \subseteq V$  be the set of *leaders*, then

$$B_{ij} = \begin{cases} 1 & \text{if } v_i = \ell_j, \\ 0 & \text{otherwise.} \end{cases}$$
 (2)

Furthermore, the state matrix A is restricted by the structure of the graph G = (V, E). Typically, each node is directly influenced only by its in-neighbors. As such, any off-diagonal term  $A_{ij}$  is non-zero if and only if there is an edge from  $v_i$  to  $v_i$ , i.e., A belongs to

$$\mathcal{A}(G) = \{ A \in \mathbb{R}^{n \times n} \mid \text{for } i \neq j, A_{ij} \neq 0 \Leftrightarrow e_{ji} \in E \},$$
 (3)

which is called the *qualitative class* of the graph G = (V, E) (Monshizadeh et al., 2014; Trefois & Delvenne, 2015). Accordingly, each  $A_{ij}$  denotes the weight of  $e_{ji}$  and the edges in G define the *structure*—location of zero and non-zero off-diagonal entries—for any  $A \in \mathcal{A}(G)$ , for instance, see Fig. 1.

# 2.3. Strong structural controllability (SSC)

Controllability of the networked system in (1), where the input matrix B is determined by the leaders  $V_{\ell} \subseteq V$  as in (2), can be checked via the *controllability matrix*, i.e.,

$$\Gamma(A, V_{\ell}) = \begin{bmatrix} B & AB & A^2B & \cdots & A^{n-1}B \end{bmatrix}. \tag{4}$$

The network is completely controllable if and only if the rank of  $\Gamma(A, V_\ell)$  is n. In that case, (A, B) is called a *controllable pair* and the system in (1) can be driven from any initial state to any desired state in finite time via a properly designed u. A network G = (V, E) with  $V_\ell$  leaders is *strong structurally controllable* if (A, B) is a controllable pair for any feasible A. In that case, the *dimension of strong structurally controllable subspace (SSCS)*, i.e., the smallest possible rank of  $\Gamma(A, V_\ell)$  under feasible values of A, is equal to n. In this paper, we will focus on cases where A belongs to the set of *distance-information preserving matrices*, which is a subset of A(G) in (3):

$$\mathcal{A}_d(G) = \{ A \in \mathcal{A} \mid [A^{d(v_j, v_i)}]_{ij} \neq 0, \forall v_i, v_j \in V : d(v_j, v_i) < \infty \}, \quad (5)$$

where  $[A^{d(v_j,v_i)}]_{ij}$  is the  $(i,j)^{th}$  entry in the  $d(v_j,v_i)^{th}$  power of A. Although  $\mathcal{A}_d(G)$  is more restrictive than  $\mathcal{A}(G)$  as per (5), it is an important and rich subset of  $\mathcal{A}(G)$ . For example, the widely studied weighted Laplacian/adjacency matrices are contained in  $\mathcal{A}_d(G)$  (e.g., see Van Waarde et al., 2017; Yazıcıoğlu et al., 2016). In fact, any  $A \in \mathcal{A}(G)$  is also contained in  $\mathcal{A}_d(G)$  if all of its off-diagonal non-zero entries have the same sign. Such a uniform sign of off-diagonal non-zero entries is sufficient but not necessary to be a contained in  $\mathcal{A}_d(G)$ . In fact, there are even networks where every matrix in  $\mathcal{A}(G)$  is also contained in  $\mathcal{A}_d(G)$ . For example,

 $A_d(G) = A(G)$  when G is a geodetic graph, i.e., an undirected graph where there is a unique shortest path between any two nodes (e.g., any tree, any cycle with an odd number of nodes, or any complete graph).

Since we focus on systems with  $A \in \mathcal{A}_d(G)$ , we define the dimension of SSCS accordingly as

$$\gamma(G, V_{\ell}) = \min_{A \in \mathcal{A}_{\ell}(G)} \operatorname{rank} \Gamma(A, V_{\ell}). \tag{6}$$

Roughly,  $\gamma(G, V_\ell)$  quantifies how much of the network can be controlled via the leaders  $V_\ell$  under any  $A \in \mathcal{A}_d$ . Computing  $\gamma(G, V_\ell)$  requires finding the minimum rank of  $\Gamma(A, V_\ell)$  that can result from any  $A \in \mathcal{A}_d(G)$ , i.e., any A that has a pattern of non-zeros determined by G as per (3) and also satisfies the additional property in (5). Such minimum rank problems are typically very challenging (e.g., Fallat & Hogben, 2007; Fazel et al., 2004; Mousavi et al., 2019) and there is no algorithm for computing the exact value of  $\gamma(G, V_\ell)$  for arbitrary G and  $V_\ell$ . This has motivated the investigation of bounds that can be used to approximate (or determine exactly in some special cases)  $\gamma(G, V_\ell)$ . We will next present two such tight lower bounds on  $\gamma(G, V_\ell)$ , which will be the main focus of our analysis in the following sections.

# 2.4. Distance-based Lower Bound: $\delta(G, V_{\ell})$

We first present the distance-based bound, which was originally proposed in Yazıcıoğlu et al. (2016) for the SSC of networks under consensus (weighted Laplacian) dynamics. While the weighted Laplacian matrices constitute a subset of  $\mathcal{A}_d$ , this distance-based bound actually holds for every  $A \in \mathcal{A}_d$  as we will show. We will first provide some definitions and then provide the bound, which is obtained from the distances of nodes to the leaders on G = (V, E).

Given any G = (V, E) with m leaders,  $V_{\ell} = \{\ell_1, \dots, \ell_m\}$ , the distance-to-leaders (DL) vector of each  $v_i \in V$  is

$$D_i = \left[\begin{array}{ccc} d(\ell_1, v_i) & d(\ell_2, v_i) & \cdots & d(\ell_m, v_i) \end{array}\right]^T \in \mathbb{Z}^m,$$

where the *j*th component of  $D_i$ , denoted by  $[D_i]_j$ , is equal to the length of the shortest path from  $\ell_j$  to  $v_i$ . Next, we provide the definition of *pseudo-monotonically increasing* sequences of DL vectors.

**Definition 1** (Pseudo-monotonically Increasing (PMI) Sequence). A sequence of distance-to-leaders vectors  $\mathcal{D}$  is PMI if for any vector  $\mathcal{D}_i$  in the sequence, there exists some  $\pi(i) \in \{1, 2, \dots, m\}$  such that

$$[\mathcal{D}_i]_{\pi(i)} < [\mathcal{D}_j]_{\pi(i)}, \quad \forall j > i. \tag{7}$$

We say that  $\mathcal{D}_i$  satisfies the *PMI property* at coordinate  $\pi(i)$  whenever  $[\mathcal{D}_i]_{\pi(i)} < [\mathcal{D}_i]_{\pi(i)}$ ,  $\forall j > i$ .

An example of DL vectors is illustrated in Fig. 2, where a PMI sequence of length six can be constructed as

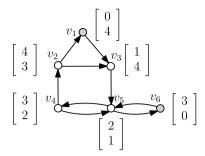
$$\mathcal{D} = \left\{ \left[ \begin{array}{c} 3 \\ \emptyset \end{array} \right], \left[ \begin{array}{c} \emptyset \\ 4 \end{array} \right], \left[ \begin{array}{c} 1 \\ 4 \end{array} \right], \left[ \begin{array}{c} 2 \\ 1 \end{array} \right], \left[ \begin{array}{c} 3 \\ 2 \end{array} \right], \left[ \begin{array}{c} 4 \\ 3 \end{array} \right] \right\},$$

where the coordinates,  $\pi(i)$ , satisfying the PMI property in (7) are circled

We next provide an extension of Yazıcıoğlu et al. (2016, Thm. 3.2), where the distance-based bound on the dimension of SSCS was derived for networks with weighted Laplacian dynamics.

