Topology Identification of Directed Dynamical Networks via Power Spectral Analysis

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***Abstract*—We address the problem of identifying the topology of an unknown weighted, directed network of LTI systems stimulated by wide-sense stationary noises of *unknown* power spectral densities. We propose several reconstruction algorithms by measuring the cross-power spectral densities of the network response to the input noises. The measurements are based on a series of node-knockout experiments where at each round the knocked out node broadcasts zero state without being eliminated from the network. Our first algorithm reconstructs the Boolean structure (i.e., existence and directions of links) of a directed network from a series of dynamical responses. Moreover, we propose a second algorithm to recover the exact structure of the network (including edge weights), as well as the power spectral density of the input noises, when an eigenvalue-eigenvector pair of the connectivity matrix is known (for example, Laplacian connectivity matrices). Finally, for the particular cases of nonreciprocal networks (i.e., networks with no directed edges pointing in opposite directions) and undirected networks, we propose specialized algorithms that result in a lower computational cost.**

***Index Terms*—Network reconstruction, networked dynamical systems, power spectral analysis, system identification.**

I. Introduction

The reconstruction of networks of dynamical systems is an important task in many realms of science and engineering, including biology [1], [2], physics [3], [4], and finance [5]. In the literature, we find a wide collection of approaches aiming to solve the network reconstruction problem. In the physics literature, we find in [3] a method to identify a network of dynamical systems which assumes that the input of each node can be individually manipulated. In [6], an approach based on Granger's causality [7] and the theory of reproducing kernel Hilbert spaces is proposed. In the statistics community, Bach and Jordan [8] used the Bayesian information criterion (BIC) to estimate sparse graphs from stationary time series. The optimization community has recently proposed a collection of papers aiming to find the sparsest network given *a priori* structural information [2], [4]. Although the assumption of sparsity is well justified in some applications, this assumptions might lead to unsuccessful topology inference, as illustrated in [9], [10]. Gonçalves *et al.* [9] investigate the necessary and sufficient conditions for reconstruction of LTI networks. Their work has been recently extended to reconstruction in the presence of intrinsic noise in [11]. On the other hand, for tree networks, several techniques for reconstruction are proposed in [5] and [12]. More recently, in a seminal work by Materassi and Salapaka [13], the authors propose a methodology for reconstruction of directed networks using locality properties of the Wiener filters. Although being applicable to many networks, this methodology is not exact when two nonadjacent nodes point towards a common node. In [14]–[16], several techniques are proposed to extract structural information of an undirected network running consensus dynamics. In particular, Nabi-Abdolyousefi *et al.* proposed in [15] a reconstruction technique based on a node-knockout procedure, where nodes are sequentially forced to broadcast a zero state (without being removed from the network).

Networked dynamical systems have been widely used to study the phenomenon of synchronization [17], [18]. Motivated by this line of research, we propose several algorithms to reconstruct the structure of a directed network of interconnected linear dynamical systems. We first propose an algorithm to find the Boolean structure of the unknown topology. This algorithm is based on the analysis of power spectral properties of the network response when the inputs are wide-sense stationary (WSS) processes of an *unknown* power spectral density (PSD). The measurements are performed via a node-knockout procedure inspired by work of Nabi-Abdolyousefi and Mesbahi [15]. Apart from recovering the Boolean structure of the network, we propose another algorithm to recover the exact structure of the network (including edge weights) when an eigenvalue-eigenvector pair of the connectivity matrix is known. This algorithm can be applied, for example, in the case of the connectivity matrix being a Laplacian matrix or the adjacency of a regular graph. Apart from general directed networks, we also propose reconstruction methodologies for directed nonreciprocal networks (networks with no directed edges pointing in opposite directions) and undirected networks. In the latter cases, we propose specialized algorithms able to recover the network structure with less computational cost.

