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, Mulitplex 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
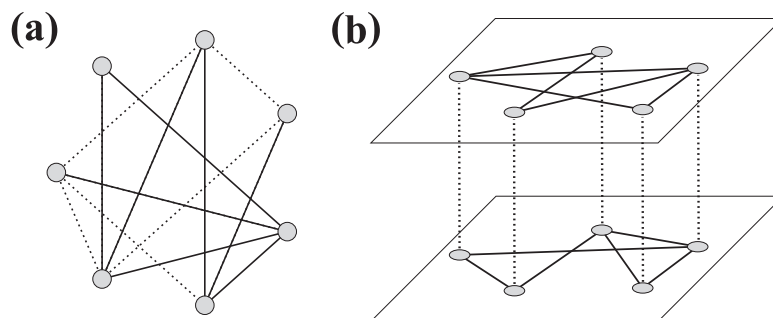
Figure 1. Examples of (a) a multiple-relation network and (b) a multiple-layer network with interconnections, with $M = 2$ layers. In (a), two relation networks (solid and dashed links) share the same set of nodes but characterize distinct relations associated with different physical variables. In (b), 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

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

where the vectors $\mathbf{x} = (x_1, \cdots, x_N)^T$ and $\mathbf{v} = (v_1, \cdots, v_N)^T$ 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]

$$
N_D = \min\left\{\operatorname{rank}(B)\right\}.
\tag{2}
$$

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:

$$\dot{\mathbf{x}} = A\mathbf{x} + B\mathbf{u}, \tag{3}$$

where the vector $\mathbf{x} = (x_1, \cdots, x_N)^T$ characterizes the states of N nodes, A denotes the coupling matrix, B is the control matrix and $\mathbf{u} = (u_1, u_2, \cdots, u_m)^T$ 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 $\mathrm{rank}[sI_N - A, B] = N$ 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:

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

where λ_i^A ($i = 1, 2, \cdots, l$) are the distinct eigenvalues of A, and $\mu(\lambda_i^A)$ is the geometric multiplicity defined as $N - \mathrm{rank}(\lambda_i^A I_N - A)$. 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 λ_i^A), so we have

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

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 $N_D^s = \max\{1, N - \mathrm{rank}(A)\}$ and for a dense network with unit link weights, we have $N_D^d = \max\{1, N - \mathrm{rank}(I_N + A)\}$ (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

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

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 $\mathrm{rank}[sI_{2N} - M, B'] = 2N$ is satisfied for any complex number s. After some elementary

algebra, we obtain

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

The necessary and sufficient controllable condition becomes then

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

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:

$$N - \mathrm{rank}(A_0) \leqslant N_D \leqslant \max_i \left\{ \mu\big(\lambda_i^{A_0}\big) \right\}, \tag{7}$$

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

$$\dot{\mathbf{y}} = M\mathbf{y} + B'\mathbf{u} \tag{8}$$

with

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

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

$$\mathrm{rank}\big[sI_{2N} - M, B'\big] = 2N \tag{9}$$

for any s, which can be simplified as

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

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

$$\mathrm{rank}\big[s^2I_N - sc_1A_1 - c_0A_0, B\big] = N. \tag{11}$$

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

$$\text{rank}(B) \geqslant N - \text{rank}\left(s^2 I_N - s c_1 A_1 - c_0 A_0\right). \tag{12}$$

Thus, for any A_0 and A_1, we can obtain

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

It is apparent that

$$\min\left\{\text{rank}\left(s^2 I_N - s c_1 A_1 - c_0 A_0\right)\right\} \leqslant \text{rank}\left(-c_0 A_0\right) = \text{rank}\left(A_0\right), \tag{13}$$

which gives the lower bound of N_D as

$$N_D = N - \min\left\{\text{rank}\left(s^2 I_N - s c_1 A_1 - c_0 A_0\right)\right\} \geqslant N - \text{rank}\left(A_0\right). \tag{14}$$