**Proposition 1.** Consider any network G = (V, E) with the leaders  $V_{\ell} \subseteq V$ . Let  $\delta(G, V_{\ell})$  be the length of longest PMI sequence of distance-to-leaders vectors with at least one finite entry. Then,

$$\delta(G, V_{\ell}) \leq \gamma(G, V_{\ell}).$$



**Fig. 2.** A network with two leaders,  $V_\ell=\{v_1,v_6\}$ , and the corresponding distance-to-leaders (DL) vectors.

**Proof.** It can be shown that for any  $A \in \mathcal{A}(G)$  and any  $v_i, v_p \in V$ ,  $[A^r]_{ip} = 0$  for every positive integer  $r < d(v_p, v_i)$  (e.g., see Van Waarde et al. (2017, Lem. 1)). Using this together with (5), for any  $A \in \mathcal{A}_d(G) \subseteq \mathcal{A}(G)$  and any  $v_i, v_p \in V$ ,

$$[A^{r}]_{ip} \begin{cases} = 0 & \text{if } 0 < r < d(v_{p}, v_{i}), \\ \neq 0 & \text{if } r = d(v_{p}, v_{i}). \end{cases}$$
(8)

Given G = (V, E) and the leaders  $V_\ell$ , let  $\mathcal{D} = \{\mathcal{D}_1, \mathcal{D}_2, \dots, \mathcal{D}_k\}$  be a PMI sequence of maximum length that can be constructed with the DL vectors with at least one finite entry. Accordingly,  $\delta(G, V_\ell) = k$ . Without any loss of generality, let us re-label the nodes based on the sequence  $\mathcal{D}$  such that  $\mathcal{D}_i$  is the DL vector of  $v_i \in V$  for all  $i \in \{1, 2, \dots, k\}$ . Now, for any  $A \in \mathcal{A}_d(G)$ , consider the following  $n \times k$  matrix:

$$\left[\begin{array}{cccc} A^{[\mathcal{D}_1]_{\pi(1)}} b_{\pi(1)} & A^{[\mathcal{D}_2]_{\pi(2)}} b_{\pi(2)} & \dots & A^{[\mathcal{D}_k]_{\pi(k)}} b_{\pi(k)} \end{array}\right], \tag{9}$$

where  $\pi(1),\ldots,\pi(k-1)$  are the coordinates of  $\mathcal{D}_1,\ldots,\mathcal{D}_{k-1}$  that satisfy the rule in  $(7),\pi(k)$  is the coordinate of any finite entry of  $\mathcal{D}_k$ , and each  $b_{\pi(i)}$  denotes the  $\pi(i)^{th}$  column of the input matrix B in (2). Accordingly,  $[\mathcal{D}_1]_{\pi(1)},\ldots,[\mathcal{D}_k]_{\pi(k)}$  are all finite values in  $\{0,1,\ldots,n-1\}$  due to the definition of distance. Hence, every column of the matrix in (9) is also a column of the controllability matrix  $\Gamma(A,V_\ell)$ . In the remainder of the proof, we will show that (9) has full column rank, which implies  $\Gamma(A,V_\ell) \geq \delta(G,V_\ell)$ . For any  $i \in \{1,2,\ldots,k\}$ , let  $v_p = \ell_{\pi(i)}$  be the  $\pi(i)^{th}$  leader. Accordingly, the ith column of (9) is

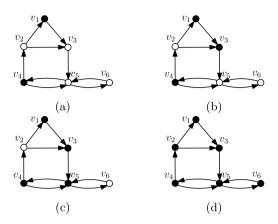
$$A^{[\mathcal{D}_i]_{\pi(i)}}b_{\pi(i)} = \left[ \begin{array}{ccc} [A^{[\mathcal{D}_i]_{\pi(i)}}]_{1p} & [A^{[\mathcal{D}_i]_{\pi(i)}}]_{2p} & \dots & [A^{[\mathcal{D}_i]_{\pi(i)}}]_{np} \end{array} \right]^T.$$

Since  $[\mathcal{D}_i]_{\pi(i)} = d(v_p, v_i)$ , (8) implies that the ith entry of  $A^{[\mathcal{D}_i]_{\pi(i)}}b_{\pi(i)}$  is non-zero. Furthermore, for every  $j \in \{i+1,\ldots,k\}$ , the jth entry of  $A^{[\mathcal{D}_i]_{\pi(i)}}b_{\pi(i)}$  is zero, i.e.,  $[A^{[\mathcal{D}_i]_{\pi(i)}}]_{jp} = 0$ , since  $[\mathcal{D}_i]_{\pi(i)} < [\mathcal{D}_j]_{\pi(i)} = d(v_p, v_j)$  due to the PMI rule in (7). Accordingly, each column of (9) contains the left-most non-zero entry in at least one row. Hence, (9) has full rank and  $\Gamma(A, V_\ell) \geq \delta(G, V_\ell)$  for any  $A \in \mathcal{A}_d(G)$ . Consequently,  $\gamma(G, V_\ell) \geq \delta(G, V_\ell)$ .

# 2.5. Zero-forcing-based Lower Bound: $\zeta(G, V_{\ell})$

We next present the zero-forcing-based lower bound on  $\gamma(G, V_{\ell})$ , which follows from the earlier studies in Monshizadeh et al. (2015, 2014). We first give the definitions of the zero forcing process and the derived set.

**Definition 2** (*Zero Forcing Process*). Given a graph G = (V, E) where each node is initially colored either *white* or *black*, zero forcing process is defined by the following coloring rule: if  $v_i \in V$  is colored black and has exactly one white out-neighbor  $v_j$ , then the color of  $v_j$  is changed to black and  $v_j$  is said to be *infected* by  $v_i$ .



**Fig. 3.** Zero forcing process. (a)  $\{v_1, v_4\}$  is the input set. (b)  $v_1$  infects  $v_3$  (as  $v_3$  is the only out-neighbor of  $v_1$ ). (c)  $v_3$  infects  $v_5$ . (d) Finally,  $v_5$  and  $v_4$  infect  $v_6$  and  $v_2$ , respectively.

**Definition 3** (*Derived Set*). Given an initial set of black nodes  $V' \subseteq V$  (called the *input set*) in a graph G = (V, E), there exists a unique derived set,  $\operatorname{dset}(G, V') \subseteq V$ , which is the resulting set of black nodes when no further color changes are possible under the zero forcing process. An input set V' is called a *zero forcing set* (ZFS) if  $\operatorname{dset}(G, V') = V$ .

These notions are illustrated in Fig. 3. Here,  $V' = \{v_1, v_4\}$  is the set of input nodes. As a result of zero forcing process, we get dset(G, V') = V (as shown in Fig. 3(d)), which means that V' is a 7FS

**Proposition 2.** For any network G = (V, E) with the leaders  $V_{\ell} \subset V$ ,

$$\zeta(G, V_{\ell}) \leq \gamma(G, V_{\ell}),$$

where  $\zeta(G, V_{\ell}) = |dset(G, V_{\ell})|$  is the size of the derived set corresponding to the input set  $V_{\ell}$ .