The rest of the technical note is organized as follows. In Section II, we introduce some preliminary definitions needed in our exposition and describe the network reconstruction problem under consideration. Section III provides several theoretical results that are the foundation for our reconstruction techniques. In Section IV, we introduce several algorithms to reconstruct the Boolean structure of a directed network (Section IV-A), the exact structure of a directed network given an eigenvalue-eigenvector pair (Section IV-B), and the structure of undirected and nonreciprocal networks (Section IV-C and D, respectively). We finish with some conclusions in Section V.

Nomenclature

I_d	$d \times d$ identity matrix.
$\mathbf{1}_d$	d-dimensional vector of all ones.
$\mathbf{e}_k$	k-th unit vector in the standard basis of $\mathbb{R}^N$.
$\mathbb{E}(\cdot)$	Expectation operator.
$R_{xy}(\tau)$	Cross-correlation function, $\mathbb{E}(x(t)y(t-\tau))$.
$R_x(\tau)$	Auto-correlation function, $\mathbb{E}(x(t)x(t-\tau))$.
$\mathcal{F}\{\cdot\}$	Fourier transform.
$S_{y_iy_j}(\omega)$	Cross-power spectral density (CPSD), $\mathcal{F}\{R_{y_iy_j}(\tau)\}$.
$S_{y_i}(\omega)$	Power spectral density (PSD), $\mathcal{F}\{R_{y_iy_i}(\tau)\}$.

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II. Preliminaries and Problem Description

A. Graph Theory

A weighted, *directed* graph is defined as the triad $\mathcal{D} \triangleq (\mathcal{V}, \mathcal{E}_d, \mathcal{F}_d)$, where $\mathcal{V} \triangleq \{v_1, \ldots, v_N\}$ denotes a set of N nodes and $\mathcal{E}_d \subseteq \mathcal{V} \times \mathcal{V}$ denotes a set of m directed edges in $\mathcal{D}$. The function $\mathcal{F}_d : \mathcal{E}_d \to \mathbb{R}_{++}$ associates *positive* real weights to the edges. We define the weighted *in-degree* of node v_i as $\deg_{in}(v_i) = \sum_{j:(v_j,v_i)\in\mathcal{E}_d} \mathcal{F}_d((v_j, v_i))$.

The *adjacency matrix* of a weighted, directed graph $\mathcal{D}$, denoted by $A_\mathcal{D} = [a_{ij}]$, is a $N \times N$ matrix defined entry-wise as $a_{ij} = \mathcal{F}_d((v_j, v_i))$ if edge $(v_j, v_i) \in \mathcal{E}_d$, and $a_{ij} = 0$ otherwise. We define the *Laplacian matrix* $L_\mathcal{D}$ as $L_\mathcal{D} = \operatorname{diag}(\deg_{in}(v_i)) - A_\mathcal{D}$. The Laplacian matrix satisfies $L_\mathcal{D}\mathbf{1} = \mathbf{0}$, i.e., the vector $\mathbf{1}/\sqrt{N}$ is an eigenvector of the Laplacian matrix with eigenvalue 0.

B. Dynamical Network Model and Problem Statement

Consider a dynamical network consisting of N linearly coupled identical nodes, with each node being an n-dimensional, LTI, SISO dynamical system. The dynamical network under study can be characterized by

$$\begin{aligned} \dot{x}_i(t) &= Ax_i(t) + b\left(\sum_{j=1}^{N} g_{ij}y_j(t) + w_i(t)\right), \\ y_i(t) &= c^T x_i(t) \end{aligned} \tag{1}$$

where $x_i(t) \in \mathbb{R}^n$ denotes the state vector describing the dynamics of node $v_i \in \mathcal{V}$. $A \in \mathbb{R}^{n\times n}$ and $b, c \in \mathbb{R}^n$ are the given state, input and output matrices corresponding to the state-space representation of each node in isolation. $w_i(t)$ and $y_i(t) \in \mathbb{R}$ are stochastic processes representing the input noise and the system output, respectively, $g_{ij} \geq 0$ is the coupling strength of a *directed* edge from v_i to v_j, which we shall assume to be *unknown*. It is worth remarking that considering identical nodes allows us to use tensor notation that simplifies our technical analysis. Relaxing this assumption as well as studying coupling strengths of dynamic form are currently under investigation.