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

$$\dot{\mathbf{x}} = A_0 \mathbf{x} + B \mathbf{u} \tag{15}$$

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

$$\text{rank}\left[s^2 I_N - (s c_1 + c_0) A_0, B\right] = N. \tag{16}$$

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

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

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

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

Therefore, when B satisfies $\text{rank}[s I_N - A_0, B] = N$ for any s, we can conclude: $\text{rank}[s I_{2N} - M, B'] = 2N$ 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

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

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

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

We thus have the following efficient criterion:

$$N_D = \max\left\{1, N - \mathrm{rank}(A_0)\right\}, \tag{17}$$

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 $\mathrm{rank}[s^2 I_N - s c_1 A_1, B] = N$, which can be satisfied for $s = 0$ if and only if $\mathrm{rank}(B) = N$, indicating that for the system $\ddot{x}_0 = c_1 A_1 \dot{x} + B\mathbf{u}$, 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

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

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 λ that satisfies $p_M(\lambda) = 0$, then λ 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

$$\lambda = \pm \sqrt{-c_0}, \tag{19}$$

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 $N_D = N - \mathrm{rank}(\lambda^2 I_N - \lambda c_1 A_1 - c_0 A_0)$ with $\lambda = \pm \sqrt{-c_0}$, yielding the following efficient criterion:

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

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

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

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

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

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]

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

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:

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

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

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

where $\delta(\lambda_i^H)$ is the algebraic multiplicity of λ_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

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

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:

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

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:

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

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:

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

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 tr (Λ) of Λ 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:

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

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

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

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 Erdö–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 $\mathrm{tr}\,(\Lambda)/N$ of interconnections [figures 3(a) and 3(b)] and (II) changing $\mathrm{tr}\,(\Lambda)/N$ by fixing link densities [figures 3(c) and 3(d)]. We see that for fixed values of $\mathrm{tr}\,(\Lambda)/N$, 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 $\mathrm{tr}\,(\Lambda)/N$. 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 $\mathrm{rank}\big[(\lambda^{\max})^2 I_N - \lambda^{\max} c_1 A_1 - c_0 A_0, B\big] = N$, 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 $\mathrm{rank}\big[\lambda^{\max} I_{2N} - H, B\big] = 2N$. 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.
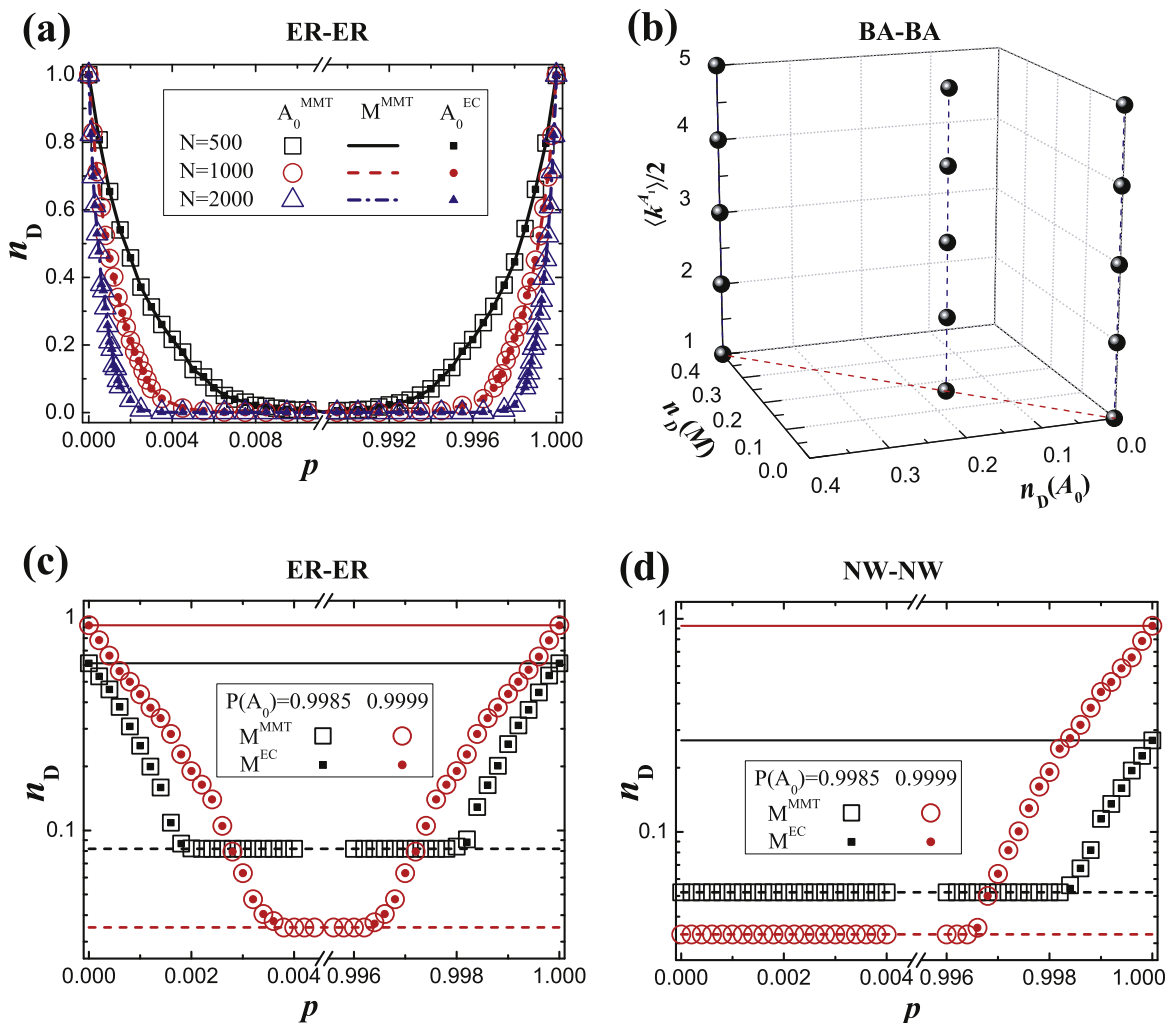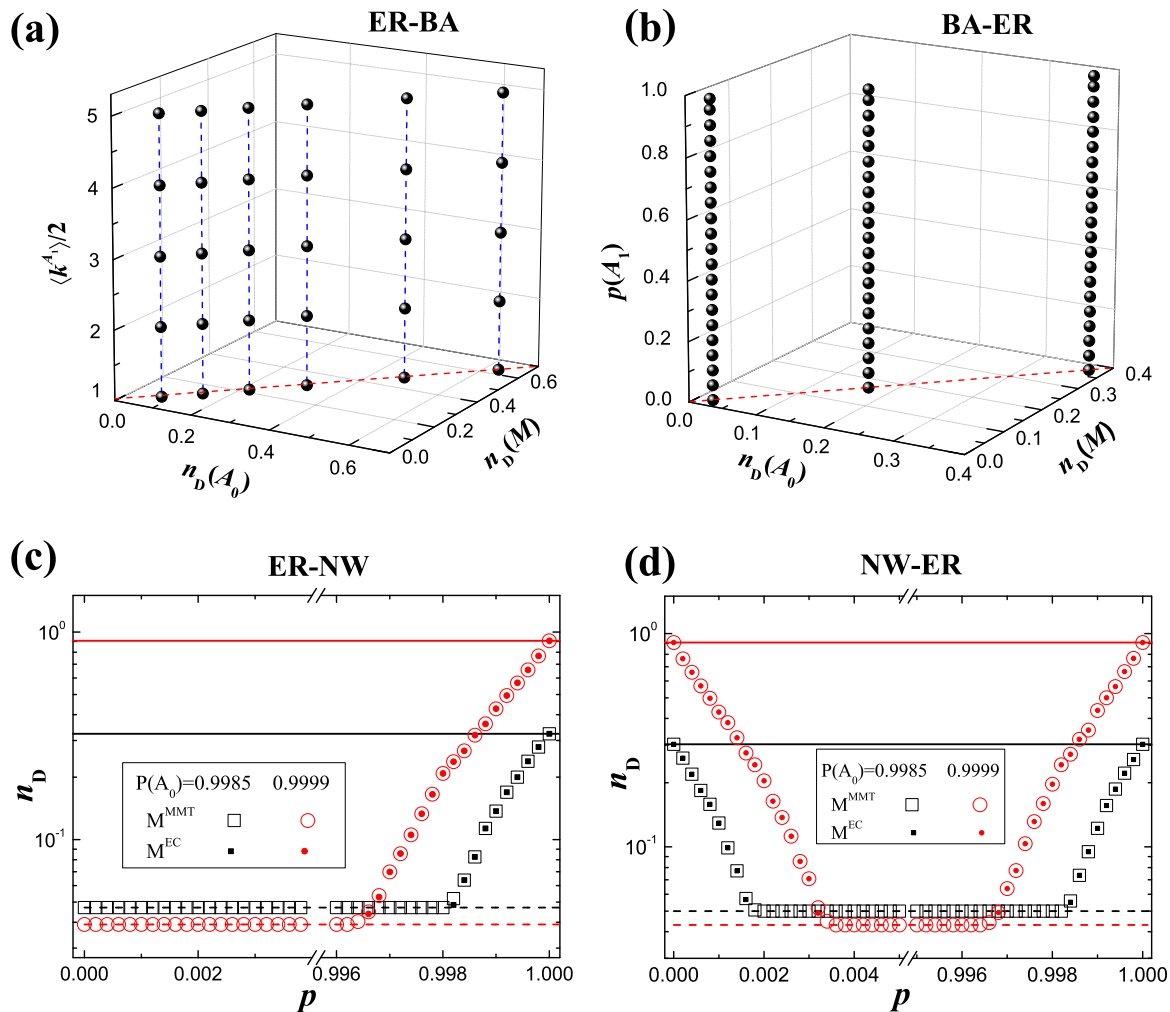
Figure 2. Controllability measure n_D of two-relation networks. (a) n_D as a function of the connection probability p of ER–ER pair with $A_0 = A_1$. (b) $n_D(M)$ of the two-relation system versus $n_D(A_0)$ of the zeroth-order layer for different half average degree $\langle k^{A_1} \rangle / 2$ of 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^{MMT} and M^{MMT} are from equation (4), and A_0^{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^{MMT} is from equation (4) and M^{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.