**Proof.** Proof mainly follows from Monshizadeh et al. (2015, Lem. 6.2), which shows that for any  $A \in \mathcal{A}(G)$  and  $V_{\ell} \subseteq V$ , the reachable/controllable subspace, i.e., the range space of the controllability matrix, remains the same when the leader set is expanded to include all the nodes in the derived set  $dset(V_{\ell})$ . More specifically,

 $range(\Gamma(A, V_{\ell})) = range(\Gamma(A, dset(G, V_{\ell}))),$ 

which implies

$$rank(\Gamma(A, V_{\ell})) = rank(\Gamma(A, dset(G, V_{\ell}))). \tag{10}$$

Furthermore, using (2) and (4), it can be shown that the rank of the controllability matrix is always lower bounded by the number of leaders. Hence,

$$|V_{\ell}| \le rank(\Gamma(A, V_{\ell})), \tag{11}$$

$$|\operatorname{dset}(G, V_{\ell})| < \operatorname{rank}(\Gamma(A, \operatorname{dset}(G, V_{\ell}))).$$
 (12)

Using (10), (11), and (12), we obtain

$$\zeta(G, V_{\ell}) \le rank(\Gamma(A, V_{\ell})), \ \forall A \in \mathcal{A}(G).$$
 (13)

Since  $A_d(G) \subseteq A(G)$ , (13) implies

$$\zeta(G, V_{\ell}) \leq \min_{A \in \mathcal{A}(G)} \operatorname{rank} \Gamma(A, V_{\ell}) \leq \gamma(G, V_{\ell}).$$
(14)

# 2.6. Computational aspects

The investigation of graph theoretic bounds on  $\gamma(G, V_\ell)$  is mainly motivated by the intractability of the exact computation of  $\gamma(G, V_\ell)$ . Hence, while the main focus of this paper is on the comparison of the values of two tight lower bounds,  $\zeta(G, V_\ell)$  and  $\delta(G, V_\ell)$ , we also briefly discuss their computational aspects prior to our analysis.

In general,  $\zeta(G, V_\ell)$  can be computed in  $O(n^2)$  time by recursively applying the coloring rule of the zero forcing process to the out-neighbors of infected nodes until no further color change is possible. Accordingly, the computation of  $\zeta(G, V_\ell)$  remains tractable as the network size or the number of leaders increases.

In comparison to  $\zeta(G, V_{\ell})$ , the exact computation of  $\delta(G, V_{\ell})$ is significantly more demanding. For any given network with nnodes and m leaders, all pair-wise distances can be computed in  $O(n^3)$  time (e.g., Floyd, 1962). Then, given the distances,  $\delta(G, V_\ell)$ can be computed in  $O(m(n \log n + n^m))$  time (Shabbir, Abbas, & Yazıcıoğlu, 2019). While this computational load scales well with increasing network size when the number of leaders is constant, it becomes intractable when the number of leaders also increases. To overcome this computational challenge, an approximation that can be obtained in  $O(mn \log n)$  time was presented in Shabbir et al. (2019). In a nutshell, this is a greedy algorithm that iteratively builds a PMI sequence of DL vectors by starting with an empty sequence and, in each iteration, adding a DL vector that minimally reduces the number of DL vectors that can be added to the sequence in the following iterations under the rule in (7). Since this approximation algorithm is based on constructing a feasible PMI sequence, the resulting value,  $\hat{\delta}(G, V_{\ell})$ , never exceeds  $\delta(G, V_{\ell})$ . Accordingly,  $\hat{\delta}(G, V_{\ell})$  can be used as a lower bound on  $\gamma(G, V_{\ell})$ , i.e.,

$$\hat{\delta}(G, V_{\ell}) \leq \delta(G, V_{\ell}) \leq \gamma(G, V_{\ell}),$$

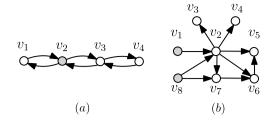
Numerical results with randomly generated networks and leader sets suggest that  $\hat{\delta}(G, V_\ell)$  is usually very close to  $\delta(G, V_\ell)$  (Shabbir et al., 2019). Furthermore, if the distance-based bound indicates complete strong structural controllability, i.e.,  $\delta(G, V_\ell) = n$ , then the approximation algorithm is also guaranteed to return  $\hat{\delta}(G, V_\ell) = n$ . We refer interested readers to Shabbir et al. (2019) for further details on the computational aspects of  $\delta(G, V_\ell)$ .

# 3. Comparison of bounds

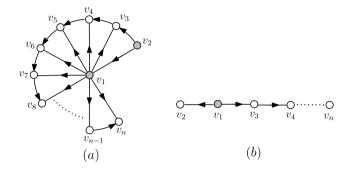
In this section, we compare the distance-based bound,  $\delta(G, V_\ell)$ , and the zero-forcing-based bound,  $\zeta(G, V_\ell)$ . It is worth mentioning that both  $\delta(G, V_\ell)$  and  $\zeta(G, V_\ell)$  are tight bounds. For instance, in the case of undirected graphs, any path graph in which one of the end nodes is a leader, or any cycle graph in which two adjacent nodes are leaders satisfy  $\zeta(G, V_\ell) = \delta(G, V_\ell) = \gamma(G, V_\ell) = n$ . Furthermore, neither of these two tight bounds is guaranteed to be at least as good as the other in all possible cases. We provide one example for  $\zeta(G, V_\ell) > \delta(G, V_\ell)$  and one example for  $\delta(G, V_\ell) > \zeta(G, V_\ell)$  in Fig. 4. In fact, as we will show in Theorem 3, for each bound there exist examples of networks where it is arbitrarily better than the other bound. Accordingly, our main goal in this section is to identify the networks when one bound may be preferable to the other.

**Theorem 3.** For any  $\alpha \geq 1$ , there exist graphs G = (V, E), G' = (V', E') and leader sets  $V_{\ell} \subseteq V$ ,  $V'_{\ell} \subseteq V'$  such that

$$\frac{\zeta(G, V_{\ell})}{\delta(G, V_{\ell})} \ge \alpha, \quad \frac{\delta(G', V_{\ell}')}{\zeta(G', V_{\ell}')} \ge \alpha. \tag{15}$$



**Fig. 4.** Two networks and their leaders show in gray. For the network in (a),  $\delta(G, V_\ell) = 3$ ,  $\zeta(G, V_\ell) = 1$ . For the network in (b),  $\delta(G, V_\ell) = 5$ ,  $\zeta(G, V_\ell) = 6$ .



**Fig. 5.** Examples where the bounds  $\zeta$  and  $\delta$  become arbitrarily larger than each other as the network size n increases.

**Proof.** While one can find many different networks and leader sets that satisfy the claim, we prove it by providing two specific network structures as shown in Fig. 5. These two networks achieve an arbitrarily large  $\zeta(G, V_\ell)/\delta(G, V_\ell)$  (Fig. 5a) or  $\delta(G', V'_\ell)/\zeta(G', V'_\ell)$  (Fig. 5b) as their sizes increase. Accordingly, for any  $\alpha \geq 1$  these networks can be built with a sufficiently large size n to obtain the pairs  $(G, V_\ell)$  and  $(G', V'_\ell)$  that satisfy (15). In the remainder of the proof, we derive the ratios of bounds and determine the sufficient size for each of these two networks to satisfy (15) for any given  $\alpha \geq 1$ .

**Network in** Fig. 5a: This network has two leaders,  $V_{\ell} = \{v_1, v_2\}$ . The graph G = (V, E) has its edge set as

$$E = \{(v_2, v_1)\} \cup \{(v_1, v_i) \mid i \geq 3\} \cup \{(v_{i-1}, v_i) \mid i \geq 3\}.$$

It can be shown that the zero forcing process starting with the input set  $\{v_1, v_2\}$  infects all the nodes in this graph. In particular, first  $v_3$  gets infected (only white out-neighbor of  $v_2$ ), then  $v_4$  gets infected (only white out-neighbor of  $v_3$ ) and so on. Accordingly,  $\zeta(G, V_\ell) = n$ . Furthermore, in this structure the DL vectors are

$$D_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \ D_2 = \begin{bmatrix} \infty \\ 0 \end{bmatrix}, \ D_3 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \ D_i = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \forall i \geq 4.$$

It can be shown that the longest PMI sequence of such DL vectors contains four vectors, i.e.,  $\delta(G, V_\ell) = 4$ . Accordingly, this network satisfies  $\zeta(G, V_\ell)/\delta(G, V_\ell) = n/4$ , which can be made arbitrarily large to satisfy (15) for any given  $\alpha \geq 1$ .