Defining the network state vector, the noise vector, and the network output vector as

$$\begin{aligned} \mathbf{x}(t) &\triangleq \left(x_1^T(t), \ldots, x_N^T(t)\right)^T \in \mathbb{R}^{Nn} \\ \mathbf{w}(t) &\triangleq \left(w_1(t), \ldots, w_N(t)\right)^T \in \mathbb{R}^{N} \\ \mathbf{y}(t) &\triangleq \left(y_1(t), \ldots, y_N(t)\right)^T \in \mathbb{R}^{N} \end{aligned}$$

respectively, we can rewrite the network dynamics in (1), as

$$\begin{aligned} \dot{\mathbf{x}}(t) &= (I_N \otimes A + \mathbf{G} \otimes bc^T)\mathbf{x}(t) + (I_N \otimes b)\mathbf{w}(t), \\ \mathbf{y}(t) &= (I_N \otimes c^T)\mathbf{x}(t) \end{aligned} \tag{2}$$

where $\mathbf{G} = [g_{ij}]$ is the *connectivity* matrix of a (possibly weighted and/or directed) network $\mathcal{D}$. For the networked dynamical system to be stable, we assume the network state matrix $I_N \otimes A + \mathbf{G} \otimes bc^T$ to be Hurwitz.

Hereafter, we will analyze the following scenario. Consider a collection of N dynamical nodes with a known LTI, SISO dynamics defined by the state-space matrices $(A, b, c^T, 0)$. The link structure of the network dynamic model, described by the connectivity matrix $\mathbf{G}$, is completely unknown. We assume the input noises, $\{w_i(t)\}_{i=1}^N$, are i.i.d. wide-sense stationary processes of *unknown* but identical power spectral densities, i.e., $S_{w_i}(\omega) = S_w(\omega)$ for all $i = 1, \ldots, N$. We are interested in identifying all the links in the network by exploiting only the information provided by the realizations of the output stochastic processes $y_1(t), \ldots, y_N(t)$. Formally, we can formulate this problem as follows.

Problem 1: Consider the dynamical network model in (2), whose connectivity matrix $\mathbf{G}$ is unknown. Assume that the only available information is a spectral characterization of the output signals $y_1(t), \ldots, y_N(t)$ in terms of power and cross-power spectral densities, $S_{y_i}(\omega)$ and $S_{y_iy_j}(\omega)$, which can be empirically estimated from the output signals.[1] Then, find the Boolean structure of the directed network, i.e., the location and direction of each edge.

It is worth remarking that we assume the input noise to be an exogenous signal of *unknown* power spectral density, $S_w(\omega)$.

III. Theoretical Results

We start by stating some assumptions we need in our subsequent developments. The following definition will be useful for determining sufficient conditions for detection of links in a network.

Definition 2—(Excitation Frequency Interval [13]): The excitation frequency interval of a vector $\mathbf{w}(t)$ of wide-sense stationary processes is defined as an interval $(-\Omega, \Omega)$, with $\Omega > 0$, such that the power spectral densities of the input components $w_i(t)$ satisfy $S_{w_i}(\omega) > 0$ for all $\omega \in (-\Omega, \Omega)$, and all $i \in \{1, 2, \ldots, N\}$.

Throughout the technical note we impose the following conditions on the input vector.

A1. The collection of signals $\{w_i(t), i = 1, \ldots, N\}$ are uncorrelated, zero-mean WSS processes with identical autocorrelation function, i.e., for any $t, \tau \in \mathbb{R}$, $R_{w_i}(\tau) = \mathbb{E}(w_i(t)w_i(t+\tau)) \triangleq R_w(\tau)$.

A2. The input noise $\mathbf{w}(t)$ presents a nonempty excitation frequency interval $(-\Omega, \Omega)$.

