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## Exact controllability of multiplex networks

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### Abstract

We develop a general framework to analyze the controllability of multiplex networks using multiple-relation networks and multiple-layer networks with interlayer couplings as two classes of prototypical systems. In the former, networks associated with different physical variables share the same set of nodes and in the latter, diffusion processes take place. We find that, for a multiple-relation network, a layer exists that dominantly determines the controllability of the whole network and, for a multiple-layer network, a small fraction of the interconnections can enhance the controllability remarkably. Our theory is generally applicable to other types of multiplex networks as well, leading to significant insights into the control of complex network systems with diverse structures and interacting patterns.

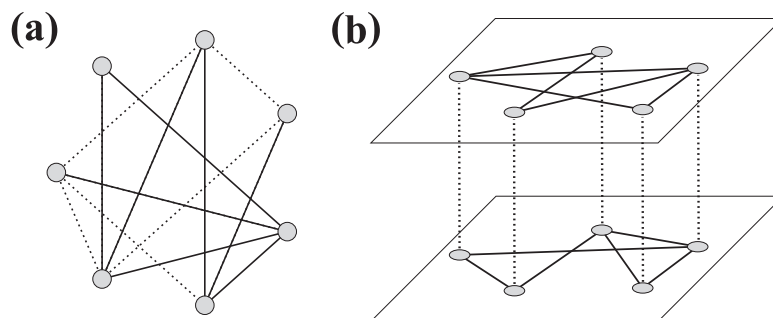
Keywords: Controllability, Multiplex networks, Diffusion

### 1. Introduction

The past decade has witnessed a great deal of effort towards understanding the dynamics of complex network systems [1]. Extensive research, however, has focused on single-layer networks with one type of nodal interactions. In a variety of complex systems, multiplex networks are becoming increasingly ubiquitous [2, 3]. For example, bus, subway and airlines constitute a



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**Figure 1.** Examples of (a) a multiple-relation network and (b) a multiple-layer network with interconnections, with  $M = 2$  layers. In (a), two relation networks (solid and dashed links) share the same set of nodes but characterize distinct relations associated with different physical variables. In (b), the interactions at each layer are independent of each other, and the interlayer connections (dashed links) are from each node in a layer to its counterpart in the other layer.

typical multiplex public transportation network, making traveling more efficient compared with the case of a single traffic mode. Communications through phones, emails, online chats and blogs represent a typical multiple-relation network in a modern society, where networks with different relations, each having its own physical function, share the same set of nodes. Multiplex networks are also quite common in biochemical systems [4]. It has been demonstrated that multiplex networks exhibit distinct dynamical properties from those in single-layer networks, examples of which include cascading failures [5–8], diffusion [9], evolutionary-game dynamics [10, 11], synchronization [12] and traffic dynamics [13]. How to control multiplex networks is a fundamental problem, but it has not been addressed despite intense recent studies of the structural controllability [14, 15] of directed complex networks [16–21].

In this paper, we present a general framework based on the maximum multiplicity theory [22, 23] to address the *exact* controllability of multiplex networks comprising multiple relations (e.g., multi-modal communication networks) and multiple interconnected layers (e.g., multi-modal transportation networks). We focus on the controllability measure defined by the minimum set of driver nodes that need to be controlled to steer the whole system toward any desired state. Our framework is generally applicable to multiplex networks of arbitrary structures and link weights. We study, in detail, duplex networks with two different relation layers that share the same set of nodes and two-layer networks with interlayer couplings as representative examples of two general classes of multiplex networks, as illustrated in figure 1. In the two-relation network, each layer characterizes interactions among one of the two types of physical variables, such as displacement (zeroth order) and velocity (first order), where the latter is the derivative of the former. A finding is that the zeroth-order layer plays the dominant role in the controllability in the sense that the layer exclusively determines the lower and upper bounds of the controllability measure. In the interconnected two-layer network, there is no dominant layer, but we find that the interlayer connections are important to facilitate the control of the whole system. Our exact controllability theory and the resulting criteria for efficiently assessing the minimal set of required controllers can be readily extended beyond duplex networks, offering a general framework for many types of multiplex networks.

The representative class of multiplex networks we treat constitutes multiple interconnected layers, where diffusion takes place in each layer. The diffusion dynamics of these types of

multiplex networks have been studied recently [9], but here we investigate these systems from the perspective of *control*. We also introduce a general method to find a minimum set of driver nodes to fully control an arbitrary network, based on the following theoretical tools: the PBH theory [22], our maximum multiplicity theory [23] and elementary column transformation as well as column canonical form. Insofar as the control matrix has been obtained, the input signal can be determined via the standard method from canonical control theory [15]. That is to say, if we find all the driver nodes, we can steer the network system to any collective state in the high-dimensional state space.

In section 2, we first introduce the notion of exact controllability by using the setting of single-layer complex networks. We next present a comprehensive theoretical framework for the exact controllability of multi-relation networks, focusing on the key quantity of the minimal number of controllers required to achieve full control of the networked system. The cases of sparse and dense connections will be treated in detail. Finally, we present an exact controllability theory for multi-layer networks with diffusion dynamics. In section 3, we present results from extensive numerical tests of our theory for a large variety of network structures. In section 5, we present a brief conclusion. Certain mathematical details are treated in a number of Appendices. In particular, in Appendix A we present a proof of the exact controllability for single-layer networks. In Appendix B, we derive a theory of exact controllability for multi-relation networks of arbitrary order. In Appendix C, we present detailed calculations of exact controllability of multiple interconnected layers with diffusion dynamics. In Appendix D, we provide details of our method for identifying the minimum set of driver nodes.

## 2. Theoretical methods

Our goal is to develop a general theoretical framework based on the maximum multiplicity theory introduced in [23] to quantify the exact controllability of multiplex networks. Without the loss of generality, we primarily use a duplex network system with two relations, as illustrated in figure 1(a). The system is described by

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{v}, \\ \dot{\mathbf{v}} &= c_0 A_0 \mathbf{x} + c_1 A_1 \mathbf{v} + \mathbf{B}\mathbf{u},\end{aligned}\tag{1}$$

where the vectors  $\mathbf{x} = (x_1, \dots, x_N)^T$  and  $\mathbf{v} = (v_1, \dots, v_N)^T$  characterize the two types of states of the same set of  $N$  nodes. The  $N \times N$  matrices  $A_0$  and  $A_1$  characterize the unweighted coupling network (transpose of adjacency matrix) associated with the zeroth-order and the first-order layer, respectively, and  $c_0$  and  $c_1$  are the interaction strengths. equation (1) can represent a mechanical system where  $\mathbf{x}$  is the vector of displacements of all nodes,  $\mathbf{v} = \dot{\mathbf{x}}$  is the corresponding velocity vector, and the input signal represents a kind of acceleration or force. Hence,  $A_0$  and  $A_1$  define two different kinds of interactions or relationships among the same set of nodes, as shown in figure 1(a). The two-relation dynamical system is also similar to a high-order consensus problem with external inputs; see, for example, [24]. Although the two-relation dynamical system used here is similar to that in [24], we focus on our ability to control the system, while [24] explored consensus dynamics with apparent difference from our work. Our goal is to find a set of  $B$  so that the number  $N_D$  is minimized with respect to controllers or independent driver nodes required to achieve full control of the system, which can be expressed as [15, 17]

$$N_D = \min \{ \text{rank}(B) \}.\tag{2}$$

In the following, we first consider the exact-controllability theory for single-layer networks, and then develop a general and detailed theory for duplex and multiplex networks.

### 2.1. Exact controllability theory for single-layer networks

We consider the following single-layer network system under control:

$$\dot{\mathbf{x}} = A\mathbf{x} + B\mathbf{u}, \quad (3)$$

where the vector  $\mathbf{x} = (x_1, \dots, x_N)^T$  characterizes the states of  $N$  nodes,  $A$  denotes the coupling matrix,  $B$  is the control matrix and  $\mathbf{u} = (u_1, u_2, \dots, u_m)^T$  is the input signal. According to the Popov-Belevitch-Hautus (PBH) rank condition [22], system (3) is fully controllable in the sense that it can be steered from any initial state to any final state in finite time, if and only if the rank condition  $\text{rank}[sI_N - A, B] = N$  holds for any complex number  $s$ , where  $I_N$  is the  $N \times N$  identity matrix. Note that in contrast to the development of a structural controllability framework [14, 17] based on the Kalman rank condition [25], here we choose the PBH condition as the base of the analysis, which, strikingly, enables us to establish an *exact* controllability framework for arbitrary complex networks.

In general, we have proved that [23] for an arbitrary single-layer network as described by  $A$ , the following relation holds:

$$N_D = \max_i \left\{ \mu(\lambda_i^A) \right\}, \quad (4)$$

where  $\lambda_i^A$  ( $i = 1, 2, \dots, l$ ) are the distinct eigenvalues of  $A$ , and  $\mu(\lambda_i^A)$  is the geometric multiplicity defined as  $N - \text{rank}(\lambda_i^A I_N - A)$ . Equation (4) is applicable to any networks with arbitrary structure and link weights. If  $A$  is diagonalizable, e.g., a symmetric matrix characterizing an undirected network, the geometric multiplicity is equal to the algebraic multiplicity or eigenvalue degeneracy  $\delta(\lambda_i^A)$  (the number of eigenvalues with identical value  $\lambda_i^A$ ), so we have

$$N_D = \max_i \left\{ \delta(\lambda_i^A) \right\}. \quad (5)$$

For sparse and dense networks, the maximum multiplicity theory leads to an efficient criterion to determine  $N_D$ , which solely depends on the rank of the coupling matrix  $A$ . In particular, for an arbitrary sparse network, we have  $N_D^s = \max\{1, N - \text{rank}(A)\}$  and for a dense network with unit link weights, we have  $N_D^d = \max\{1, N - \text{rank}(I_N + A)\}$  (See Appendix A).

