Supplementary Material for Manuscript ID IEEE $TCNS\ 23-0126$

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September 11, 2023

This Supplementary Material is organized as follows. In Section I, the proposed "Minimum-cost Flow based Driver-node Identification" (MFDI) method is compared with the existing methods in terms of the minimum number of driver nodes required to ensure the structural controllability of two-layer multiplex networks. In Section II, we demonstrate that using the method designed for single-layer networks on two-layer networks can result in the allocation of driver nodes that violates the constraint.

1 Comparative Analysis of MFDI with Existing Techniques

To the best of our knowledge, our work is the first to study the problem of finding the minimum number of driver nodes to ensure the structural controllability of multiplex networks. Our work shares a common interest in the structural controllability of multiplex networks with several other significant studies but features some distinct characteristics [14,18,19]. In [14], the authors examined finding the minimum number of controllers on multiplex multi-time-scale networks within discrete dynamics, providing a solution using the max flow method. However, this work may not be directly comparable to our work and existing works on continuous dynamics [18,19] due to the significant difference in the dynamics framework. In the following, we shall conduct the comparisons between the MFDI algorithm and the algorithms proposed in [18,19] from problem formulation and numerical results perspectives.

In [18,19], the authors delved into the problem of finding the minimum number of controllers required to ensure target controllability on two-layer multiplex networks. These two studies respectively employed a maximum flow algorithm and a minimum-cost maximum flow algorithm, respectively. When their methods are applied to the problem of structural controllability, the target set is considered as the whole network's node sets. Specifically, their formulation of the problem is as follows. In a two-layer multiplex network with

n nodes in each layer, of which the wiring diagram is $\bar{A} = \begin{bmatrix} \bar{A}_{11} & \mathbf{0} \\ \bar{A}_{21} & \bar{A}_{22} \end{bmatrix} \in \{0,\star\}^{2n \times 2n}$, the problem can be formulated as

$$\min_{\bar{B}_1 \in \{0,\star\}^{n \times m}} m,$$
s. t. $\bar{B} = \begin{bmatrix} \bar{B}_1 \\ \mathbf{0} \end{bmatrix} \in \{0,\star\}^{2n \times m},$

$$\dot{\mathbf{x}}(t) = \bar{A}\mathbf{x}(t) + \bar{B}\mathbf{u}(t),$$

$$(S1)$$

$$(\bar{A}, \bar{B}) \text{ is structurally controllable.}$$

where m represents the number of external controllers.

In our paper, we study the problem of finding the minimum number of driver nodes necessary to ensure the structural controllability of multiplex networks. On a two-layer multiplex network, of which the wiring diagram is denoted as $\bar{A} = \begin{bmatrix} \bar{A}_{11} & \mathbf{0} \\ \bar{A}_{21} & \bar{A}_{22} \end{bmatrix} \in \{0,\star\}^{2n\times 2n}$, we tackle the optimization problem

$$\min_{\bar{B}_1 \in \{0,\star\}^{n \times n}} \|\bar{B}\|_0,$$
s. t.
$$\bar{B} = \begin{bmatrix} \bar{B}_1 \\ \mathbf{0} \end{bmatrix} \in \{0,\star\}^{2n \times n},$$

$$\dot{\mathbf{x}}(t) = \bar{A}\mathbf{x}(t) + \bar{B}\mathbf{u}(t),$$

$$(S2)$$

$$(\bar{A}, \bar{B}) \text{ is structurally controllable.}$$

The main distinction between formulations (S1) and (S2) is that while (S1) focuses on finding the minimum number of controllers, (S2) is concerned with identifying the minimum number of driver nodes required to ensure the structural controllability of multiplex networks. Both equations (S1) and (S2) impose a constraint that controllers can only be connected to nodes in the first layer.

The proposed "Minimum-cost Flow based Driver-node Identification" (MFDI) method is compared with the methods described in [18,19] in terms of the driver nodes required to ensure the structural controllability of two-layer multiplex networks. The results of comparisons on synthetic multiplex networks are presented in Table S1, where each layer consists of n nodes and μ_i denotes the average nodal degree in the i^{th} layer. In Table S1, each value is represented as the mean \pm standard deviation calculated from 100 independent simulations. Moreover, Table S2 showcases the comparisons made on real-life multiplex networks where each layer consists of n nodes and $|E_i|$ denotes the number of edges in the i^{th} layer. The real-life network datasets are accessible on the website of CoMuNe Laboratory¹, the Research Unit of Bruno Kessler Foundations Center for Information and Communication Technologies. For those networks with more than two layers, we only use the data of the first two layers in the simulations. In Table S2, each real-life multiplex network is represented where n marks the number of nodes in each layer, and $|E_i|$ denotes the number of edges in the i^{th} layer.