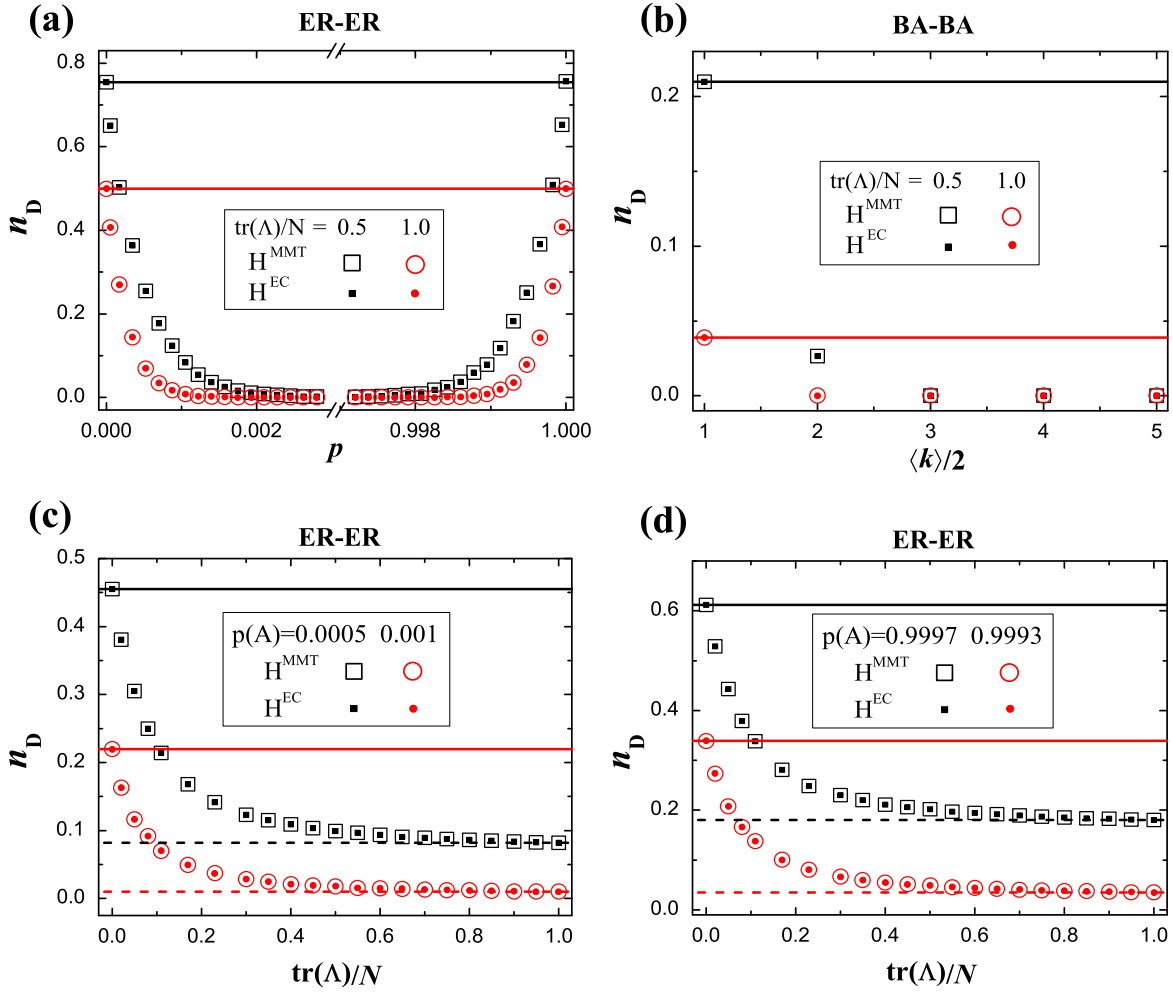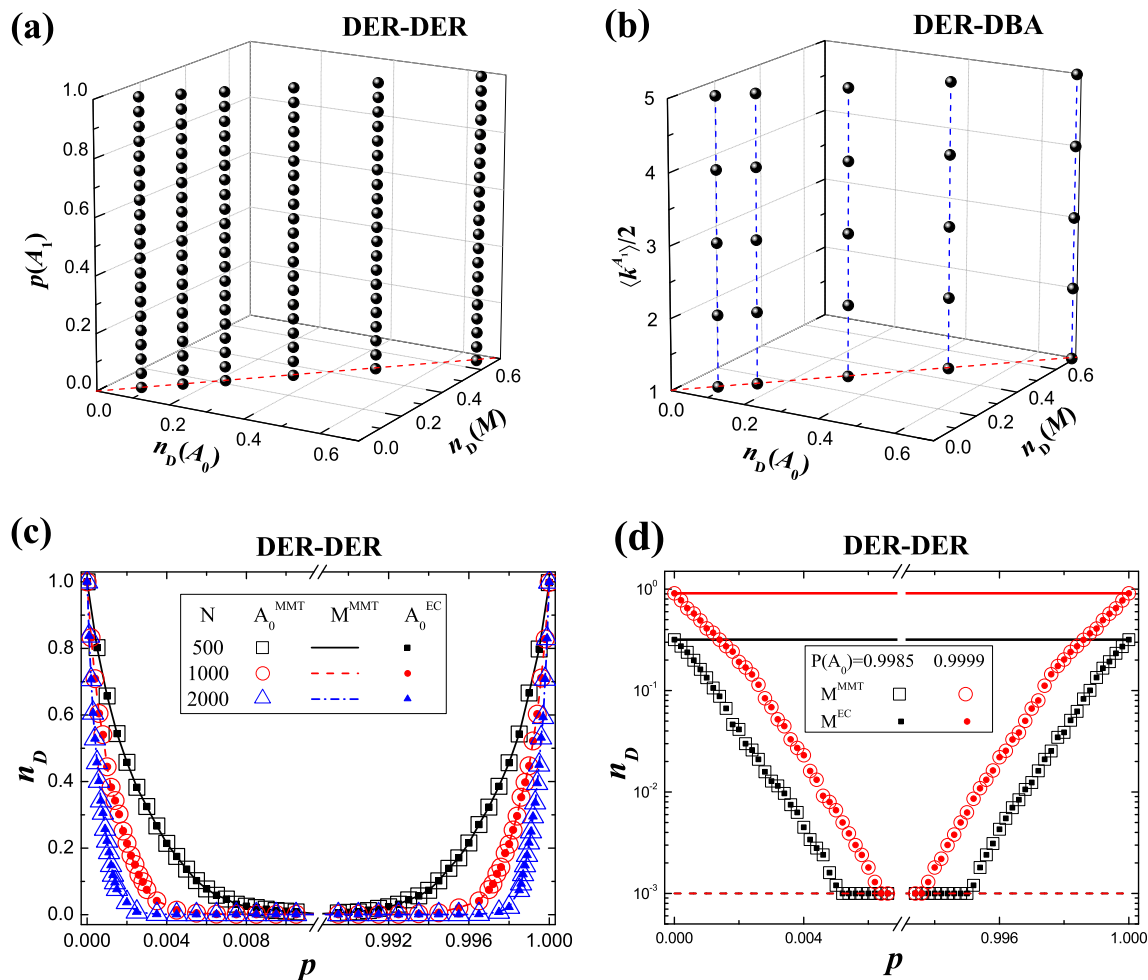
Figure 3. Controllability measure n_D of two-layer networks. (a) n_D as a function of the connecting probability p for fixed fraction tr $(\Lambda)/N$ of interconnections of ER–ER pair. (b) n_D as a function of half of the average degree $\langle k \rangle/2$ for fixed tr $(\Lambda)/N$ of BA–BA pair. (c) and (d), n_D as a function of the fraction 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^{MMT} in (a)–(d) refers to the exact controllability from equation (5). For tr $(\Lambda)/N = 1.0$, H^{EC} denotes the results obtained from equation (28) and (29) for sparse and dense connections of both layers, respectively. For tr $(\Lambda)/N < 1.0$, H^{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^{MMT} is the n_D measure of the zeroth-order layer A_0 obtained by the maximum multiplicity theory equation (4), M^{MMT} is the n_D value of the duplex from the maximum multiplicity theory equation (4), and A_0^{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^{MMT} is the controllability measure of the duplex from equation (4) and M^{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.
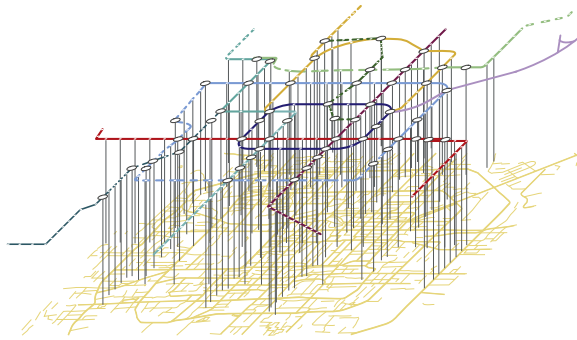
Figure 6. A real bus-subway two-layer network in Beijing, China. For better visualization, we set the subway network to be the upper layer and the bus network to be the lower layer. In the subway layer, the colors represent different subway lines. In the bus layer, there are a large number of different 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