**Network in Fig. 5**b: This network has a single leader,  $V'_{\ell} = \{v_1\}$ . The graph G' = (V', E') has its edge set as

$$E' = \{(v_1, v_2), (v_1, v_3)\} \cup \{(v_{i-1}, v_i) \mid i \geq 4\}.$$

The zero forcing process starting with the input set  $\{v_1\}$  does not infect any other node since  $v_1$  has two followers as outneighbors. Accordingly,  $\zeta(G',V'_\ell)=1$ . Furthermore, the DL vectors in this network are

$$D_1 = \begin{bmatrix} 0 \end{bmatrix}$$
,  $D_2 = D_3 = \begin{bmatrix} 1 \end{bmatrix}$ ,  $D_i = \begin{bmatrix} i-2 \end{bmatrix}$ ,  $\forall i \geq 4$ .

It can be shown that the longest PMI sequence of such DL vectors is  $\{[0], [1], \ldots, [n-2]\}$ . Accordingly,  $\delta(G', V'_\ell) = n-1$  and this network satisfies  $\delta(G', V'_\ell)/\zeta(G', V'_\ell) = n-1$ , which can get arbitrarily large by increasing n to satisfy (15) for any given  $\alpha \geq 1$ .

One important implication of Theorem 3 is that although  $\zeta(G,V_\ell)$  and  $\delta(G,V_\ell)$  are both tight lower bounds on the dimension of SSCS, i.e., there exist networks such that  $\delta(G,V_\ell)=\gamma(G,V_\ell)$  or  $\zeta(G,V_\ell)=\gamma(G,V_\ell)$ , these lower bounds can also be arbitrarily smaller than  $\gamma(G,V_\ell)$  in some cases. How well these two lower bounds typically approximate  $\gamma(G,V_\ell)$  for arbitrary networks and leader sets is currently an open problem.

**Corollary 4.** For any  $\alpha \geq 0$ , there exist graphs G = (V, E), G' = (V', E') and leader sets  $V_{\ell} \subseteq V$ ,  $V'_{\ell} \subseteq V'$  such that

$$\frac{\gamma(G,V_\ell)}{\delta(G,V_\ell)} \geq \alpha, \ \frac{\gamma(G',V'_\ell)}{\zeta(G',V'_\ell)} \geq \alpha.$$

**Proof.** As per Theorem 3, there exist graphs G = (V, E), G' = (V', E') and leader sets  $V_{\ell} \subseteq V$ ,  $V'_{\ell} \subseteq V'$  such that  $\zeta(G, V_{\ell})/\delta(G, V_{\ell})$  and  $\delta(G', V'_{\ell})/\zeta(G', V'_{\ell})$  are arbitrarily large. Since  $\zeta$  and  $\delta$  are both lower bounds on  $\gamma$ , i.e.,  $\zeta(G, V_{\ell}) \leq \gamma(G, V_{\ell})$  and  $\delta(G', V'_{\ell}) \leq \gamma(G', V'_{\ell})$ , such networks also yield arbitrarily large values for  $\gamma(G, V_{\ell})/\delta(G, V_{\ell})$  and  $\gamma(G', V'_{\ell})/\zeta(G', V'_{\ell})$ .

Our focus in the remainder of this paper will be on comparing  $\delta(G,V_\ell)$  and  $\zeta(G,V_\ell)$  and developing a novel lower bound on  $\gamma(G,V_\ell)$  that combines the strengths of these two state-of-the-art bounds.

#### 3.1. Advantages of using the distance-based bound

We will present two results, Theorems 5 and 6, identifying some rich families of cases where  $\delta(G,V_\ell) > \zeta(G,V_\ell)$ . Later in Section 5, we will also provide numerical results showing that  $\delta(G,V_\ell)$  is actually significantly greater than  $\zeta(G,V_\ell)$  in many cases that are not limited to those captured by Theorems 5 and 6. Our first result in this section shows that  $\delta(G,V_\ell)$  is greater than  $\zeta(G,V_\ell)$  whenever each leader has at least two followers as outneighbors. Note that this condition is very likely to occur when a small number of leaders are scattered over a large graph where most nodes have an in-degree of two or more (e.g., most regular graphs, random graphs, scale-free networks).

**Theorem 5.** Consider any graph G = (V, E) with n nodes and m leaders  $V_{\ell} \subseteq V$ . If each leader has at least two followers as out-neighbors, then  $\delta(G, V_{\ell}) > \zeta(G, V_{\ell})$ .

**Proof.** If every leader has outgoing links to at least two followers, then none of the followers will be forced when only the leaders are the black nodes. Accordingly, the  $dset(G, V_\ell) = V_\ell$  and  $\zeta(G, V_\ell) = m$ . On the other hand, we can always find a PMI sequence of DL vectors whose length is greater than m in such a case. As an example, consider the following sequence that has a length of m+1: 1) start with the DL vectors of leaders in any order, 2) add the DL vector of a follower who has a distance of one to one of the leaders. Since each leader is the only node who has a distance of zero to itself, those self-distance entries can be selected as the entries that satisfy the PMI rule. Hence, the longest possible PMI sequence would have a length of at least m+1, which implies  $\delta(G, V_\ell) > \zeta(G, V_\ell)$ .

Our next result shows that for any single-leader network where each follower has a finite distance to the leader,  $\delta(G, V_{\ell}) < n$  ensures that  $\delta(G, V_{\ell}) > \zeta(G, V_{\ell})$ .

**Theorem 6.** For any G = (V, E) with n nodes and a single leader  $V_{\ell} = \{v_{\ell}\}$  such that  $d(v_{\ell}, v_i) < \infty$  for all  $v_i \in V$ ,

$$\delta(G, V_{\ell}) < n \Rightarrow \delta(G, V_{\ell}) > \zeta(G, V_{\ell}). \tag{16}$$

**Proof.** Since the left side of (16) can never be true for n=1, we focus on networks with  $n\geq 2$  and we will prove the claim via contradiction. Suppose that  $\delta(G,V_\ell)< n$  and  $\zeta(G,V_\ell)\geq \delta(G,V_\ell)$ . Note that if  $v_\ell$  has more than one follower as out-neighbor, then the zero forcing process starting with the input set  $\{v_\ell\}$  would not propagate and we would have  $\zeta(G,V_\ell)=1$ . Furthermore, for any network with a single leader  $v_\ell\in V$  such that  $d(v_\ell,v_i)<\infty$  for all  $v_i\in V$ ,

$$\delta(G, \{v_{\ell}\}) = \max_{v_{\ell} \in V} d(v_{\ell}, v_{\ell}) + 1, \tag{17}$$

which is always greater than one. Hence, if  $\zeta(G,V_\ell) \geq \delta(G,V_\ell)$ , then  $v_\ell$  must have only one out-neighbor, say  $v_i$ , who will be infected by  $v_\ell$  under the zero forcing process. Now, if n=2 (there are no other followers), then we end up with  $\delta(G,V_\ell)=\zeta(G,V_\ell)=2$ , which contradicts with  $\delta(G,V_\ell)<1$ . On the other hand, if n>2 then we can repeat the same reasoning by removing  $v_\ell$  from the network, since  $v_\ell$  has no impact on the infection of nodes at distance of two or more from itself, and treating the remaining network as a system with a single leader  $v_i$  with  $d(v_i,v_j)<\infty$  for every  $v_j\neq v_\ell$  ( $v_i$  being the only outneighbor of  $v_\ell$  implies that the paths from  $v_\ell$  to all other nodes go through  $v_i$ , hence  $d(v_i,v_j)<\infty$ ). Accordingly, we can show that if  $\zeta(G,V_\ell)\geq\delta(G,V_\ell)$ , then each follower must have a distinct distance to  $v_\ell$ , which implies  $\delta(G,V_\ell)=\zeta(G,V_\ell)=n$  and results in a contradiction with  $\delta(G,V_\ell)< n$ .