¹https://manliodedomenico.com/data.php

Table S1: Comparisons between the number of driver nodes obtained by different methods on two-layer synthetic multiplex networks (n=1000)

	maximum flow	minimum-cost maximum	proposed MFDI
	algorithm [18]	flow algorithm [19]	algorithm
ER-ER, $\mu_1 = 2$, $\mu_2 = 2$	330.99 ± 10.48	330.99 ± 10.48	$\textbf{330.62}\pm\textbf{10.11}$
ER-ER, $\mu_1 = 3$, $\mu_2 = 3$	131.44 ± 9.10	131.44 ± 9.10	$\textbf{127.95}\pm\textbf{8.87}$
ER-ER, $\mu_1 = 4$, $\mu_2 = 4$	44.04 ± 5.52	44.04 ± 5.52	$\textbf{41.88} \pm \textbf{5.40}$
ER-ER, $\mu_1 = 5$, $\mu_2 = 5$	18.10 ± 4.33	18.10 ± 4.33	$\textbf{14.28}\pm\textbf{3.55}$
ER-ER, $\mu_1 = 8$, $\mu_2 = 8$	6.64 ± 2.17	6.64 ± 2.17	$\textbf{1.36}\pm\textbf{0.66}$
SF-SF, $\mu_1 = 2$, $\mu_2 = 2$	776.58 ± 7.89	776.58 ± 7.89	$\textbf{775.16}\pm\textbf{7.37}$
SF-SF, $\mu_1 = 3$, $\mu_2 = 3$	693.82 ± 8.92	693.82 ± 8.92	$\textbf{692.28}\pm\textbf{8.21}$
SF-SF, $\mu_1 = 10$, $\mu_2 = 10$	301.46 ± 9.85	301.46 ± 9.85	$\textbf{300.66} \pm \textbf{9.88}$
SF-SF, $\mu_1 = 15$, $\mu_2 = 15$	129.81 ± 8.07	129.81 ± 8.07	$\textbf{128.64} \pm \textbf{8.16}$
SF-SF, $\mu_1 = 20$, $\mu_2 = 20$	26.41 ± 7.07	26.41 ± 7.07	$\textbf{23.22}\pm\textbf{6.93}$
SF-SF, $\mu_1 = 30$, $\mu_2 = 30$	6.28 ± 1.71	6.28 ± 1.71	$\textbf{1.00}\pm\textbf{0.00}$

Table S2: Comparisons between the Number of Driver Nodes Obtained by Different Methods on Two-layer Real-life Multiplex Networks

	maximum flow minimum-cost maximum		proposed MFDI	
	algorithm [18]	flow algorithm [19]	algorithm	
CKM physicians' innovation [43]	133	133	127	
$n = 246, E _1 = 480, E _2 = 565$	100	100		
Lazega law firm [44]	9	9	6	
$n = 71, E _1 = 892, E _2 = 575$	J	3		
C. Elegans connectome [47]	135	135	60	
$n = 279, E _1 = 1031, E _2 = 1639$	100	100		
C. Elegans GPI [48]	3817	3817	3810	
$n = 3879, E _1 = 5557, E _2 = 313$	3011	9011	3610	
Arabidopsis GPI [48]	6597	6597	6564	
$n = 6980, E _1 = 13857, E _2 = 4411$	0001	0001	0004	

From Tables S1 and S2, it can be observed that the proposed MFDI consistently finds the smallest number of driver nodes on either synthetic or real-life networks. However, it's important to note that we should not claim our algorithm "outperforms" the algorithms in [18,19] because their optimization targets are different from ours.

2 Applying Single-Layer Methods to Two-Layer Networks

The fundamental distinction between identifying the minimum number of driver nodes required to ensure structural controllability in single-layer and two-layer multiplex networks is that, in the latter, the driver nodes must be situated in the first layer. Casting a two-layer network into a single-layer network and using the method in [22] on two-layer networks may result in the allocation of driver nodes that violates this constraint. We further elucidate this with mathematical formulations and supportive empirical data.

Specifically, in [22], the authors studied the problem of finding the minimum number of driver nodes on single-layer networks, which could be formulated as

$$\min_{\bar{B} \in \{0, \star\}^{n \times n}} ||\bar{B}||_{0},$$
s. t. $\dot{\mathbf{x}}(t) = \bar{A}\mathbf{x}(t) + \bar{B}\mathbf{u}(t),$

$$(\bar{A}, \bar{B}) \text{ is structurally controllable,}$$
(S3)

where $\bar{A} \in \{0,\star\}^{n\times n}$ denotes the wiring diagram of the network, and $\|\bar{B}\|_0$ denotes the number of non-zero entries in B, i.e., the number of driver nodes. This problem was solved by a minimum-weighted maximum matching method.