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 $\mathrm{rank}[\lambda_i I_N - A, B] = N$ holds. In terms of the rank inequality, we have

$$N = \mathrm{rank}\left[\lambda_i I_N - A, B\right] \leqslant \mathrm{rank}\left(\lambda_i I_N - A\right) + \mathrm{rank}(B), \tag{A1}$$

such that

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

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 λ_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

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

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 λ_i. For a sparse network without self-loops, it can be proved that [23]

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

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

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

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

$$\begin{aligned}
\dot{\mathbf{x}}_0 &= \mathbf{x_1} \\
\dot{\mathbf{x}}_1 &= \mathbf{x_2} \\
&\ \vdots \\
\dot{\mathbf{x}}_{n-1} &= A_0 \mathbf{x}_0 + A_1 \mathbf{x}_1 + \cdots + A_{n-1} \mathbf{x}_{n-1} + B\mathbf{u},
\end{aligned} \tag{A6}$$

where A_i $(i = 0, 1, \cdots, n - 1)$ 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: $N - \text{rank}(A_0) \leqslant N_D$, where $\lambda_i^{A_0}$ $(i = 1, 2, \cdots, N)$ 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 $(i = 0, 1, \cdots, n - 1)$, $N_D = N - \min_s\{\text{rank}(f_0(s))\}$ 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 $(i = 1, \cdots, n - 1)$, we have $N_D = N - \text{rank}[f_0(s)]$, where s

satisfies $s^n + 1 = 0$.

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

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

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

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

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

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

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

for any complex number s.

We can implement elementary transformation on $[sI_{nN} - M, B']$, as follows. First, from the nth column to first column, we multiply $-s$ by the ith 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 $[sI_{nN} - M, B']$:

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

where

$$f_0(s) = I_N s^n - A_{n-1}s^{n-1} - A_{n-2}s^{n-2} - \cdots - sA_1 - A_0,$$

$$f_1(s) = I_N s^{n-1} - A_{n-1}s^{n-2} - A_{n-2}s^{n-3} - \cdots - sA_2 - A_1,$$

$$f_2(s) = I_N s^{n-2} - A_{n-1}s^{n-3} - A_{n-2}s^{n-4} - \cdots - sA_3 - A_2,$$

$$\vdots$$

$$f_{n-1}(s) = s(sI_N - A_{n-1}) - A_{n-2},$$

$$f_n(s) = sI_N - A_{n-1}. \tag{A10}$$

Secondly, from the first row to $(n - 1)$ th row, we multiply $f_i(s)$ by the ith row and add the result to the nth 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 $[sI_{nN} - M, B']$:

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

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

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

for any s. This means

$$\mathrm{rank}\big[f_0(s), B\big] = N \qquad (A13)$$

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

$$N_D = \max_s \left\{ N - \mathrm{rank}\big(f_0(s)\big) \right\} = N - \min_s \left\{ \mathrm{rank}\big(f_0(s)\big) \right\}. \qquad (A14)$$

Apparently,

$$\min_s \left\{ \mathrm{rank}\big(f_0(s)\big) \right\} \leqslant \mathrm{rank}\big(A_0\big) \qquad (A15)$$

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

$$N_D \geqslant N - \mathrm{rank}\big(A_0\big). \qquad (A16)$$

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

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

- If s satisfies $s^{n-1} + s^{n-2} + \cdots + s + 1 = 0$, then $s \neq 0$ and $s^n \neq 0$, so
$$\mathrm{rank}\big[f_0(s), B\big] = \mathrm{rank}\big[I_N s^n, B\big] = N;$$

- For other s that satisfies $s^{n-1} + s^{n-2} + \cdots + s + 1 \neq 0$, we have
$$\mathrm{rank}\big[f_0(s), B\big] = \mathrm{rank}\left[\frac{s^n}{s^{n-1} + s^{n-2} + \cdots + s + 1}I_N - A_0, B\right].$$

This means that if B satisfies $\mathrm{rank}[sI_N - A_0, B] = N$ for all complex numbers s, then $\mathrm{rank}[sI_{nN} - M, B'] = nN$ for $s \in C$, 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 $N_D = \mu(0) = N - \mathrm{rank}(A_0)$.