### 2.2. Exact controllability theory for two-relation networks of second order

Consider now the two-relation network system (1). In order to find  $N_D$ , we use the transformation  $\mathbf{y} = (\mathbf{x}^T, \mathbf{v}^T)^T$  to write the system as

$$\dot{\mathbf{y}} = M\mathbf{y} + B'\mathbf{u} = \begin{bmatrix} 0 & I_N \\ c_0 A_0 & c_1 A_1 \end{bmatrix} \mathbf{y} + \begin{bmatrix} 0 \\ B \end{bmatrix} \mathbf{u}, \quad (6)$$

where  $0$  represents the zero matrix of proper dimension and  $M \in R^{2N \times 2N}$ . It can be verified that system (6) possesses the same controllability measure as system (1). Note that half of the control matrix  $B'$  has zero elements and, consequently, the structural-controllability theory [14, 17] is not applicable. The PBH condition stipulates that system (6) is controllable if and only if  $\text{rank}[sI_{2N} - M, B'] = 2N$  is satisfied for any complex number  $s$ . After some elementary

algebra, we obtain

$$\text{rank}[sI_{2N} - M, B'] = N + \text{rank}[s^2I_N - sc_1A_1 - c_0A_0, B].$$

The necessary and sufficient controllable condition becomes then

$$\text{rank}[s^2I_N - sc_1A_1 - c_0A_0, B] = N,$$

which is determined by both layers  $A_0$  and  $A_1$ , so that  $N_D$  is affected by the interplay between them. We explore such interplay in terms of two categories: (I)  $A_0 = A_1$  (special case) and (II)  $A_0 \neq A_1$  (general case).

**2.2.1. Lower and upper bounds of  $N_D$ .** We find that the lower and upper bounds of  $N_D$  are determined exclusively by the properties of  $A_0$ :

$$N - \text{rank}(A_0) \leq N_D \leq \max_i \left\{ \mu(\lambda_i^{A_0}) \right\}, \quad (7)$$

where  $\max_i \{\mu(\lambda_i^{A_0})\}$  is the maximum geometric multiplicity determined by  $A_0$ , suggesting that the network property of the zeroth-order layer plays the key role in the controllability of the whole system. The proof of (7) proceeds, as follows.

Applying the transformation  $\mathbf{y} = (\mathbf{x}^T, \mathbf{v}^T)^T$ , system (4) can be rewritten as

$$\dot{\mathbf{y}} = M\mathbf{y} + B'\mathbf{u} \quad (8)$$

with

$$M = \begin{bmatrix} 0 & I_N \\ c_0A_0 & c_1A_1 \end{bmatrix}, B' = \begin{bmatrix} 0 \\ B \end{bmatrix}.$$

Here 0 represents some zero matrix with proper dimension. According to the PBH rank condition, system (8) is controllable if and only if

$$\text{rank}[sI_{2N} - M, B'] = 2N \quad (9)$$

for any  $s$ , which can be simplified as

$$\begin{aligned} \text{rank}[sI_{2N} - M, B'] &= \text{rank} \begin{bmatrix} sI_N & -I_N & 0 \\ -c_0A_0 & sI_N - c_1A_1 & B \end{bmatrix} \\ &= \text{rank} \begin{bmatrix} sI_N & -I_N & 0 \\ s(sI_N - c_1A_1) - c_0A_0 & 0 & B \end{bmatrix} \\ &= \text{rank} \begin{bmatrix} 0 & -I_N & 0 \\ s(sI_N - c_1A_1) - c_0A_0 & 0 & B \end{bmatrix} \\ &= N + \text{rank}[s^2I_N - sc_1A_1 - c_0A_0, B], \end{aligned} \quad (10)$$

indicating that system (8) is controllable if and only if

$$\text{rank}[s^2I_N - sc_1A_1 - c_0A_0, B] = N. \quad (11)$$

Note that the minimum number of controllers or independent drivers is defined as  $N_D = \min \{\text{rank}(B)\}$ . According to equation (11), we have

$$\text{rank}(B) \geq N - \text{rank}(s^2 I_N - sc_1 A_1 - c_0 A_0). \quad (12)$$

Thus, for any  $A_0$  and  $A_1$ , we can obtain

$$\begin{aligned} N_D &= \min \left\{ \text{rank}(B) \right\} = \max \left\{ N - \text{rank}(s^2 I_N - sc_1 A_1 - c_0 A_0) \right\} \\ &= N - \min \left\{ \text{rank}(s^2 I_N - sc_1 A_1 - c_0 A_0) \right\}. \end{aligned}$$

It is apparent that

$$\min \left\{ \text{rank}(s^2 I_N - sc_1 A_1 - c_0 A_0) \right\} \leq \text{rank}(-c_0 A_0) = \text{rank}(A_0), \quad (13)$$

which gives the lower bound of  $N_D$  as

$$N_D = N - \min \left\{ \text{rank}(s^2 I_N - sc_1 A_1 - c_0 A_0) \right\} \geq N - \text{rank}(A_0). \quad (14)$$

Finally, we obtain the lower and the upper bounds as given by (7). It is noteworthy that the bounds are determined solely by the zeroth-order network, and they hold for any  $A_0$  and  $A_1$ , either sparse or dense.

**2.2.2. The case of  $A_0 = A_1$ .** For the special case  $A_0 = A_1$ , we can prove that system (8) has the same controllability measure and drivers as the single-layer system

$$\dot{\mathbf{x}} = A_0 \mathbf{x} + B \mathbf{u} \quad (15)$$

but with different control signal  $\mathbf{u}$ . This result is rigorous and valid for any  $A_0$ ,  $c_0$ , and  $c_1$  in the absence of self-loops. The proof proceeds, as follows.

Under the condition  $A_1 = A_0$ , equation (11) can be rewritten as

$$\text{rank} \left[ s^2 I_N - (sc_1 + c_0) A_0, B \right] = N. \quad (16)$$

- If  $s = -c_0/c_1$ , for any  $B$ , we have

$$\text{rank} \left[ s^2 I_N - (sc_1 + c_0) A_0, B \right] = \text{rank} \left[ \begin{pmatrix} c_0 \\ c_1 \end{pmatrix}^2 I_N, B \right] = N.$$

- If  $s \neq -c_0/c_1$ , we have

$$\text{rank} \left[ s^2 I_N - (sc_1 + c_0) A_0, B \right] = \text{rank} \left[ \frac{s^2}{sc_1 + c_0} I_N - A_0, B \right] = N.$$

Therefore, when  $B$  satisfies  $\text{rank}[sI_N - A_0, B] = N$  for any  $s$ , we can conclude:  $\text{rank}[sI_{2N} - M, B'] = 2N$  for all  $s$ , indicating that system (4) has the same controllability and input matrix as system (15). Nevertheless, system (4) has a different input signal  $\mathbf{u}$  from that associated with system (15).

**2.2.3. The case of  $A_0 \neq A_1$ . Sparse  $A_0$ .** When the network  $A_0$  is sparse, the network corresponding to  $M$  is sparse as well, since  $M$  contains three sparse parts  $0_N$ ,  $I_N$  and  $c_0 A_0$ , where  $0_N$  represents a zero matrix of order  $N$ . So,  $N_D$  associated with  $M$ , according to the exact

controllability of single network [equation (A4)], becomes

$$N_D = \max\{1, 2N - \text{rank}(M)\},$$

where  $\text{rank}(M)$  can be calculated as

$$\begin{aligned} \text{rank}(M) &= \text{rank} \begin{bmatrix} 0 & I_N \\ c_0 A_0 & c_1 A_1 \end{bmatrix} = \text{rank} \begin{bmatrix} 0 & I_N \\ c_0 A_0 & 0 \end{bmatrix} \\ &= \text{rank}[0, I_N] + \text{rank}[c_0 A_0, 0] = \text{rank}(I_N) + \text{rank}(c_0 A_0) \\ &= N + \text{rank}(A_0). \end{aligned}$$

We thus have the following efficient criterion:

$$N_D = \max\{1, N - \text{rank}(A_0)\}, \quad (17)$$

regardless of the link density of  $A_1$ . This suggests that, when  $A_0$  is sparse, the controllability of system (4) is solely determined by  $A_0$ .

As a special case, if  $A_0 = 0$  and  $A_1 \neq 0$ , equation (11) becomes  $\text{rank}[s^2 I_N - s c_1 A_1, B] = N$ , which can be satisfied for  $s = 0$  if and only if  $\text{rank}(B) = N$ , indicating that for the system  $\dot{\mathbf{x}}_0 = c_1 A_1 \dot{\mathbf{x}} + B \mathbf{u}$ , the number of driver nodes required is  $N_D = N$ .

**Dense  $A_0$ .** We next analyze the detailed dependence of  $N_D$  on the interplay between  $A_0$  and  $A_1$ . In general,  $N_D$  for the two-layer network system (4) under control is given by

$$N_D = \min \left\{ \text{rank}(B) \right\} = \max_s \left\{ N - \text{rank}(s^2 I_N - s c_1 A_1 - c_0 A_0) \right\}. \quad (18)$$

The key to calculating  $N_D$  lies in identifying the eigenvalue  $s$  associated with the maximum geometric multiplicity of matrix  $M$ . We treat the two cases where  $A_1$  is sparse and dense, separately.

*Sparse  $A_1$ .* According to equation (10), the characteristic polynomial of  $M$  is  $p_M(\lambda) = |\lambda^2 I_N - \lambda c_1 A_1 - c_0 A_0|$ , where  $|\cdot|$  represents the determinate. This means that, if we find  $\lambda$  that satisfies  $p_M(\lambda) = 0$ , then  $\lambda$  is an eigenvalue of  $M$ . From the exact-controllability formula, we already have that, for dense  $A_0$ , the maximum geometric multiplicity occurs at the eigenvalue  $\lambda = -1$ . Thus, in the absence of  $A_1$  ( $A_1 = 0$ ),  $p_M(\lambda)$  becomes

$$p_M(\lambda) = \left| \lambda^2 I_N - c_0 A_0 \right| = c_0^N \left| \frac{\lambda^2}{c_0} I_N - A_0 \right| = c_0^N p_{A_0} \left( \frac{\lambda^2}{c_0} \right),$$

where  $p_{A_0}(\lambda)$  is the characteristic polynomial of  $A_0$  containing the factor  $\lambda + 1$  resulting from the eigenvalue of  $\lambda = -1$  associated with the maximum geometric multiplicity. This leads to the characteristic polynomial factor  $\lambda^2/c_0 + 1$  in  $p_M(\lambda)$ . The solution to the equation  $\lambda^2/c_0 + 1 = 0$  gives the eigenvalue

$$\lambda = \pm \sqrt{-c_0}, \quad (19)$$

which corresponds to the maximum geometric multiplicity of  $M$ . When  $A_1$  is present but is sparse, we can check that  $A_1$  has little effect on such crucial eigenvalues of  $M$ . Hence, in the case where  $A_0$  is dense and  $A_1$  is sparse, the controllability measure can be determined as  $N_D = N - \text{rank}(\lambda^2 I_N - \lambda c_1 A_1 - c_0 A_0)$  with  $\lambda = \pm \sqrt{-c_0}$ , yielding the following efficient criterion:



$$N_D = N - \text{rank}(c_0 I_N \pm c_1 \sqrt{-c_0} A_1 + c_0 A_0). \quad (20)$$

Dense  $A_1$ . We then turn to the case of dense  $A_1$ , where the eigenvalue associated with the maximum multiplicity of a single network is  $-1$  as well. Substituting  $A_1 = A_0$  into the characteristic polynomial  $p_M(\lambda)$ , we have

$$\begin{aligned} p_M(\lambda) &= \left| \lambda^2 I_N - \lambda c_1 A_0 - c_0 A_0 \right| = \left| \lambda^2 I_N - (\lambda c_1 + c_0) A_0 \right| \\ &= (\lambda c_1 + c_0)^N \left| \frac{\lambda^2}{\lambda c_1 + c_0} I_N - A_0 \right| = (\lambda c_1 + c_0)^N p_{A_0} \left( \frac{\lambda^2}{\lambda c_1 + c_0} \right). \end{aligned}$$