In our paper, we study the problem of finding the minimum number of driver nodes needed to ensure the structural controllability of multiplex networks, where the driver nodes can only be situated on the first layer of the network. On a two-layer multiplex network, of which the wiring diagram is denoted as $\bar{A} = \begin{bmatrix} \bar{A}_{11} & \mathbf{0} \\ \bar{A}_{21} & \bar{A}_{22} \end{bmatrix} \in \{0, \star\}^{2n \times 2n}$, the problem is formulated as

$$\min_{\bar{B}_1 \in \{0, \star\}^{n \times n}} \|\bar{B}\|_0,$$
s. t.
$$\bar{B} = \begin{bmatrix} \bar{B}_1 \\ \mathbf{0} \end{bmatrix} \in \{0, \star\}^{2n \times n},$$

$$\dot{\mathbf{x}}(t) = \bar{A}\mathbf{x}(t) + \bar{B}\mathbf{u}(t),$$

$$(S4)$$

$$(\bar{A}, \bar{B}) \text{ is structurally controllable.}$$

We shall then illustrate that the minimum-weighted maximum matching method in [22] may violate the constraints in our problem (S4). In order to keep the dimensions consistent,

we rewrite the formulation (S3) as

$$\min_{\bar{B} \in \{0, \star\}^{2n \times n}} \|\bar{B}\|_{0},$$
s. t. $\dot{\mathbf{x}}(t) = \bar{A}\mathbf{x}(t) + \bar{B}\mathbf{u}(t),$

$$(\bar{A}, \bar{B}) \text{ is structurally controllable,}$$
(S5)

where $\bar{A} \in \{0,\star\}^{2n\times 2n}$. The distinction between (S4) and (S5) is that (S5) does not confine the locations of driver nodes. As such, the lower half of $\bar{B} \in \{0,\star\}^{2n\times n}$ obtained by using minimum-weighted maximum matching method [22] may contain non-zero entries, violating the restriction set in (S4). Table S3 records the proportion of instances where the method proposed in [22] fails to meet the constraints of our problem (S4) on synthetic networks. This implies the scenarios where the lower half of the obtained $\bar{B} \in \{0,\star\}^{2n \times n}$ has non-zero entries. In Table S3, μ_i represents the mean degree of the i^{th} layer. For each network configuration, the result is generated from simulations run on 100 independent networks. Table S4 illustrates cases from real-life multiplex networks, assessing whether the calculated $\bar{B} \in \{0,\star\}^{2n\times n}$ obtained using the minimum-weighted maximum matching method [22], violates the constraints outlined in (S4). The real-life network datasets are accessible on the website of CoMuNe Laboratory², the Research Unit of Bruno Kessler Foundations Center for Information and Communication Technologies. For those networks with more than two layers, we only use the data of the first two layers in the simulations. In Table S4, for each real-life multiplex network, n denotes the number of nodes in each layer and $|E_i|$ denotes the number of edges in the i^{th} layer. The symbol \checkmark denotes that \bar{B} , calculated using the minimum-weighted maximum matching method, complies with the constraints specified in (S4). Conversely, X indicates that the calculated B violates the constraints.

²https://manliodedomenico.com/data.php

Table S3: The proportion of instances where the calculated B using the minimum-weighted maximum matching method [22] on synthetic networks fails to comply with the constraints specified in problem (S4)

two-layer ER-ER multiplex networks, $n=1000$	$\mu_1 = 2$	$\mu_1 = 3$	$\mu_1 = 4$	$\mu_1 = 5$
$\mu_2 = 2$	100%	100%	100%	100%
$\mu_2 = 3$	100%	100%	100%	100%
$\mu_2 = 4$	84%	83%	94%	100%
$\mu_2 = 5$	46%	42%	43%	67%
two-layer SF-SF multiplex networks, $n=1000$	$\mu_1 = 2$	$\mu_1 = 3$	$\mu_1 = 4$	$\mu_1 = 5$
$\mu_2 = 2$	100%	100%	100%	100%
$\mu_2 = 3$	100%	100%	100%	100%
$\mu_2 = 4$	92%	100%	100%	100%
$\mu_2 = 5$	86%	95%	100%	100%

Table S4: Assessment of constraint violations in (S4) by the minimum-weighted maximum matching method [22] on real-life multiplex networks

CKM physicians' innovation [43], $n=246$, $ E _1=480$, $ E _2=565$	
Lazega law firm [44], $n = 71$, $ E _1 = 892$, $ E _2 = 575$	1
C. Elegans connectome [47], $n=279, E _1=1031, E _2=1639$	X
C. Elegans GPI [48], $n = 3879$, $ E _1 = 5557$, $ E _2 = 313$	X
Arabidopsis GPI [48], $n=6980, E _1=13857, E _2=4411$	X

From Tables S3 and S4, it can be seen that on either synthetic or real-life networks, results generated by the minimum-weighted maximum matching method [22] may not fulfill the constraints in (S4).

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