In our derivation, we will invoke the following variation of the matrix inversion lemma [20]:

Lemma 3 (Sherman-Morrison-Woodbury): Assume that the matrices D and $I + WD^{-1}UE$ are nonsingular. Then, the following identity holds:

$$(D + UEW)^{-1} = D^{-1} - D^{-1}UE(I + WD^{-1}UE)^{-1}WD^{-1}$$

where E, W, D, and U are matrices of compatible dimensions and I is the identity matrix.

Based on Woodbury's formula, we derive an expression that provides an explicit relationship between the (cross-)power spectral densities of two stochastic outputs, $y_i(t)$ and $y_j(t)$, when we inject a noise $w_k(t)$ into node k with power spectral density $S_w(\omega)$.

Lemma 4: Consider the continuous-time networked dynamical system (2). Then, under assumptions (A1)–(A2), the following identity holds:

$$\mathbf{S}(\omega) = S_w(\omega)\left(\frac{I_N}{|h(\mathbf{j}\omega)|^2} + \mathbf{G}^T\mathbf{G} - \frac{\mathbf{G}}{h^*(\mathbf{j}\omega)} - \frac{\mathbf{G}^T}{h(\mathbf{j}\omega)}\right)^{-1} \tag{3}$$

where $\mathbf{S}(\omega) \triangleq [S_{y_iy_j}(\omega)]$ is the matrix of output CPSD's, and $h(\mathbf{j}\omega) \triangleq c^T(\mathbf{j}\omega I_n - A)^{-1}b$ is the nodal transfer function.

Proof: The $N \times N$ transfer matrix, $H(\mathbf{j}w) \triangleq [H_{ji}(\mathbf{j}\omega)]$, of the state-space model in (2) is given by

$$\begin{aligned} H(\mathbf{j}\omega) &= (I_N \otimes c^T)(\mathbf{j}\omega I_{Nn} - I_N \otimes A - \mathbf{G} \otimes bc^T)^{-1}(I_N \otimes b) \\ &= (I_N \otimes c^T)(I_N \otimes (\mathbf{j}\omega I_n - A) - \mathbf{G} \otimes bc^T)^{-1}(I_N \otimes b). \end{aligned} \tag{4}$$

[1]One can use, for example, Bartletts averaging method [19] to produce periodogram estimates of power and cross-power spectral densities, $S_{y_i}(\omega)$ and $S_{y_iy_j}(\omega)$.

Assume that we inject a noise signal into the k-th node, i.e., $\mathbf{w}(t) = w_k(t)\mathbf{e}_k$. Hence, the power spectral density measured on the output of node i is equal to $S_{y_i}(\omega) = H_{ki}(\omega)H^*_{ki}(\omega)S_{w_k}(\omega)$. On the other hand, the transfer functions from input $w_k(t)$ to the outputs $y_i(t)$ and $y_j(t)$ are, respectively, $Y_i(\mathbf{j}\omega)/W_k(\mathbf{j}\omega) = H_{ki}(\mathbf{j}\omega)$ and $Y_j(\mathbf{j}\omega)/W_k(\mathbf{j}\omega) = H_{kj}(\mathbf{j}\omega)$, where $Y_i(\mathbf{j}\omega)$ and $W_k(\mathbf{j}\omega)$ are the Fourier transforms of $y_i(t)$ and $w_k(t)$, respectively. Hence, $Y_j(\mathbf{j}\omega)/Y_i(\mathbf{j}\omega) = H^{-1}_{ki}(\mathbf{j}\omega)H_{kj}(\mathbf{j}\omega)$, which implies $S_{y_iy_j}(\omega) = (H_{kj}(\mathbf{j}\omega)H^{-1}_{ki}(\mathbf{j}\omega))^* S_{y_i}(\omega)$. Since $S_{w_k}(\omega) = S_w(\omega)$ for all k, we have that $S_{y_iy_j}(\omega) = H_{ki}(\mathbf{j}\omega)H^*_{kj}(\mathbf{j}\omega)S_w(\omega)$. Assume that we inject noise signals satisfying assumptions (A1)–(A2) into all the nodes in the network, i.e., $\mathbf{w}(t) = \sum_{k=1}^N w_k(t)\mathbf{e}_k$. Hence, we can apply superposition to obtain