We see that  $\lambda c_1 + c_0 \neq 0$  and, hence, the characteristic polynomial suggests the existence of a factor  $\lambda^2/(\lambda c_1 + c_0) + 1$ . Solving the equation  $\lambda^2/(\lambda c_1 + c_0) + 1 = 0$  gives the eigenvalue associated with the maximum geometric multiplicity as

$$\lambda = \frac{-c_1 \pm \sqrt{c_1^2 - 4c_0}}{2}. \quad (21)$$

We see that, when  $A_1$  is dense, there is little difference from case of dense  $A_0$ , validating the approximation used in the derivation of the eigenvalue of  $M$ . Consequently, for dense  $A_1$ ,  $\lambda = (-c_1 \pm \sqrt{c_1^2 - 4c_0})/2$  becomes the eigenvalue of the maximum geometric multiplicity. The controllability measure is thus given by the following efficient criterion:

$$N_D = N - \text{rank} \left[ \left( \frac{-c_1 \pm \sqrt{c_1^2 - 4c_0}}{2} \right)^2 I_N - c_1 \frac{-c_1 \pm \sqrt{c_1^2 - 4c_0}}{2} A_1 - c_0 A_0 \right]. \quad (22)$$

The above treatment of the two-relation network can be extended to multi-relation networks of arbitrary order. See Appendix D.

### 2.3. Exact controllability theory for multiple-layer networks with diffusion dynamics

We consider the general setting of multiple-layer networks in which two types of diffusion dynamics occur with  $a$  in each layer and among  $M$  layers, respectively. There are in total  $M \times N$  nodes and the state  $x_i^K(t)$  of each node is indexed by a layer  $K$  and a number  $i$  within each layer. The equations describing the multiple-layer diffusion system are [9]

$$\dot{\mathbf{x}}_i^K = D_K \sum_{j=1}^N a_{ij}^K \mathbf{x}_j^K + \sum_{l=1}^M D_{Kl} c_{ii}^{Kl} (\mathbf{x}_i^l - \mathbf{x}_i^K) + \sum_{j=1}^m b_{ij}^K u_j, \quad (23)$$

where  $D_K$  is a diffusion constant within layer  $K$ ,  $a_{ij}^K = a_{ji}^K$  represents the connections in the layer,  $D_{Kl}$  stands for the interlayer diffusion constant,  $c_{ii}^{Kl}$  represents the interconnections between  $K$  and  $l$  layers, and  $b_{ij}^K u_j$  denotes the control at layer  $K$ . Without loss of generality, we consider the case of  $M = 2$ . Denoting the inter-diffusion constant  $D_{12} = D_{21}$  by  $D_x$ , we can rewrite equation (23) in the matrix form:

$$\dot{\mathbf{x}} = H\mathbf{x} + B\mathbf{u} = \begin{bmatrix} D_1 A_1 - D_x \Lambda & D_x \Lambda \\ D_x \Lambda & D_2 A_2 - D_x \Lambda \end{bmatrix} \mathbf{x} + B\mathbf{u}, \quad (24)$$

where  $A_1$  and  $A_2$  are the adjacency matrices of each layer, the diagonal matrix  $\Lambda$  represents the interlayer couplings with  $\Lambda_{ii} = c_{ii}^{12} = c_{ii}^{21}$ , and  $\mathbf{x} = (\mathbf{x}_1^1, \dots, \mathbf{x}_N^1, \mathbf{x}_1^2, \dots, \mathbf{x}_N^2)^T$  represents the

states of  $2N$  nodes. If interconnections exist between all pairs of corresponding nodes, we have  $\Lambda = I_N$ , where  $I_N$  is unit matrix of dimension  $N$ . Since  $H$  is symmetric, according to the exact controllability theory [equation (5)], we have

$$N_D = \max_i \left\{ \delta(\lambda_i^H) \right\}, \quad (25)$$

where  $\delta(\lambda_i^H)$  is the algebraic multiplicity of  $\lambda_i^H$ . Analogous to the two-relation network, we are able to derive the lower and upper bounds of  $N_D$ . In particular, we rewrite  $H$  as

$$H = H_1 + H_2 = \begin{bmatrix} D_1 A_1 & 0 \\ 0 & D_2 A_2 \end{bmatrix} + \begin{bmatrix} -D_x \Lambda & D_x \Lambda \\ D_x \Lambda & -D_x \Lambda \end{bmatrix}. \quad (26)$$

The two bounds are given in terms of the eigenvalue properties of  $H_0$  ( $H_0$  with  $\Lambda = I_N$  equals to  $H$ ) and  $H_1$ :

$$\max_i \left\{ \delta(\lambda_i^{H_0}) \right\} \leq N_D \leq \max_i \left\{ \delta(\lambda_i^{H_1}) \right\}. \quad (27)$$

In contrast to the two-relation network, here the bounds are determined by both layers. To reveal the impact of interconnections on  $N_D$ , we consider two cases: (I)  $\Lambda = I_N$  (full interconnections) and (II)  $\Lambda \neq I_N$  (partial interconnections). We set  $D_2 = D_1$  to simplify the formulation of  $N_D$ .

For case (I), we consider two subcategories: (i)  $A_1$  and  $A_2$  are both sparse and (ii) they are both dense. For (i), we can derive from the characteristic polynomial that there are two eigenvalues:  $\lambda_1 = 0$  and  $\lambda_2 = -2D_x$  corresponding to identical maximum algebraic multiplicity. Inserting the eigenvalues into equation (4) leads to the efficient criterion:

$$N_D = 2N - \text{rank}(H) = 2N - \text{rank}(2D_x I_{2N} + H). \quad (28)$$

For (ii), the two eigenvalues are  $\lambda_1 = -D_1$  and  $\lambda_2 = -D_1(1 + 2D_x)$ , which are associated with identical maximum algebraic multiplicity. We obtain the following efficient criterion:

$$N_D = 2N - \text{rank}(D_1 I_{2N} + H) = 2N - \text{rank}[D_1(1 + 2D_x)I_{2N} + H]. \quad (29)$$

For case (II)  $\Lambda \neq I_N$ , we explore the effect of the fraction of interconnections on  $N_D$  by simply setting  $D_1$ ,  $D_2$  and  $D_x$  to be unity. In this case, the trace  $\text{tr}(\Lambda)$  of  $\Lambda$  is less than or equal to  $N$  due to partial interconnections. There are also two subcategories: (i)  $A_1$  and  $A_2$  are both sparse and (ii) they are both dense. Our theoretical analysis indicates that for (i), zero becomes the key eigenvalue, yielding the following efficient criterion:

$$N_D = 2N - \text{rank}(H). \quad (30)$$

For (ii), the eigenvalue becomes  $-1$ , leading to

$$N_D = 2N - \text{rank}(I_{2N} + H). \quad (31)$$

Appendix C presents detailed derivations of equation (28)-(31).

### 3. Numerical results

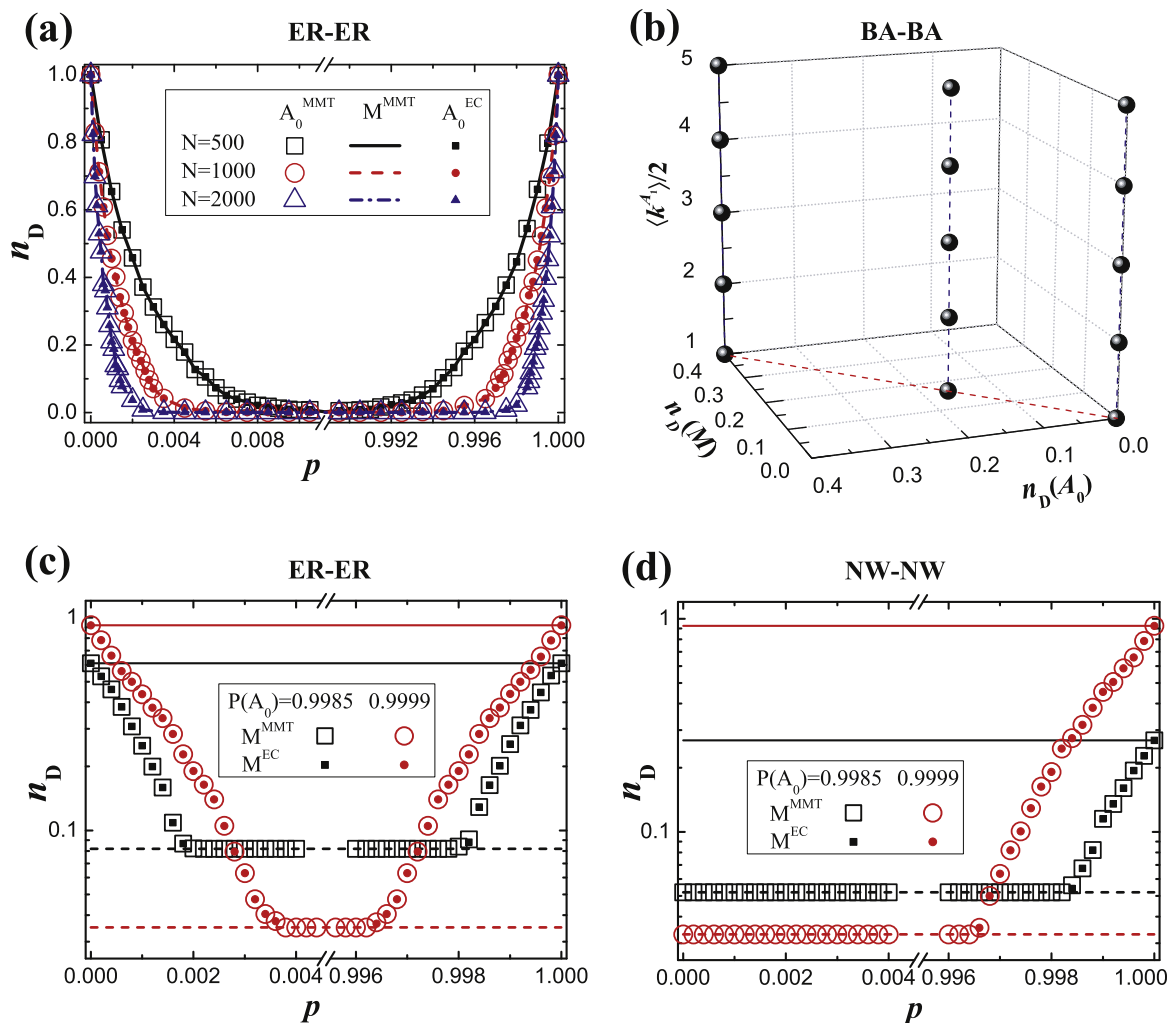
*Random, scale-free, and small-world double-relation networks.* We numerically validate our exact controllability theory using Erdős–Rényi (ER) random [26], Barabási–Albert (BA)