**Remark 1.** In light of (17), the only connected undirected network with a single-leader that yields  $\delta(G,V_\ell)=n$  is a path graph with a terminal node being the leader. Hence, Theorem 6 implies that  $\delta(G,V_\ell)>\zeta(G,V_\ell)$  for all other connected undirected networks with a single-leader.

# 3.2. Advantages of using the zero-forcing-based bound

One advantage of using a zero-forcing-based approach is that  $\zeta(G,V_\ell)$  is actually a lower bound on  $rank(\varGamma(A,V_\ell))$  for every  $A\in \mathcal{A}(G)$  as per (14). In this regard, it differs from  $\delta(G,V_\ell)$ , which is a lower bound on  $rank(\varGamma(A,V_\ell))$  only for  $A\in \mathcal{A}_d(G)\subseteq \mathcal{A}(G)$ . Furthermore, as we will formally show below,  $\zeta(G,V_\ell)$  is better at verifying complete SSC. More specifically, we show that if  $\delta(G,V_\ell)=n$ , then  $V_\ell$  must be a zero forcing set. Note that the converse is not true in general, i.e., it is possible to have a zero forcing set  $V_\ell$  such that  $\delta(G,V_\ell)< n$ , as already shown by the example in Fig. 4b. Clearly, such examples do not exist for single-leader networks due to Theorem 6.

**Theorem 7.** For any graph G = (V, E) with n nodes and any set of m leaders  $V_{\ell} \subseteq V$ ,

$$\delta(G, V_{\ell}) = n \Rightarrow \zeta(G, V_{\ell}) = n.$$

**Proof.** The claim is trivial for the cases when  $V_\ell = V$  since  $\delta(G,V) = \zeta(G,V) = n$ . Hence we focus on  $V_\ell \subset V$  (n>m) in the proof. Let  $\mathcal{D} = [\mathcal{D}_1 \ \mathcal{D}_2 \ \cdots \ \mathcal{D}_n]$  be a PMI sequence consisting of all the distance-to-leaders (DL) vectors such the first  $|V_\ell|$  vectors belong to the leaders. Note that there is no loss of generality here since for any PMI sequence of DL vectors, the vectors belonging to the leaders can be moved to the beginning of the sequence and the distance of each leader to itself (zero) satisfies the PMI rule. Without any loss of generality, let the nodes be re-labeled based on the order of their DL vectors in the sequence, i.e.,  $\mathcal{D}_i$  is the

DL vector of  $v_i \in V$  for all i = 1, 2, ..., n. Furthermore, let  $\pi(i)$  denote the dimension of  $\mathcal{D}_i$  that satisfies the PMI rule, i.e.,

$$[\mathcal{D}_i]_{\pi(i)} < [\mathcal{D}_i]_{\pi(i)}, \quad \forall i > i. \tag{18}$$

Due to Yazıcıoğlu et al. (2016, Lem. 4.1), if  $\mathcal{D}$  is the longest possible PMI sequence of DL vectors, then it must satisfy

$$[\mathcal{D}_i]_{\pi(i)} = \min_{j \geq i} [\mathcal{D}_j]_{\pi(i)}, \forall i \in \{1, \dots, n-1\}.$$

For each  $i \in \{m+1,\ldots,n\}$ , let  $W_i = \{v_i,\ldots,v_n\} \subseteq V$  be the owners of the DL vectors in the subsequence of  $\mathcal{D}$  starting with the ith entry. We will show that

$$\forall i > m, \exists k < i : \mathcal{N}_k \cap W_i = \{v_i\},\tag{19}$$

where  $\mathcal{N}_k$  is the set of out-neighbors of  $v_k$ . Note that (19) would imply that if all the nodes  $\{v_1,\ldots,v_{i-1}\}$  are infected, then  $v_i$  becomes infected under the zero forcing process. Accordingly, we can conclude that  $\zeta(G,V_\ell)=n$  since starting with all the leaders being infected, all the followers would eventually become infected.

Note that (19) clearly holds for i=n since  $W_n=\{v_n\}$  and  $v_n$  must have at least one in-neighbor in  $\{v_1,\ldots,v_{n-1}\}$  as otherwise its DL vector would be all  $\infty$  and not included in any PMI sequence, leading to the contradiction  $\delta(G,V_\ell)< n$ . Now, for the sake of contradiction, suppose that (19) is not true for some  $i\in\{m+1,\ldots,n-1\}$ . Let  $v_k$  be any in-neighbor of  $v_i$  such that

$$[\mathcal{D}_k]_{\pi(i)} = [\mathcal{D}_i]_{\pi(i)} - 1.$$

Clearly such a neighbor always exists:  $v_k$  is either the leader  $\ell_{\pi(i)}$  or another follower on the shortest path from  $\ell_{\pi(i)}$  to  $v_i$ . Furthermore, k < i due to (18). Now suppose that  $v_k$  has another out-neighbor  $v_i$  such that j > i. Then,

$$[\mathcal{D}_i]_{\pi(i)} \leq [\mathcal{D}_k]_{\pi(i)} + 1 = [\mathcal{D}_i]_{\pi(i)},$$

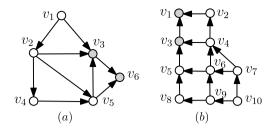
which contradicts with (18). Hence, (19) must be true, and it implies that  $\zeta(G,V_\ell)=n$ .

In light of Theorem 7, the zero-forcing-based approach is a better choice for verifying complete strong structural controllability, especially since there exist cases such as the example in Fig. 5a, where complete SSC can be inferred via the zero-forcing-based bound but not via the distance-based bound, i.e.,  $\delta(G, V_\ell) < \zeta(G, V_\ell) = n$ .

It should be noted that having a zero forcing set as the leaders, i.e.,  $\zeta(G,V_\ell)=n$ , is not necessary for the zero-forcing-based to outperform the distance-based bound. For instance, the example in Fig. 4b shows a network where  $\delta(G,V_\ell)<\zeta(G,V_\ell)< n$ . However, whether there exists a rich family of such examples remains as an open question. Our numerical results in Section 5 suggest that  $\delta(G,V_\ell)<\zeta(G,V_\ell)< n$  may occur in rare cases since none of the randomly generated graphs and leader sets therein resulted in such an inequality.

# 4. Combined Bound: $\delta(G, \operatorname{dset}(G, V_{\ell}))$

Our analysis so far has shown that both the distance-based bound,  $\delta(G,V_\ell)$ , and the zero-forcing-based bound,  $\zeta(G,V_\ell)$ , have their own merits. Given these results, it is only natural to ask if it is possible to find a novel bound that combines the strengths of distance-based and zero-forcing-based methods. In this regard, one trivial approach is taking the maximum of the two bounds. While guaranteed to be at least as good as either of the bounds alone, this approach does not reveal any additional information compared to the two original bounds. In this section, we present a novel bound that fuses the strengths of distance-based and zero-forcing-based approaches and sometimes outperforms both original bounds. More specifically, we show that the length of the



**Fig. 6.** Two networks and their leaders (gray). In (a):  $\delta(G, \text{dset}(G, V_\ell)) = 5$ ,  $\delta(G, V_\ell) = 4$ ,  $\zeta(G, V_\ell) = 3$ . In (b):  $\delta(G, \text{dset}(G, V_\ell)) = 9$ ,  $\delta(G, V_\ell) = 6$ ,  $\zeta(G, V_\ell) = 5$ .

longest PMI sequence of distances to the derived set of leaders provides a tight lower bound on the dimension of SSCS, i.e.,

$$\delta(G, \operatorname{dset}(G, V_{\ell})) \leq \gamma(G, V_{\ell}).$$

We show that this novel bound is always at least as good as, and sometimes better than, the individual bounds.