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

If A_0 is dense and A_i $(i = 1, \cdots, n-1)$ are sparse, we can get $p_M(\lambda) = p_{A_0}(\lambda^n)$ by setting $A_i = 0$ $(i = 1, \cdots, n-1)$. 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 $N_D = N - \mathrm{rank}(f_0(s))$.

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

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

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

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

or equivalently $s^n + s^{n-1} + s^{n-2} + \cdots + s + 1 = 0$, which gives $N_D = N - \mathrm{rank}(f_0(s))$ This completes our proof. It is noteworthy that the matrices A_i $(i = 0, 1, \cdots, n-1)$ 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:

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

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 λ_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 λ_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 λ associated with the maximum geometric multiplicity. Thus $p_H(\lambda)$ has factors λ/D 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

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

or

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

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

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

or

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

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,

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

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

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

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

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

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:

$$p_H(\lambda) = \left| \lambda I_{3N} - H \right|$$

$$= \begin{vmatrix} (\lambda + 2)I_N - A_1 & -I_N & -I_N \\ -I_N & (\lambda + 2)I_N - A_1 & -I_N \\ -I_N & -I_N & (\lambda + 2)I_N - A_1 \end{vmatrix}$$

$$= \begin{vmatrix} -I_N & (\lambda + 2)I_N - A_1 & -I_N \\ -I_N & -I_N & (\lambda + 2)I_N - A_1 \\ (\lambda + 2)I_N - A_1 & -I_N & -I_N \end{vmatrix}$$

$$= \begin{vmatrix} -I_N & (\lambda + 2)I_N - A_1 & -I_N \\ 0 & -(\lambda + 3)I_N + A_1 & (\lambda + 3)I_N - A_1 \\ 0 & [(\lambda + 2)I_N - A_1]^2 - I & -(\lambda + 3)I_N + A_1 \end{vmatrix}$$

$$= \begin{vmatrix} -I_N & (\lambda + 2)I_N - A_1 & -I_N \\ 0 & -(\lambda + 3)I_N + A_1 & (\lambda + 3)I_N - A_1 \\ 0 & [(\lambda + 3)I_N - A_1][(\lambda + 1)I_N - A_1] & -(\lambda + 3)I_N + A_1 \end{vmatrix}$$

$$= \left| (\lambda + 3)I_N - A_1 \right|^2 \begin{vmatrix} -I_N & (\lambda + 2)I_N - A_1 & -I_N \\ 0 & -I_N & I_N \\ 0 & (\lambda + 1)I_N - A_1 & -I_N \end{vmatrix}$$

$$= \left| (\lambda + 3)I_N - A_1 \right|^2 \begin{vmatrix} -I_N & (\lambda + 2)I_N - A_1 & -I_N \\ 0 & \lambda I_N - A_1 & 0 \\ 0 & [(\lambda + 1)I_N - A_1] & -I_N \end{vmatrix}$$

$$= \left| (\lambda + 3)I_N - A_1 \right|^2 \left| \lambda I_N - A_1 \right| = p_{A_1}(\lambda) p_{A_1}^2(\lambda + 3).$$

From this result, we can infer that if A_1 has the eigenvalue λ_0 with algebraic multiplicity $\delta(\lambda_0)$, H must have the eigenvalue λ_0 with algebraic multiplicity $\delta(\lambda_0)$ and the eigenvalue λ_{0-3} with algebraic multiplicity $2\delta(\lambda_0 - 3)$. This means that, when A_1 has the eigenvalue λ_0 associated with the maximum multiplicity, the eigenvalue of H corresponding to the maximum multiplicity is λ_{0-3}. So, when A_1, A_2 and A_3 are sparse, i.e., $\lambda_0 = 0$, the three-layer network has

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

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

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

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:

$$\text{rank}\left[\lambda^{\max} I_N - A, B\right] = N. \tag{A26}$$

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 $\mu(\lambda^{\max})$, aresult 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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