scale-free [27] and Newman-Watts (NW) small-world networks [28]. Figure 2 shows the controllability measure  $n_D \equiv N_D/N$  of the networks with two types of relations [figure 1(a) and equation (1)] with respect to different cases in terms of the zeroth-order layer  $A_0$  and the first-order layer  $A_1$ . For  $A_0 = A_1$  [figure 2(a)]  $n_D$  of the duplex network is exactly the same as that of the single network  $A_0$ , as predicted. For  $A_0 \neq A_1$  and  $A_0$  is sparse [figure 2(b)],  $n_D(M)$  of the duplex network is exactly equal to  $n_D(A_0)$  of layer  $A_0$ , regardless of the average degree of layer  $A_1$ , in agreement with our prediction. If  $A_0 \neq A_1$  and  $A_0$  is dense [figures 2(c) and 2(d)],  $n_D$  is a result of the interplay between the two layers. The lower and upper bounds are explicit and determined solely by  $A_0$ , as predicted by our theory. An interesting finding is that  $n_D$  can be either a non-monotonic [figures 2(a) and 2(c)] or a monotonic [figure 2(d)] function of the link density of two layers, depending on the structural property of each layer. All the results from the maximum multiplicity theory are in excellent agreement with our efficient criteria.

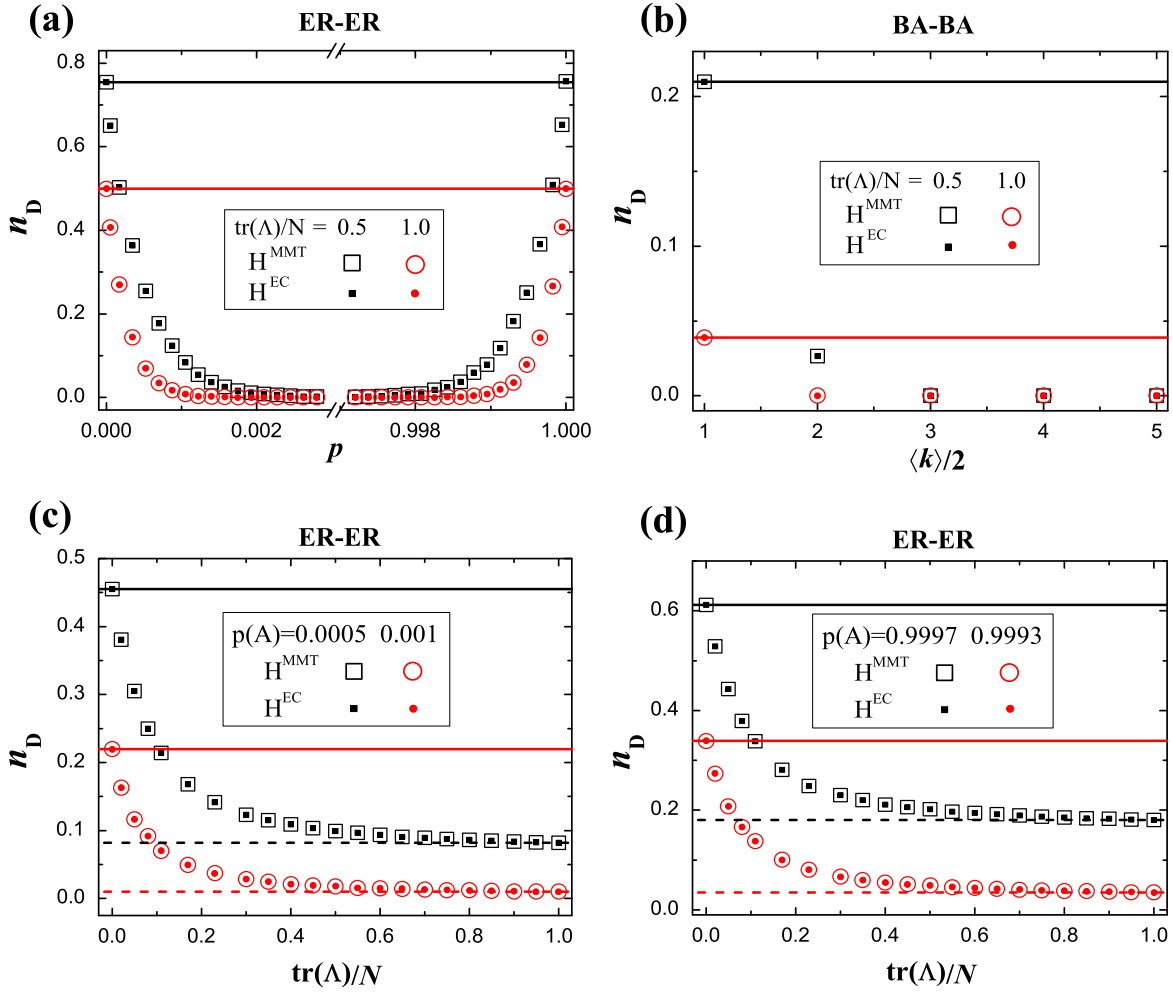
Figure 3 shows  $n_D$  of duplex networks with two interconnected layers  $A_1$  and  $A_2$  [figure 1(b) and equation (24)]. We find that there is no dominant layer in the sense that  $A_1$  and  $A_2$  play the same role in determining  $n_D$ . Two cases are considered: (I) adjusting link densities of both layers by fixing the fraction  $\text{tr}(\Lambda)/N$  of interconnections [figures 3(a) and 3(b)] and (II) changing  $\text{tr}(\Lambda)/N$  by fixing link densities [figures 3(c) and 3(d)]. We see that for fixed values of  $\text{tr}(\Lambda)/N$ ,  $n_D$  can be either a non-monotonic or a monotonic function of the link density, depending on the structural property of each layer. Interestingly, as shown in figures 3(c) and 3(d), the presence of a small fraction of interconnections can considerably improve the system's controllability compared with that for isolated layers, as demonstrated by the rapid decrease of  $n_D$  for small values of  $\text{tr}(\Lambda)/N$ . The results from the maximum multiplicity theory and the lower and upper bounds again are in exact agreement with those from our efficient criteria.

*Control implementation.* To address this issue, we offer a general method to identify the minimum set of driver nodes required to fully control multiplex networks. In particular, for the network system (8), the control matrix  $B$  associated with a minimum set of drivers satisfies  $\text{rank}[(\lambda^{\max})^2 I_N - \lambda^{\max} c_1 A_1 - c_0 A_0, B] = N$ , where  $\lambda^{\max}$  is the eigenvalue corresponding to the maximum geometric multiplicity. We implement elementary column transformation on the matrix  $(\lambda^{\max})^2 I_N - \lambda^{\max} c_1 A_1 - c_0 A_0$  to obtain the column canonical form of the matrix that reveals a set of linearly-dependent rows. The nodes corresponding to the linearly-dependent rows are the drivers. For the two-layer network system (24), the condition becomes  $\text{rank}[\lambda^{\max} I_{2N} - H, B] = 2N$ . Driver nodes can be identified as well via the column canonical form of  $\lambda^{\max} I_{2N} - H$ . For more details, see Appendix D.

*Undirected networks.* figure 4 shows the controllability  $n_D$  of undirected two-relation networks with different combinations of two layers. In particular, figures 4(a) and 4(b) show  $n_D$  of ER-BA and BA-ER duplex for the case where the zeroth-order layer  $A_0$  is sparse. We see that  $n_D(M)$  of the duplex is always equal to  $n_D(A_0)$ , regardless of the connection density of the first-order layer  $A_1$ , which is analogous to the observation in figure 2, further validating our theoretical prediction. In contrast, if the zeroth-order layer  $A_0$  is dense,  $n_D$  of the duplex depends on both layers, as shown in figures 4(c) and 4(d) for ER-NW and NW-ER pairs. Both the upper and lower bounds of exact controllability are successfully predicted analytically, as well as the controllability in between, providing stronger support for the validity of our theory.