**Theorem 8.** Consider any network G = (V, E) with the leaders  $V_{\ell} \subseteq V$ . Then,

$$\delta(G, V_{\ell}), \zeta(G, V_{\ell}) < \delta(G, dset(G, V_{\ell})) < \gamma(G, V_{\ell}).$$

**Proof.** First, we show that  $\delta(G, \operatorname{dset}(G, V_{\ell})) \leq \gamma(G, V_{\ell})$ . In light of (6) and (10),

$$\gamma(G, \operatorname{dset}(G, V_{\ell})) = \gamma(G, V_{\ell}). \tag{20}$$

Due to Proposition 1,

$$\delta(G, \operatorname{dset}(G, V_{\ell})) \le \gamma(G, \operatorname{dset}(G, V_{\ell})). \tag{21}$$

Using (20) and (21), we get  $\delta(G, \operatorname{dset}(G, V_{\ell})) \leq \gamma(G, V_{\ell})$ .

Next, we show that  $\delta(G, \operatorname{dset}(G, V_\ell)) \geq \zeta(G, V_\ell)$ . Since the DL vectors of leaders can always be included in the beginning of a PMI sequence (self-distances are uniquely zero),  $\delta(G, V') \geq |V'|$  for any  $V' \subset V$ . Hence,

$$\delta(G, \operatorname{dset}(G, V_{\ell})) \ge |\operatorname{dset}(G, V_{\ell})| = \zeta(G, V_{\ell}).$$

Finally, we show that  $\delta(G, \operatorname{dset}(G, V_\ell)) \geq \delta(G, V_\ell)$ . Since the initial set of infected nodes (input nodes) are always contained in the derived set, we have  $V_\ell \subseteq \operatorname{dset}(G, V_\ell)$ . Accordingly, for any PMI sequence  $\mathcal D$  of DL vectors under the leader set  $V_\ell$ , there is an equally long PMI sequence of DL vectors  $\mathcal D'$  under the leader set  $\operatorname{dset}(G, V_\ell)$ , which has the DL vectors of the same nodes in the same order as  $\mathcal D$ . Hence, the longest possible PMI sequence of DL vectors with the additional leaders cannot be shorter, i.e.,

$$\delta(G, \operatorname{dset}(G, V_{\ell})) \geq \delta(G, V_{\ell}).$$

**Remark 2.** While Theorem 8 shows that the combined bound is at least as good as the distance-based and zero-forcing-based bounds, it should also be emphasized that there exist cases where the combined bound is strictly better than the two original bounds, i.e.,  $\delta(G, \operatorname{dset}(G, V_\ell)) > \delta(G, V_\ell)$ ,  $\zeta(G, V_\ell)$ . We provide two such examples in Fig. 6.

# 4.1. Comparison with the original bounds

We conclude this section by presenting some results that compare  $\delta(G, \operatorname{dset}(G, V_\ell))$  to  $\delta(G, V_\ell)$  and  $\zeta(G, V_\ell)$ . Our first result is a corollary showing that if each leader has two followers as out-neighbors, then the combined bound is equal to the distance-based bound and strictly larger than the zero-forcing-based bound.

**Corollary 9.** Consider any graph G = (V, E) with the leaders  $V_{\ell} \subseteq V$ . If each leader has at least two followers as out-neighbors, then  $\delta(G, \operatorname{dset}(G, V_{\ell})) = \delta(G, V_{\ell}) > \zeta(G, V_{\ell})$ .

**Proof.** If each leader has at least two followers as out-neighbors, then none of the followers are infected by the leaders, i.e.,  $\operatorname{dset}(G, V_\ell) = V_\ell$ . Accordingly,  $\delta(G, \operatorname{dset}(G, V_\ell)) = \delta(G, V_\ell)$  and the strict inequality  $\delta(G, \operatorname{dset}(G, V_\ell)) > \zeta(G, V_\ell)$  follows from Theorem 5.

Next, we show that the combined bound can verify complete SSC, i.e.,  $\delta(G, \operatorname{dset}(G, V_\ell)) = n$ , if and only if the leader set is a zero forcing set, i.e.,  $\zeta(G, V_\ell) = n$ . Accordingly, the combined bound is better than the distance-based bound and equivalent to the zero-forcing-based bound for verifying complete SSC.

**Corollary 10.** For any graph G = (V, E) with n nodes and any set of leaders  $V_{\ell} \subseteq V$ ,

$$\delta(G, dset(G, V_{\ell})) = n \iff \zeta(G, V_{\ell}) = n.$$

**Proof** ( $\Rightarrow$ :). In light of Theorem 7, we have

$$\delta(G, \operatorname{dset}(G, V_{\ell})) = n \Rightarrow \zeta(G, \operatorname{dset}(G, V_{\ell})) = n. \tag{22}$$

Since  $dset(G, V_{\ell})$  is the equilibrium of zero forcing process,

$$\zeta(G, \operatorname{dset}(G, V_{\ell})) = |\operatorname{dset}(G, V_{\ell})| = \zeta(G, V_{\ell}). \tag{23}$$

Accordingly, (22) and (23) together imply

$$\delta(G, \operatorname{dset}(G, V_{\ell})) = n \Rightarrow \zeta(G, V_{\ell}) = n.$$

( $\Leftarrow$ :) If  $\zeta(G, V_\ell) = n$ , then  $\operatorname{dset}(G, V_\ell) = V$ . Note that  $\delta(G, \operatorname{dset}(G, V_\ell)) = \delta(G, V) = n$  since any sequence of the corresponding DL vectors would be a PMI sequence as the unique zero in each vector (distance of the node to itself) would satisfy the rule in (7). ■

In the following result, we provide a sufficient condition for the combined bound to outperform the zero-forcing-based bound. More specifically,  $\delta(G, \operatorname{dset}(G, V_\ell)) > \zeta(G, V_\ell)$  for any strongly connected network and any leader set such that  $\zeta(G, V_\ell) < n$ . Since these are mild conditions on the network and the leader set, the combined bound is likely to outperform the zero-forcing-based bound in most cases, which is also supported by the numerical results in Section 5.

**Theorem 11.** For any strongly connected G = (V, E) with n nodes and any set of leaders  $V_{\ell} \subseteq V$ ,

$$\zeta(G, V_{\ell}) < n \Rightarrow \delta(G, dset(G, V_{\ell})) > \zeta(G, V_{\ell}).$$

**Proof.** If  $\zeta(G, V_\ell) < n$ , then  $\operatorname{dset}(G, V_\ell) \subset V$ . Note that on a strongly connected graph, for any such  $\operatorname{dset}(G, V_\ell) \subset V$  there exists some  $v_i \in \operatorname{dset}(G, V_\ell)$  who has an out-neighbor  $v_j \notin \operatorname{dset}(G, V_\ell)$ , i.e.,  $d(v_i, v_j) = 1$ . Accordingly, given the vectors of distances to the nodes in  $\operatorname{dset}(G, V_\ell)$ , one can always construct a PMI sequence of length at least  $|\operatorname{dset}(G, V_\ell)| + 1$  by starting with the distance vectors of all the nodes in  $\operatorname{dset}(G, V_\ell)$  in any order (self-distances of zero satisfy the PMI rule) and continuing with the distance vector of  $v_i$ . Hence,

$$\zeta(G, V_{\ell})\langle n \Rightarrow \delta(G, \operatorname{dset}(G, V_{\ell}))\rangle |\operatorname{dset}(G, V_{\ell})| = \zeta(G, V_{\ell}).$$

We will conclude this section with a couple of results comparing the combined bound with the distance-based bound. First, we show that these two bounds are typically equal in single-leader networks.

**Theorem 12.** For any G = (V, E) with a single leader  $v_{\ell} \in V$  such that  $d(v_{\ell}, v_i) < \infty$  for all  $v_i \in V$ , we have  $\delta(G, dset(G, V_{\ell})) = \delta(G, V_{\ell})$ .

**Proof.** Since  $V_{\ell} \subseteq \operatorname{dset}(G, V_{\ell})$ , it can be easily shown that  $\delta(G, \operatorname{dset}(G, V_{\ell})) \geq \delta(G, V_{\ell})$ , i.e., adding more leaders cannot reduce the length of the longest PMI sequence of DL vectors. Accordingly, in the remainder of the proof we will show that it must also be true that  $\delta(G, V_{\ell}) \geq \delta(G, \operatorname{dset}(G, V_{\ell}))$ , which together with  $\delta(G, \operatorname{dset}(G, V_{\ell})) \geq \delta(G, V_{\ell})$  implies  $\delta(G, \operatorname{dset}(G, V_{\ell})) = \delta(G, V_{\ell})$ . There are three possible cases depending on  $\operatorname{dset}(G, V_{\ell})$ , and we analyze them separately:

Case 1: If  $\operatorname{dset}(G, V_{\ell}) = V_{\ell}$ , then clearly  $\delta(G, \operatorname{dset}(G, V_{\ell})) = \delta(G, V_{\ell})$ .

Case 2: If  $\operatorname{dset}(G, V_\ell) = V$ , then clearly  $\delta(G, \operatorname{dset}(G, V_\ell)) = |V|$ . Furthermore, in that case (16) implies  $\delta(G, V_\ell) = |\operatorname{dset}(G, V_\ell)| = |V|$  as otherwise  $\delta(G, V_\ell)$  would have to be larger than |V|, which is not possible. Hence,  $\delta(G, \operatorname{dset}(G, V_\ell)) = \delta(G, V_\ell)$ .

Case 3: If  $V_{\ell} \subset \delta(G, \operatorname{dset}(G, V_{\ell})) \subset V$ , then  $v_{\ell}$  must have only one out-neighbor, say  $v_j$ , as otherwise  $\delta(G, \operatorname{dset}(G, V_{\ell})) = V_{\ell}$ . Since  $v_j$  is the only out-neighbor of  $v_{\ell}$ , it is also the only node with a distance of one to  $v_{\ell}$  and any path from  $v_{\ell}$  to any other node  $v_{\ell}$  has to go through  $v_i$ . Accordingly,

$$d(v_{\ell}, v_k) = d(v_j, v_k) + 1, \forall v_k \notin \{v_{\ell}, v_j\}.$$

Once  $v_j$  is infected, another node becomes infected only if  $v_j$  has a unique uninfected out-neighbor, say  $v_i \neq v_\ell$ . Note that  $v_i$  would also be the only node with a distance of two to  $v_\ell$  and

$$d(v_{\ell}, v_{k}) = d(v_{i}, v_{k}) + 2, \forall v_{k} \notin \{v_{\ell}, v_{i}, v_{i}\}.$$

By following this induction, we can show that each node in  $\operatorname{dset}(G, V_\ell)$  has a distinct distance to  $v_\ell$ . Furthermore, for every  $v_q \in \operatorname{dset}(G, V_\ell)$  we have

$$d(v_{\ell}, v_k) = d(v_q, v_k) + d(v_{\ell}, v_q), \forall v_k \notin \operatorname{dset}(G, V_{\ell}). \tag{24}$$

In light of (24),  $d(v_\ell, v_k) > d(v_\ell, v_q)$  for every  $v_q \in \operatorname{dset}(G, V_\ell)$  and  $v_k \notin \operatorname{dset}(G, V_\ell)$ . Furthermore, for any  $v_k, v_k' \notin \operatorname{dset}(G, V_\ell)$ , if  $d(v_\ell, v_k) = d(v_\ell, v_k')$ , then  $d(v_q, v_k) = d(v_q, v_k')$  for any  $v_q \in \operatorname{dset}(G, V_\ell)$ . Hence, such  $v_k, v_k'$  would have identical DL vectors under the leader set  $\operatorname{dset}(G, V_\ell)$ , which cannot be included together in a PMI sequence as per the rule in (18). Accordingly, every DL vector in the longest PMI sequence under the leader set  $\operatorname{dset}(G, V_\ell)$  must have a distinct entry as the distance to  $v_\ell$ . Hence, an equally long PMI sequence can be constructed by only using the distances to  $v_\ell$ , which implies  $\delta(G, V_\ell) \geq \delta(G, \operatorname{dset}(G, V_\ell))$ .

Finally, we provide a sufficient condition for the combined bound to outperform the distance-based bound.

**Theorem 13.** For any G = (V, E) with a leader set  $V_{\ell} \subseteq V$ , if  $dset(G, V_{\ell})$  contains any two nodes with identical DL vectors, then  $\delta(G, dset(G, V_{\ell})) > \delta(G, V_{\ell})$ .

**Proof.** Any PMI seq under the leader set  $V_{\ell}$  is also a valid PMI seq under the leader set  $\delta(G, \operatorname{dset}(G, V_{\ell}))$ . Let  $D_i = D_j$  for some  $v_i, v_j \in V$ . Consider the longest PMI seq under  $V_{\ell}, \mathcal{D}$ , which cannot contain both  $D_i$  and  $D_j$  due the PMI rule. Without loss of generality let  $D_i$  be the vector not contained in  $\mathcal{D}$ . By appending  $D_i$  to the beginning of  $\mathcal{D}$  we obtain a sequence  $\mathcal{D}' = \{D_i, \mathcal{D}_1, \mathcal{D}_2, \dots \mathcal{D}_{|\mathcal{D}|}\}$ . Note that  $\mathcal{D}'$  is a valid PMI seq under  $\operatorname{dset}(G, V_{\ell})$  since the self-distance of  $v_i$  satisfies the rule. As such, we obtain  $\delta(G, \operatorname{dset}(G, V_{\ell})) > \delta(G, V_{\ell})$ .

Note that the condition in Theorem 13 is sufficient but not necessary for the combined bound to outperform the distance-based bound. For example, while  $\delta(G, \operatorname{dset}(G, V_\ell)) > \delta(G, V_\ell)$  for both examples in Fig. 6, only the one in Fig. 6b satisfies this sufficient condition.

#### 5. Numerical results

In this section, we present two sets of numerical results. In the first part, we compare the bounds numerically for randomly generated networks and leader sets. In the second part, we demonstrate an application of the bounds where the goal is to select a minimal set of leaders that guarantee a desired level of SSC.

## 5.1. Comparison of the bounds

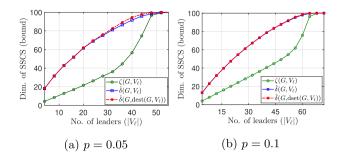
We compare the lower bounds on the dimension of strong structurally controllable subspace on Erdös–Rényi (ER) and Barabási–Albert (BA) graphs. ER graphs are the ones in which any two nodes are adjacent with a probability p. BA graphs are obtained by adding nodes to an existing graph one at a time. Each new node is adjacent to  $\varepsilon$  existing nodes that are chosen with probabilities proportional to their degrees.

In all the simulations, we consider undirected graphs with n=100 nodes. In Figs. 7 and 8, we plot the distance-based, zero-forcing-based, and combined lower bounds on the dimension of SSCS as a function of number of leaders  $|V_\ell|=m$ . We select the leader nodes randomly. Each point on the plots corresponds to the average of 100 randomly generated instances. For each graph G and leader set  $V_\ell$ , we compute the exact value of  $\zeta(G,V_\ell)$ , and we use the greedy approximation algorithm (underestimation) in Shabbir et al. (2019) for the distance-based computations, i.e.,  $\hat{\delta}(G,V_\ell)$  and  $\hat{\delta}(G,\operatorname{dset}(G,V_\ell))$ , due to the large number of leaders. While this approximation was numerically shown to be very close to the actual value in most cases (Shabbir et al., 2019), the gap between  $\delta(G,V_\ell)$  and  $\zeta(G,V_\ell)$  may be larger than shown in Figs. 7 and 8.