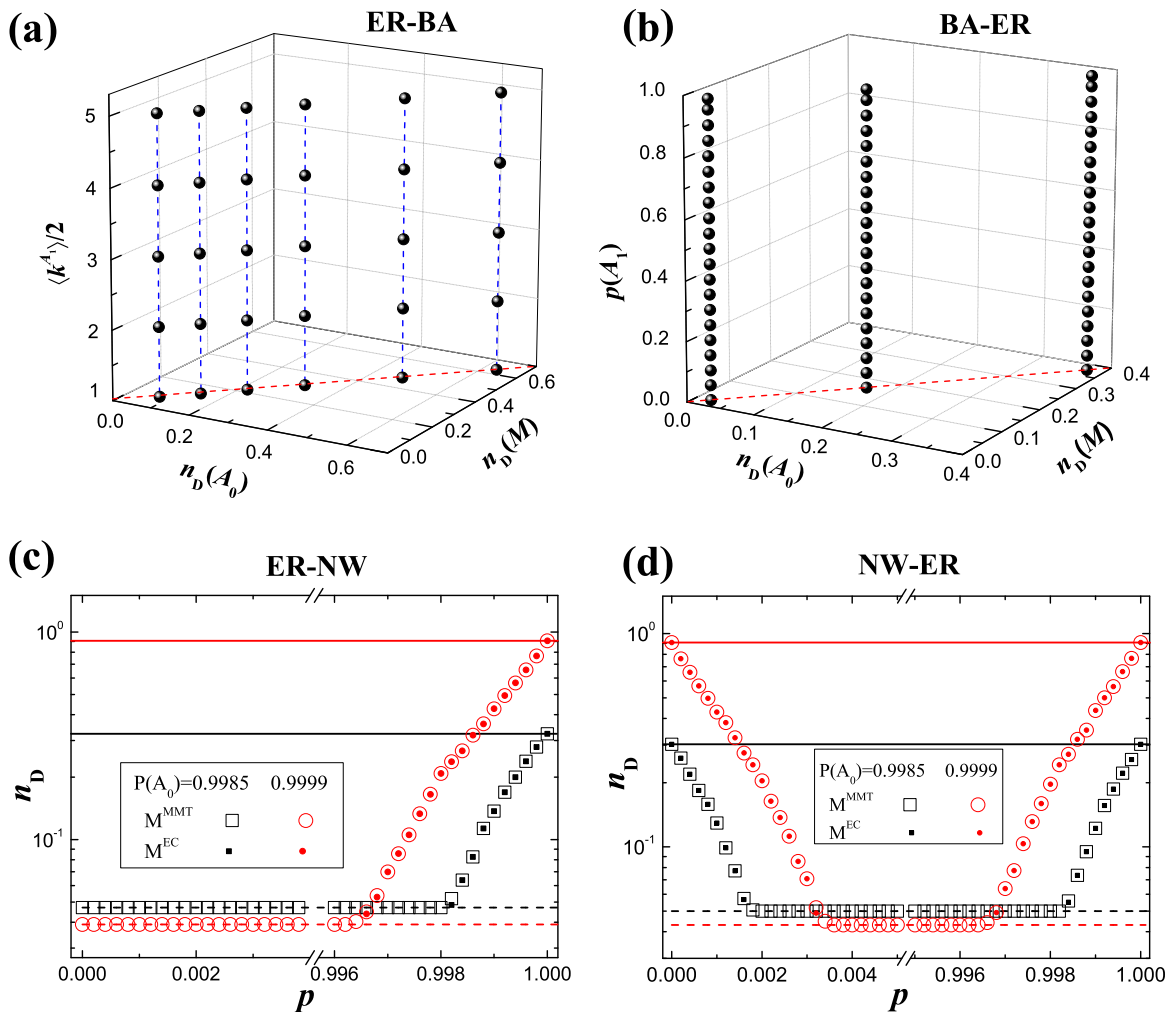


**Figure 2.** Controllability measure  $n_D$  of two-relation networks. (a)  $n_D$  as a function of the connection probability  $p$  of ER–ER pair with  $A_0 = A_1$ . (b)  $n_D(M)$  of the two-relation system versus  $n_D(A_0)$  of the zeroth-order layer for different half average degree  $\langle k^{A_1} \rangle / 2$  of the first-order layer  $A_1$ , where  $A_0$  is sparse in the BA–BA pair. (c)  $n_D$  as a function of the connecting probability  $p$  of  $A_1$  for ER–ER pair, where  $A_0$  is dense. (d)  $n_D$  as a function of random shortcut probability  $p$  in  $A_1$  for NW–NW pair, where  $A_0$  is dense. Here, superscript MMT and EC denote the maximum multiplicity theory and the efficient criteria, respectively. In (a),  $A_0^{\text{MMT}}$  and  $M^{\text{MMT}}$  are from equation (4), and  $A_0^{\text{EC}}$  denotes the results from the efficient criteria for sparse and dense connections. In (b),  $n_D(M)$  and  $n_D(A_0)$  are obtained from equation (4) and (17), and the dashed line is for eye guidance. In (c) and (d), the solid and dashed lines represent the upper and lower bounds of  $n_D$  obtained from equation (7), where the quantity  $M^{\text{MMT}}$  is from equation (4) and  $M^{\text{EC}}$  is from equation (20) and (22) for sparse and dense  $A_1$ , respectively.  $P(A_0)$  in (c) is the connecting probability of  $A_0$ , and in (d) it is the random shortcut probability in  $A_0$ . Both  $A_0$  and  $A_1$  are undirected and unweighted networks. Data points are the average of 50 independent realizations. In (b)–(d),  $N = 2000$ . We set  $c_0$  and  $c_1$  to be unity and have checked that  $n_D$  is insensitive to their values.

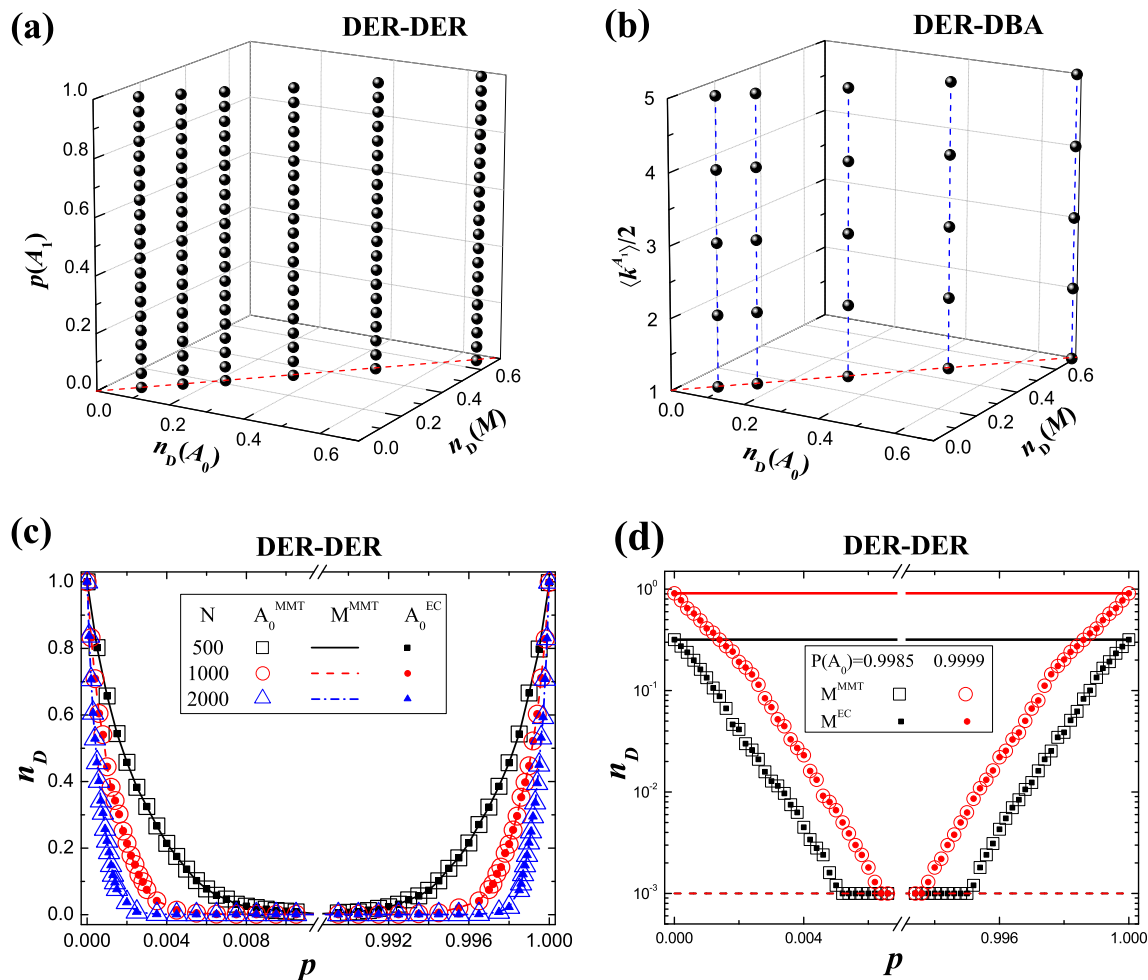


**Figure 3.** Controllability measure  $n_D$  of two-layer networks. (a)  $n_D$  as a function of the connecting probability  $p$  for fixed fraction  $\text{tr}(\Lambda)/N$  of interconnections of ER–ER pair. (b)  $n_D$  as a function of half of the average degree  $\langle k \rangle/2$  for fixed  $\text{tr}(\Lambda)/N$  of BA–BA pair. (c) and (d),  $n_D$  as a function of the fraction  $\text{tr}(\Lambda)/N$  of interconnections for fixed connection densities  $p(A)$  in both layers. The solid and dashed lines represent the upper and lower bounds of  $n_D$  obtained from equation (27). Both layers have identical average degrees.  $H^{\text{MMT}}$  in (a)–(d) refers to the exact controllability from equation (5). For  $\text{tr}(\Lambda)/N = 1.0$ ,  $H^{\text{EC}}$  denotes the results obtained from equation (28) and (29) for sparse and dense connections of both layers, respectively. For  $\text{tr}(\Lambda)/N < 1.0$ ,  $H^{\text{EC}}$  denotes the results from equation (30) and (31) for sparse and dense connections of both layers, respectively. Both layers are undirected with size  $N = 2000$ , and 50 independent realizations are used.