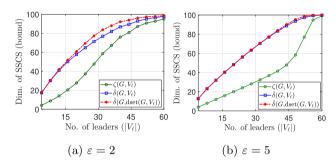
In all the plots in Figs. 7 and 8, we observe that the distancebased bound  $\delta(G, V_{\ell})$  starts above the zero-forcing-based bound  $\zeta(G, V_{\ell})$ , which is expected due to Theorem 6 (or Remark 1). Furthermore,  $\delta(G, V_{\ell})$  is usually significantly larger than  $\zeta(G, V_{\ell})$ , especially when the number of leaders is small. This can be explained by Theorem 5 since most of the nodes in these networks have degrees of two or more. In the ER graphs the expected degree of each node is approximately pn, and each node in the BA graphs has a degree of  $\varepsilon$  or more. Indeed, all the plots show a linear trend in  $\zeta(G, V_{\ell})$  when the number of leaders is small, indicating  $\zeta(G, V_{\ell}) \approx |V_{\ell}|$ . Note that when  $\zeta(G, V_{\ell}) = |V_{\ell}|$ , trivially  $\delta(V, \operatorname{dset}(G, V_{\ell})) = \delta(G, V_{\ell})$ , which explains why the distancebased and combined bounds mostly overlap until the number of leaders is sufficiently large and the zero-forcing-based bound departs from the initial linear regime where  $\zeta(G, V_{\ell}) \approx |V_{\ell}|$ . While the difference between the combined bound  $\delta(V, \operatorname{dset}(G, V_{\ell}))$  and  $\delta(G, V_{\ell})$  was observed to be small in these simulations, it is worth emphasizing that  $\delta(V, \operatorname{dset}(G, V_{\ell}))$  is the only bound guaranteed to be at least as good as the other two in all possible cases (Theorem 8) and the improvement with respect to  $\delta(G, V_{\ell})$  may be significant for other families of networks (e.g., networks where  $\zeta(G, V_{\ell})$  is arbitrarily larger than  $\delta(G, V_{\ell})$  as given in Theorem 3). Finally, we see in all the plots that the three bounds approach each other as they all increase toward n, which is expected due to Theorem 7 and Corollary 10.

# 5.2. Using the bounds for leader selection

One standard problem in networked dynamical systems is to find an optimal set of leaders (actuation nodes) to achieve properties such as controllability or robustness (e.g., Clark et al., 2017; Pasqualetti et al., 2014; Summers et al., 2015; Tzoumas et al., 2015). In this part, we demonstrate the performance of the lower bounds in such an application. Given a network G = (V, E)



**Fig. 7.** Comparison of the zero-forcing-based bound  $\zeta(G, V_\ell)$  and the approximate values of the distance-based  $\delta(G, V_\ell)$  and combined  $\delta(G, \operatorname{dset}(G, V_\ell))$  bounds in ER graphs.



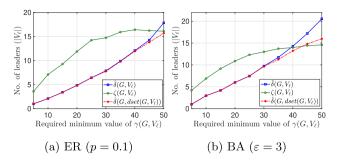
**Fig. 8.** Comparison of the zero-forcing-based bound  $\zeta(G, V_\ell)$  and the approximate values of the distance-based  $\delta(G, V_\ell)$  and combined  $\delta(G, \operatorname{dset}(G, V_\ell))$  bounds in BA graphs.

of *n* agents, we consider the problem of finding a minimal set of leaders,  $V_{\ell} \subseteq V$ , such that  $\gamma(G, V_{\ell})$  is at least k, i.e.,

$$\begin{array}{ll}
\text{minimize} & |V_{\ell}| \\
V_{\ell} \subseteq V \\
\text{subject to} & \gamma(G, V_{\ell}) \ge k,
\end{array}$$
(25)

where  $k \in \{1, 2, ..., n\}$  encodes the required minimum level of SSC. Here, the special case k = n corresponds to imposing complete SSC, whereas smaller values of k can be used in applications where complete SSC is unnecessary (e.g., Li et al., 2020; Van Waarde et al., 2017). There are two major challenges to solving (25): 1) it is an intractable combinatorial optimization problem in general, 2) there is no algorithm for determining the exact value of  $\gamma(G, V_{\ell})$  for arbitrary G and  $V_{\ell}$ . Here, we discuss one possible way of using the tight lower bounds on  $\gamma(G, V_{\ell})$  to address these challenges and approximately solve (25). The approach is to choose one of the bounds and use it with a standard greedy algorithm to select a minimal set of leaders. More specifically, an initially empty leader set is grown by adding the node that maximally improves the selected bound in each iteration until the value of the bound is at least k, which implies that the resulting leader set  $V_{\ell}$  satisfies  $\gamma(G, V_{\ell}) \geq k$ . We test this approach on various networks and report the results in Fig. 9.

Each data point in Fig. 9 corresponds to an average of 35 randomly generated instances of the corresponding type of graph with n=50 nodes. For Erdös–Rényi (ER) random graphs, p=0.1, and for Barabási–Albert (BA) graphs  $\varepsilon=3$ . The value of required minimum  $\gamma(G,V_\ell)$ , k in (25), varies from 5 to 50. Similar to the previous set of simulations, the approximations  $\hat{\delta}(G,V_\ell)$  and  $\hat{\delta}(G, \operatorname{dset}(G,V_\ell))$  are used for the distance-based computations. Among the two original bounds, in alignment with the comparison results in Figs. 7 and 8, we observe that the greedy leader selection algorithm performs better (selects fewer leaders) with  $\hat{\delta}(G,V_\ell)$  for a wide range of k, whereas it performs better with  $\xi(G,V_\ell)$  when k gets close to n. On the other hand, when the combined bound  $\hat{\delta}(G,\operatorname{dset}(G,V_\ell))$  is used, the resulting number



**Fig. 9.** Number of leaders selected by the greedy heuristic is shown for each bound as a function of the required minimum value of  $\gamma(G, V_{\ell})$  in (25) for ER and BA graphs with 50 nodes.

of leaders is similar to  $\hat{\delta}(G, V_\ell)$  for small values of k and similar to  $\zeta(G, V_\ell)$  for large values of k. Accordingly, using  $\hat{\delta}(G, \text{dset}(G, V_\ell))$  is observed to result in the smallest number of leaders in most cases as shown in Fig. 9.

#### 6. Conclusion

In this paper, we focused on the dimension of the strong structurally controllable subspace (SSCS) of networks. We compared two tight lower bounds on the dimension of SSCS: one based on the distances of nodes to the leaders and the other based on the zero forcing process. We showed that for each bound there exist networks where it is arbitrarily better than the other bound. We then characterized various cases where the distance-based lower bound is guaranteed to be greater than the zero-forcing-based bound. On the other hand, we also showed that, for any network of n nodes, any set of leaders that makes the distance-based bound equal to *n* is necessarily a zero forcing set. These results indicate that while the zero-forcing-based approach may be a better choice for verifying complete strong structural controllability (SSC), the distance-based approach is usually better when the leaders do not constitute a zero forcing set. We also derived a novel bound by combining these two approaches. This new bound is always at least as good as, and in some cases strictly better than, the maximum of the two previous bounds. We showed that the combined bound outperforms the zero-forcing-based bound on any strongly connected graph unless the leader set is a zero forcing set, equals the distance-based bound on most singleleader networks, and outperforms the distance-based bound if the derived set,  $dset(G, V_{\ell})$ , contains multiple nodes with identical distances to the leaders. Finally, we numerically compared the bounds on various networks.

As a future direction, we plan to improve the proposed combined bound, for example, by utilizing the invariance of controllable subspace to the addition/removal of links between the leaders (Yazıcıoğlu & Egerstedt, 2013). Obtaining a formal characterization of cases where the zero-forcing-based bound is guaranteed to be greater than the distance-based bound is another direction we plan to explore. Furthermore, the distance-based bound was recently utilized for analyzing the robustness-controllability trade-off in networks (Abbas, Shabbir, Yazıcıoğlu, & Akber, 2020). We intend to use the combined bound for further exploration of such trade-offs.

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