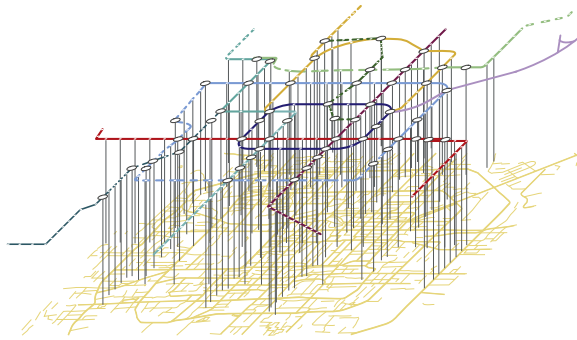
*Directed networks.* figure 5 shows the controllability  $n_D$  of directed two-relation duplex for different combinations of ER random network and BA scale-free networks. The directions of links are randomly set for the BA and for ER networks, bidirectional links are possible among nodes, and each directed link is established according to the connecting probability  $p$ . figure 5(a) and 5(b) show that  $n_D(M)$  is always equal to  $n_D(A_0)$  if  $A_0$  is sparse, regardless of the connection density of  $A_1$ , analogous to the results of undirected networks. Figure 5(c) shows that for the case of  $A_0 = A_1$ , regardless of whether  $A_0$  is sparse or dense,  $n_D$  values of



**Figure 4.** Controllability measure  $n_D(M)$  of the undirected, two-relation network versus the controllability measure  $n_D(A_0)$  of the sparse zeroth-order layer  $A_0$  for (a) undirected ER–BA pair, where  $\langle k^{A_1} \rangle$  is the average degree of the first-order undirected BA network  $A_1$  and (b) undirected BA–ER pair, where  $p(A_1)$  is the randomly connecting probability of  $A_1$ . Here, the red dashed lines represent  $n_D(M) = n_D(A_0)$ . We see that  $n_D(M) = n_D(A_0)$  always holds, regardless of the connection density of  $A_1$ . (c)  $n_D$  versus the probability  $p$  of randomly adding shortcuts in the first-order layer  $A_1$  for ER–NW pair, for dense zeroth-order layer  $A_0$ , where  $P(A_0)$  is the random connecting probability of  $A_0$ . (d)  $n_D$  versus the randomly connecting probability  $p$  of  $A_1$  for NW–ER pair, for dense layer  $A_0$ , where  $P(A_0)$  is the random shortcut probability of  $A_0$ . In (a) and (b), the values of  $n_D(M)$  and  $n_D(A_0)$  are obtained by the maximum multiplicity theories in equation (4) and equation (5), respectively. We have checked that  $n_D(A_0)$  from equation (5) is the same as those from the efficient criterion equation (A4). In (c) and (d), the solid and dashed lines represent the upper and lower bounds of  $n_D$  obtained from equation (7). The quantity  $M^{MMT}$  denotes the controllability measure of the duplex from equation (4), and  $M^{EC}$  denotes the controllability measure of the duplex calculated from the efficient criteria equation (20) and equation (22) for sparse and dense  $A_1$  layers, respectively. Each data point is the average over 50 independent realizations, and the network size  $N$  is 2000.



**Figure 5.** Controllability measure  $n_D(M)$  of the directed, two-relation network versus the controllability measure  $n_D(A_0)$  of the sparse zeroth-order layer  $A_0$  for (a) DER–DER pair, where  $p(A_1)$  is the connecting probability of directed ER network  $A_1$  and (b) DER–DBA pair, where  $\langle k^{A_1} \rangle$  is the average degree of the first-order directed BA network  $A_1$ . Here, the red dashed lines represent  $n_D(M) = n_D(A_0)$ . We see that  $n_D(M) = n_D(A_0)$  always holds, regardless of the connection density of  $A_1$ . (c)  $n_D$  versus the random connecting probability  $p$  of DER–DER pair, when  $A_0 = A_1$ . (d)  $n_D$  versus the random connecting probability  $p$  of layer  $A_1$  for DER–DER pair, when layer  $A_0$  is dense, where  $P(A_0)$  is the random connecting probability of  $A_0$ . In (a) and (b), the quantities  $n_D(M)$  and  $n_D(A_0)$  are obtained by the maximum multiplicity theories, equation (4). We have checked that the values of  $n_D(A_0)$  from equation (4) are the same as those from the efficient criterion equation (A4). In (c), the quantity  $A_0^{\text{MMT}}$  is the  $n_D$  measure of the zeroth-order layer  $A_0$  obtained by the maximum multiplicity theory equation (4),  $M^{\text{MMT}}$  is the  $n_D$  value of the duplex from the maximum multiplicity theory equation (4), and  $A_0^{\text{EC}}$  denotes the values of  $n_D$  from the efficient criteria of equation (A4) and equation (A5) for sparse and dense connection, respectively. In (d), the solid and dashed lines represent the upper and lower bounds of  $n_D$  obtained from equation (7),  $M^{\text{MMT}}$  is the controllability measure of the duplex from equation (4) and  $M^{\text{EC}}$  denotes the controllability measure calculated from the efficient criteria equation (20) and equation (22) for sparse and dense  $A_1$  layers, respectively. Each data point is the average over 50 independent realizations, and the network sizes  $N$  in (a), (b) and (d) are 2000.



**Figure 6.** A real bus-subway two-layer network in Beijing, China. For better visualization, we set the subway network to be the upper layer and the bus network to be the lower layer. In the subway layer, the colors represent different subway lines. In the bus layer, there are a large number of different bus lines, so that we don't distinguish them by different colors. Interlayer connections represented by vertical lines represent the existence of transfer stations between bus and subway at a specific location. The bus-subway network is a typical two-layer network, the controllability of which can be calculated by our theoretical tools.

the directed duplex networks exhibit quite similar qualitative behaviors to those for undirected duplex networks. Figure 5(d) shows  $n_D$  of the directed duplex if  $A_0$  is dense, where the value of  $n_D$  depends on both layers, similar to the undirected duplex. All the numerical results of  $n_D$ , as well as the lower and upper bounds are in excellent agreement with the analytical prediction.

#### 4. A real two-layer network of public traffic system

We apply our controllability criteria to a two-layer public traffic network consisting of a bus network and a subway network in Beijing, China. The structure of the two-layer network is shown in figure 6. In the bus layer, there are 2267 bus stations in total, and in the layer of subway, there are 188 subway stations in total. For the bus network, if there is a direct bus line between two bus stations (without any more stations between them), they are connected by an undirected link. The links in the subway network represent the same meaning as those of the bus network. Interlayer connections between the two layers stand for the existence of transfer stations between bus and subway at a location. We find that there are 97 interlayer connections.

Although the number of nodes in the subway layer is less than that in the bus layer, our theoretical tools are still available to calculate  $n_D$ . We first calculate the  $n_D$  of each layer individually by using the exact controllability theory for a single layer, yielding that  $n_D$  of bus layer is 0.0543 and that of subway layer is 0.0213. These results demonstrate that each layer is of high controllability. We then use the exact controllability theory for two layer networks to calculate the bus-subway network.  $n_D$  of the two-layer network is 0.0424, indicating that the controllability of the bus-subway network is in between that of each single layer. It is noteworthy that the structural controllability theory is not applicable in the bus-subway network, because the two-layer network is undirected.



## 5. Conclusion

To summarize, we have developed a general theoretical framework based on the maximum multiplicity theory to assess the exact controllability of multiplex networks. The framework, as an alternative to but going much beyond the recently introduced structural controllability theory, is applicable to arbitrary single and multiplex networks, including weighted/unweighted, directed/undirected and connected/disconnected networks/layers. Applying the framework to two general classes of prototypical duplex networks, we find that for the two-relation network, the zeroth-order layer plays the dominant role in controllability. However, in the interconnected two-layer network, the controllability bounds are determined by the interplay between two layers, and the presence of a small fraction of interconnections can considerably improve the system's controllability. We have also introduced a general method to identify the minimum set of driver nodes to achieve full control of the multiplex network.

We wish to make two remarks. (1) The controllability measure of certain complex networks can also be approximately calculated by a known method from statistical physics, the cavity method [29–31]. (2) Our framework based on the maximum multiplicity theory is sufficiently distinct from the recently introduced structural controllability theory for complex networks [17], where it was proved that the structural controllability of any directed network as characterized by the structural matrix is determined by the maximum matching of the network topology. In contrast, our framework is applicable to any network, including directed, undirected, weighted, unweighted, connected or disconnected networks with many components. In this regard, our framework offers a more general theoretical tool to study multiplex networks that are the subject of intense and extensive recent research in a wide range of fields.

Although we focus our study on the two representative classes of multiplex networks, our framework is applicable to any multiplex network with arbitrary architecture, insofar as such a network can be mathematically represented in a matrix form. Our theory thus offers an approach, more general than any previous one, toward understanding and controlling complex multiplex networks of significant physical interest.

## Acknowledgements

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## Appendix A: Proof of exact Controllability theory for arbitrary single-layer networks

Although the exact controllability theory has been proved in our previously published work [23], here we offer a simpler proof of the theory. According to the PBH rank condition, system (1) is controllable if and only if for each  $\lambda_i \in \sigma(A)$ , the relation  $\text{rank}[\lambda_i I_N - A, B] = N$  holds. In terms of the rank inequality, we have

$$N = \text{rank}[\lambda_i I_N - A, B] \leq \text{rank}(\lambda_i I_N - A) + \text{rank}(B), \quad (\text{A1})$$

such that

$$\text{rank}(B) \geq N - \text{rank}(\lambda_i I_N - A). \quad (\text{A2})$$

Equation (A2) will be satisfied if  $\text{rank}(B)$  is larger than or equal to the maximum value of  $N - \text{rank}(\lambda_i I_N - A)$  for all eigenvalues  $\lambda_i$ . Consequently, the minimum value of  $\text{rank}(B)$  is the maximum value of  $N - \text{rank}(\lambda_i I_N - A)$ . That is, we can define the minimum number  $N_D$  of controllers or independent drivers, which is equal to  $\min \{\text{rank}(B)\}$ , as

$$N_D = \max_i \left\{ N - \text{rank}(\lambda_i I_N - A) \right\} = \max_i \left\{ \mu(\lambda_i) \right\}. \quad (\text{A3})$$

If  $A$  is diagonalizable, e.g., it is a symmetric matrix, then  $\delta(\lambda_i) = \mu(\lambda_i)$ , yielding

$$N_D = \max_i \left\{ \delta(\lambda_i) \right\}.$$

where  $\delta(\lambda_i)$  is the algebraic multiplicity of  $\lambda_i$ . For a sparse network without self-loops, it can be proved that [23]

$$N_D = \max \{1, N - \text{rank}(A)\}. \quad (\text{A4})$$

For a densely connected network, it can be proved that [23]

$$N_D = \max \{1, N - \text{rank}(I_N + A)\}. \quad (\text{A5})$$

## Appendix B: Exact controllability theory for multiple-relation networks of arbitrary order

Our theory for two-relation networks can be generalized to multi-relation networks of arbitrary orders, as described by

$$\begin{aligned} \dot{\mathbf{x}}_0 &= \mathbf{x}_1 \\ \dot{\mathbf{x}}_1 &= \mathbf{x}_2 \\ &\vdots \\ \dot{\mathbf{x}}_{n-1} &= A_0 \mathbf{x}_0 + A_1 \mathbf{x}_1 + \cdots + A_{n-1} \mathbf{x}_{n-1} + B \mathbf{u}, \end{aligned} \quad (\text{A6})$$

where  $A_i$  ( $i = 0, 1, \dots, n-1$ ) denotes the coupling matrix corresponding to  $\mathbf{x}_i$ .

For the general system (A6), we prove that

- The lower bound and the upper bound always exist, determined by the zeroth-order network  $A_0$ :  $N - \text{rank}(A_0) \leq N_D$ , where  $\lambda_i^{A_0}$  ( $i = 1, 2, \dots, N$ ) are the eigenvalues of  $A_0$ .
- If  $A_0 = A_1 = \cdots = A_{n-1}$ , then  $N_D = \max_i \{\mu(\lambda_i^{A_0})\}$ , which is exclusively determined by the zeroth-order network  $A_0$ .
- For general  $A_i$  ( $i = 0, 1, \dots, n-1$ ),  $N_D = N - \min_s \{\text{rank}(f_0(s))\}$  where  $s \in C$  with  $f_0(x) = I_N x^n - A_{n-1} x^{n-1} - A_{n-2} x^{n-2} - \cdots - x A_1 - A_0$ .

If  $A_0$  is sparse, regardless of the structure of other layers, we have  $N_D = N - \text{rank}(A_0)$ , the lower bound as determined by the rank of zeroth-order network  $A_0$ .

If  $A_0 = 0$ , then  $N_D = N$ , which means that, if the zeroth-order network does not exist, all nodes need to be controlled to realize full control.

If  $A_0$  is dense with sparse  $A_i$  ( $i = 1, \dots, n-1$ ), we have  $N_D = N - \text{rank}[f_0(s)]$ , where  $s$

satisfies  $s^n + 1 = 0$ .

If all of  $A_i$  ( $i = 0, 1, \dots, n - 1$ ) are dense, we have  $N_D = N - \text{rank}(f_0(s))$  where  $s$  satisfies  $s^n + s^{n-1} + \dots + s + 1 = 0$ .

**Proof.** Without changing the controllability, system (A6) can be transformed into

$$\dot{\mathbf{y}} = M\mathbf{y} + B'\mathbf{u} \tag{A7}$$

with  $\mathbf{y} = (\mathbf{x}_0^T, \mathbf{x}_1^T, \dots, \mathbf{x}_{n-1}^T)^T$ ,  $B' = (0, 0, \dots, 0, B^T)^T$  and

$$M = \begin{bmatrix} 0 & I_N & 0 & \dots & 0 & 0 \\ 0 & 0 & I_N & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & I_N \\ A_0 & A_1 & A_2 & \dots & A_{n-2} & A_{n-1} \end{bmatrix}.$$

From the PBH rank condition, the system is fully controllable if and only if

$$\text{rank}[sI_{nN} - M, B'] = \text{rank} \begin{bmatrix} sI_N & -I_N & 0 & \dots & 0 & 0 & 0 \\ 0 & sI_N & -I_N & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & sI_N & -I_N & 0 \\ -A_0 & -A_1 & -A_2 & \dots & -A_{n-2} & sI_N - A_{n-1} & B \end{bmatrix} = nN \tag{A8}$$

for any complex number  $s$ .

We can implement elementary transformation on  $[sI_{nN} - M, B']$ , as follows. First, from the  $n$ th column to first column, we multiply  $-s$  by the  $i$ th column and add the result to the  $(i - 1)$  th column so as to give the following matrix  $M_1$  that has the same rank as  $[sI_{nN} - M, B']$ :

$$M_1 = \begin{bmatrix} 0 & -I_N & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & -I_N & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & -I_N & 0 \\ f_0(s) & f_1(s) & f_2(s) & \dots & f_{n-1}(s) & f_n(s) & B \end{bmatrix}, \tag{A9}$$

where

$$\begin{aligned} f_0(s) &= I_N s^n - A_{n-1} s^{n-1} - A_{n-2} s^{n-2} - \dots - sA_1 - A_0, \\ f_1(s) &= I_N s^{n-1} - A_{n-1} s^{n-2} - A_{n-2} s^{n-3} - \dots - sA_2 - A_1, \\ f_2(s) &= I_N s^{n-2} - A_{n-1} s^{n-3} - A_{n-2} s^{n-4} - \dots - sA_3 - A_2, \\ &\vdots \\ f_{n-1}(s) &= s(sI_N - A_{n-1}) - A_{n-2}, \\ f_n(s) &= sI_N - A_{n-1}. \end{aligned} \tag{A10}$$

Secondly, from the first row to  $(n - 1)$  th row, we multiply  $f_i(s)$  by the  $i$ th row and add the result to the  $n$ th row with  $f_i(s) = sf_{i+1}(s) - A_i$ ,  $f_{n-1}(s) = sI_N - A_{n-1}$ , which yields the following matrix  $M_2$  with the same rank as  $[sI_{nN} - M, B']$ :

$$M_2 = \begin{bmatrix} 0 & -I_N & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & -I_N & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & -I_N & 0 \\ f_0(s) & 0 & 0 & \cdots & 0 & 0 & B \end{bmatrix} \quad (\text{A11})$$

According to the PBH rank condition, the general  $n$ th-order system is controllable if and only if

$$nN = \text{rank}[sI_{nN} - M, B'] = \text{rank}[M_2] = (n - 1)N + \text{rank}[f_0(s), B] \quad (\text{A12})$$

for any  $s$ . This means

$$\text{rank}[f_0(s), B] = N \quad (\text{A13})$$

should be satisfied for any  $s$ . From the definition  $N_D = \min \{\text{rank}(B)\}$ , we can have

$$N_D = \max_s \left\{ N - \text{rank}(f_0(s)) \right\} = N - \min_s \left\{ \text{rank}(f_0(s)) \right\}. \quad (\text{A14})$$

Apparently,

$$\min_s \left\{ \text{rank}(f_0(s)) \right\} \leq \text{rank}(A_0) \quad (\text{A15})$$

can be proven to be valid, analogous to the two-layer case. This thus gives the lower bound

$$N_D \geq N - \text{rank}(A_0). \quad (\text{A16})$$

In the case of  $A_i = A_0$  ( $i = 1, 2, \dots, n - 1$ ), we have

$$\text{rank}[f_0(s), B] = \text{rank}\left[ I_N s^n - (s^{n-1} + s^{n-2} + \cdots + s + 1)A_0, B \right].$$

- If  $s$  satisfies  $s^{n-1} + s^{n-2} + \cdots + s + 1 = 0$ , then  $s \neq 0$  and  $s^n \neq 0$ , so

$$\text{rank}[f_0(s), B] = \text{rank}[I_N s^n, B] = N;$$

- For other  $s$  that satisfies  $s^{n-1} + s^{n-2} + \cdots + s + 1 \neq 0$ , we have

$$\text{rank}[f_0(s), B] = \text{rank}\left[ \frac{s^n}{s^{n-1} + s^{n-2} + \cdots + s + 1} I_N - A_0, B \right].$$

This means that if  $B$  satisfies  $\text{rank}[sI_N - A_0, B] = N$  for all complex numbers  $s$ , then  $\text{rank}[sI_{nN} - M, B'] = nN$  for  $s \in \mathbb{C}$ , i.e.,  $N_D = \max_i \{\mu(\lambda_i^{A_0})\}$ .

If  $A_0$  is sparse,  $M$  is sparse as well. In this case,  $s = 0$  is the eigenvalue associated with the maximum geometric multiplicity of  $M$ . Therefore, we have  $N_D = \mu(0) = N - \text{rank}(A_0)$ .

If  $A_0 = 0$ , we have  $\text{rank}(A_0) = 0$ , leading to  $N_D = N - \text{rank}(A_0) = N$ .

If  $A_0$  is dense and  $A_i$  ( $i = 1, \dots, n - 1$ ) are sparse, we can get  $p_M(\lambda) = p_{A_0}(\lambda^n)$  by setting  $A_i = 0$  ( $i = 1, \dots, n - 1$ ). Due to the fact that  $-1$  corresponds to the maximum multiplicity of dense  $A_0$ , the eigenvalue  $s$  of  $M$  associated with the maximum multiplicity satisfies  $s^n + 1 = 0$ , yielding  $N_D = N - \text{rank}(f_0(s))$ .

If all  $A_i$ 's ( $i = 0, 1, \dots, n - 1$ ) are dense,  $-1$  becomes the eigenvalue corresponding to the maximum multiplicity. By setting  $A_i = A_0$  ( $i = 1, \dots, n - 1$ ), we can derive

$$p_M(\lambda) = (\lambda^{n-1} + \lambda^{n-2} + \dots + \lambda + 1)^{N-1} p_{A_0} \left( \frac{\lambda^n}{\lambda^{n-1} + \lambda^{n-2} + \dots + \lambda + 1} \right).$$

Since  $-1$  corresponds to the maximum multiplicity of dense  $A_0$ , the eigenvalue  $s$  of  $M$  associated with the maximum multiplicity satisfies

$$\frac{s^n}{s^{n-1} + s^{n-2} + \dots + s + 1} + 1 = 0,$$

or equivalently  $s^n + s^{n-1} + s^{n-2} + \dots + s + 1 = 0$ , which gives  $N_D = N - \text{rank}(f_0(s))$ . This completes our proof. It is noteworthy that the matrices  $A_i$  ( $i = 0, 1, \dots, n-1$ ) are the adjacency matrices of the respective networks.

### Appendix C: Calculations of exact controllability of multiple interconnected layers

We provide detailed theoretical calculations for the controllability of a two-layer network system with interlayer connections as described in the matrix form equation (23) for the two cases: full interlayer and partial interlayer connections. We also treat the case of three interconnected layers.

*Full interlayer connections.* We have  $\Lambda = I_N$  and thus

$$H_2 = H_0 = \begin{bmatrix} -D_x I_N & D_x I_N \\ D_x I_N & -D_x I_N \end{bmatrix}.$$

To calculate the characteristic polynomial of  $H$  so as to identify the key eigenvalues, we set  $A_2 = A_1$  and the calculation proceeds, as follows:

$$\begin{aligned} p_H(\lambda) &= |\lambda I_{2N} - H| \\ &= \begin{vmatrix} (\lambda + D_x)I_N - D_1 A_1 & -D_x I_N \\ -D_x I_N & (\lambda + D_x)I_N - D_1 A_1 \end{vmatrix} \\ &= \left| [(\lambda + D_x)I_N - D_1 A_1]^2 - D_x^2 I_N \right| \\ &= \left| [(\lambda + D_x)I_N - D_1 A_1 - D_x I_N][(\lambda + D_x)I_N - D_1 A_1 + D_x I_N] \right| \\ &= |\lambda I_N - D_1 A_1| |(\lambda + 2D_x)I_N - D_1 A_1| \\ &= D_1^{2N} p_{A_1} \left( \frac{\lambda}{D_1} \right) p_{A_1} \left( \frac{\lambda + 2D_x}{D_1} \right). \end{aligned}$$

This result suggests that there is a one-to-one correspondence between the eigenvalues of matrix  $A_1$  and that of matrix  $H$ . We can thus predict the eigenvalue of  $H$  associated with the maximum multiplicity based on such correspondence. In particular, assuming that  $\lambda_0$  is the eigenvalue of  $A_1$ , i.e., the characteristic polynomial  $p_{A_1}(\lambda)$  has a factor  $\lambda - \lambda_0$ , the characteristic polynomial of matrix  $H$  must contain factors  $\lambda/D_1 - \lambda_0$  and  $(\lambda + 2D_x)/D_1 - \lambda_0$ , leading to two eigenvalues  $D_1 \lambda_0$  and  $D_1(\lambda_0 - 2D_x)$  with the same multiplicity as that of  $\lambda_0$  in  $A_1$ .

When both  $A_1$  and  $A_2$  are sparse, the eigenvalue associated with the maximum multiplicity is  $\lambda_0 = 0$ , i.e.,  $p_{A_1}(\lambda)$  has a factor  $\lambda$  associated with the maximum geometric multiplicity. Thus  $p_H(\lambda)$  has factors  $\lambda/D_1$  and  $(\lambda + 2D_x)/D_1$ , indicating that the eigenvalues associated with the

maximum geometric multiplicity of  $H$  are  $\lambda_1 = 0$  and  $\lambda_2 = -2D_x$ , resulting from  $\lambda/D_1 = 0$  and  $(\lambda + 2D_x)/D_1 = 0$ , respectively. Therefore,  $N_D$  of the two-layer network when  $A_1$  and  $A_2$  are both sparse is

$$N_D = \mu(0) = 2N - \text{rank}(H) \quad (\text{A17})$$

or

$$N_D = \mu(-2D_x) = 2N - \text{rank}(2D_x I_{2N} + H). \quad (\text{A18})$$

When  $A_1$  and  $A_2$  are dense, the eigenvalue corresponding to the maximum geometric multiplicity is  $\lambda_0 = -1$  and  $p_{A_1}(\lambda)$  has a factor  $\lambda + 1$  associated with the maximum geometric multiplicity, accounting for the fact that  $p_H(\lambda)$  has factors  $\frac{\lambda}{D_1} + 1$  and  $\frac{\lambda + 2D_x}{D_1} + 1$ . The eigenvalues associated with the maximum geometric multiplicity of  $H$  become  $\lambda_1 = -D_1$  and  $\lambda_2 = -D_1(1 + 2D_x)$ , resulting from  $\frac{\lambda}{D_1} + 1 = 0$  and  $\frac{\lambda + 2D_x}{D_1} + 1 = 0$ , respectively.  $N_D$  of the two-layer network when both  $A_1$  and  $A_2$  are dense is

$$N_D = \mu(-D_1) = 2N - \text{rank}(D_1 I_{2N} + H), \quad (\text{A19})$$

or

$$N_D = \mu(-D_1(1 + 2D_x)) = 2N - \text{rank}(D_1(1 + 2D_x)I_{2N} + H). \quad (\text{A20})$$

*Partial-interlayer connections.* We set  $D_2 = D_1 = D_x = 1$  and explore the impact of the fraction of interlayer connections on the controllability of the two-layer network. In this case,  $H_1 = \begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix}$  and  $H_2 = \begin{bmatrix} -\Lambda & \Lambda \\ \Lambda & -\Lambda \end{bmatrix}$ . If there are a small fraction  $\text{tr}(\Lambda)/N$  of interlayer connections,  $H_2$  can be regarded as perturbations to  $H_1$  and the eigenvalue corresponding to the maximum multiplicity is mainly determined by  $H_1$ . Thus, when both  $A_1$  and  $A_2$  are sparse, the eigenvalue of  $H$  as determined by  $H_1$  is 0 as well. We then have, for the two-layer network,

$$N_D = \mu(0) = 2N - \text{rank}(H), \quad (\text{A21})$$

Analogously, when both  $A_1$  and  $A_2$  are dense, the eigenvalue of  $H_1$  corresponding to the maximum multiplicity is  $-1$ , leading to

$$N_D = \mu(-1) = 2N - \text{rank}(I_{2N} + H). \quad (\text{A22})$$

*Exact controllability of networks of three interconnected layers.* We can analytically calculate the eigenvalues associated with the maximum multiplicity for a three-layer network with full interlayer connections. The coupling matrix of the network becomes

$$H = H_1 + H_2 = \begin{bmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_3 \end{bmatrix} + \begin{bmatrix} -2I_N & I_N & I_N \\ I_N & -2I_N & I_N \\ I_N & I_N & -2I_N \end{bmatrix}, \quad (\text{A23})$$

where  $H_1$  and  $H_2$  denote the intra- and inter-coupling matrices, respectively.

The eigenvalues can be solved from the characteristic polynomial of  $H$  by setting  $A_1 = A_2 = A_3$ , as follows:

$$\begin{aligned}
p_H(\lambda) &= |\lambda I_{3N} - H| \\
&= \begin{vmatrix} (\lambda + 2)I_N - A_1 & -I_N & -I_N \\ -I_N & (\lambda + 2)I_N - A_1 & -I_N \\ -I_N & -I_N & (\lambda + 2)I_N - A_1 \end{vmatrix} \\
&= \begin{vmatrix} -I_N & (\lambda + 2)I_N - A_1 & -I_N \\ -I_N & -I_N & (\lambda + 2)I_N - A_1 \\ (\lambda + 2)I_N - A_1 & -I_N & -I_N \end{vmatrix} \\
&= \begin{vmatrix} -I_N & (\lambda + 2)I_N - A_1 & -I_N \\ 0 & -(\lambda + 3)I_N + A_1 & (\lambda + 3)I_N - A_1 \\ 0 & [(\lambda + 2)I_N - A_1]^2 - I & -(\lambda + 3)I_N + A_1 \end{vmatrix} \\
&= \begin{vmatrix} -I_N & (\lambda + 2)I_N - A_1 & -I_N \\ 0 & -(\lambda + 3)I_N + A_1 & (\lambda + 3)I_N - A_1 \\ 0 & [(\lambda + 3)I_N - A_1][(\lambda + 1)I_N - A_1] & -(\lambda + 3)I_N + A_1 \end{vmatrix} \\
&= |(\lambda + 3)I_N - A_1|^2 \begin{vmatrix} -I_N & (\lambda + 2)I_N - A_1 & -I_N \\ 0 & -I_N & I_N \\ 0 & (\lambda + 1)I_N - A_1 & -I_N \end{vmatrix} \\
&= |(\lambda + 3)I_N - A_1|^2 \begin{vmatrix} -I_N & (\lambda + 2)I_N - A_1 & -I_N \\ 0 & \lambda I_N - A_1 & 0 \\ 0 & [(\lambda + 1)I_N - A_1] & -I_N \end{vmatrix} \\
&= |(\lambda + 3)I_N - A_1|^2 |\lambda I_N - A_1| = p_{A_1}(\lambda) p_{A_1}^2(\lambda + 3).
\end{aligned}$$

From this result, we can infer that if  $A_1$  has the eigenvalue  $\lambda_0$  with algebraic multiplicity  $\delta(\lambda_0)$ ,  $H$  must have the eigenvalue  $\lambda_0$  with algebraic multiplicity  $\delta(\lambda_0)$  and the eigenvalue  $\lambda_{0-3}$  with algebraic multiplicity  $2\delta(\lambda_0 - 3)$ . This means that, when  $A_1$  has the eigenvalue  $\lambda_0$  associated with the maximum multiplicity, the eigenvalue of  $H$  corresponding to the maximum multiplicity is  $\lambda_{0-3}$ . So, when  $A_1, A_2$  and  $A_3$  are sparse, i.e.,  $\lambda_0 = 0$ , the three-layer network has

$$N_D = \mu(-3) = 3N - \text{rank}(3I_{3N} + H). \quad (\text{A24})$$

If  $A_1, A_2$  and  $A_3$  are dense, the eigenvalue  $\lambda_0 = -1$  corresponds to the maximum multiplicity, leading to

$$N_D = \mu(-4) = 3N - \text{rank}(4I_{3N} + H). \quad (\text{A25})$$

#### Appendix D: Method for identifying minimum set of driver nodes

The method for identifying a minimum set of driver nodes presented in the main text is generally applicable to any complex network systems that can be characterized in a matrix

form, for which a rigorous mathematical proof based on the PBH theory [22] and elementary matrix transformations has been provided in [23]. Consider an arbitrary network described by matrix  $A$ . The minimum number of driver nodes  $N_D$  is determined by the maximum geometric multiplicity  $\mu(\lambda^{\max})$  occurring at the eigenvalue  $\lambda^{\max}$ , which is ensured by the maximum multiplicity theory (4). Hence, the control matrix  $B$  needed to achieve full control should satisfy the PBH rank condition by substituting  $\lambda^{\max}$  for the complex number  $s$ , as follows:

$$\text{rank}[\lambda^{\max} I_N - A, B] = N. \quad (\text{A26})$$

Our goal then becomes that of identifying the minimum set of driver nodes in  $B$  to ensure the condition (A26). Note that  $\text{rank}[\lambda^{\max} I_N - A]$  is exclusively determined by the number of linearly-independent rows. If we are able to find all linearly-independent rows, the rest of the rows in  $A$  that violate the full rank condition can then be identified. This can be realized by implementing elementary column transformation on the matrix  $\lambda^{\max} I_N - A$ , which yields the column canonical form of matrix  $\lambda^{\max} I_N - A$ , revealing the linear dependence among the rows. The rows linearly-dependent on the others correspond to the driver nodes needed to achieve and maintain full control. The number of the identified nodes is  $N - \text{rank}(\lambda^{\max} I_N - A)$ , which is nothing but the maximum geometric multiplicity  $\mu(\lambda^{\max})$  of the eigenvalue  $\lambda^{\max}$ . Note that each column in  $B$  can at most eliminate one linear correlation. Thus the minimum number of columns of  $B$ , i.e.,  $\min\{\text{rank}(B)\}$  is the same as the number  $\mu(\lambda^{\max})$  of drivers. This means that the minimum number  $N_D$  of drivers as defined by  $N_D = \min\{\text{rank}(B)\}$  is exactly equal to the maximum geometric multiplicity  $\mu(\lambda^{\max})$ , a result of our maximum multiplicity theory obtained by performing elementary transformation on the matrix  $\lambda^{\max} I_N - A$ .

Note that there are no restrictions on the application of the method to complex networks, insofar as such a network can be mathematically represented in a matrix form. For the two classes of multiplex networks in the main text, this method allows us to find all driver nodes by using the transformed matrices of the multiple-relation networks and the multiple-layer networks, respectively.

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