$$\begin{aligned}\frac{S_{y_iy_j}(\omega)}{S_w(\omega)} &= \sum_{k=1}^N H^*_{kj}(\mathbf{j}\omega)H_{ki}(\mathbf{j}\omega)\\ &= \sum_{k=1}^N \mathbf{e}_k^T H^*(\mathbf{j}\omega)\mathbf{e}_j\mathbf{e}_i^T H(\mathbf{j}\omega)\mathbf{e}_k\\ &= \sum_{k=1}^N \mathrm{Tr}\left(H^*(\mathbf{j}\omega)\mathbf{e}_j\mathbf{e}_i^T H(\mathbf{j}\omega)\mathbf{e}_k\mathbf{e}_k^T\right)\\ &= \mathrm{Tr}\left(H^*(\mathbf{j}\omega)\mathbf{e}_j\mathbf{e}_i^T H(\mathbf{j}\omega)\sum_{k=1}^N \mathbf{e}_k\mathbf{e}_k^T\right)\\ &= \mathbf{e}_i^T H(\mathbf{j}\omega)H^*(\mathbf{j}\omega)\mathbf{e}_j \qquad (5)\end{aligned}$$

for any $\omega \in (-\Omega, \Omega)$, where we used the identity $\sum_{k=1}^N \mathbf{e}_k\mathbf{e}_k^T = I_N$ in our derivation.

Let us define the matrices $W \triangleq I_N \otimes c^T$, $U \triangleq I_N \otimes b$, $E \triangleq -\mathbf{G}$, and $D \triangleq I_N \otimes (\mathbf{j}\omega I_n - A)$. Then, we can rewrite the transfer matrix $H(\mathbf{j}\omega)$ in (4) as

$$H(\mathbf{j}\omega) = W(D + UEW)^{-1}U. \qquad (6)$$

Also, we have that $h(\mathbf{j}\omega)I_N = WD^{-1}U$. Then, applying Lemma 3 to (6), we can rewrite the transfer matrix, as follows:

$$\begin{aligned}H(\mathbf{j}\omega) &= h(\mathbf{j}\omega)\left(I_N + \mathbf{G}\left(I_N - h(\mathbf{j}\omega)\mathbf{G}\right)^{-1} h(\mathbf{j}\omega)I_N\right)\\ &= h(\mathbf{j}\omega)\left(I_N + \mathbf{G}\left(\frac{I_N}{h(\mathbf{j}\omega)} - \mathbf{G}\right)^{-1}\right)\\ &= h(\mathbf{j}\omega)\left(I_N + \left(\mathbf{G} - \frac{I_N}{h(\mathbf{j}\omega)} + \frac{I_N}{h(\mathbf{j}\omega)}\right)\right.\\ &\qquad\qquad \left.\times\left(\frac{I_N}{h(\mathbf{j}\omega)} - \mathbf{G}\right)^{-1}\right)\\ &= h(\mathbf{j}\omega)\left(I_N - I_N + \frac{1}{h(\mathbf{j}\omega)}\left(\frac{I_N}{h(\mathbf{j}\omega)} - \mathbf{G}\right)^{-1}\right)\\ &= \left(\frac{I_N}{h(\mathbf{j}\omega)} - \mathbf{G}\right)^{-1}.\end{aligned}$$

Substituting above into (5), we reach the statement of our lemma. ■

In the following section, we will use this lemma to reconstruct an unknown network structure $\mathbf{G}$ from the empirical CPSD's of the outputs. We will also show that, assuming that we know one eigenvalue-eigenvector pair of $\mathbf{G}$, we can recover the weighted and directed graph $\mathcal{D}$ (not only its Boolean structure, but also its weights), as well as the PSD of the noise, $S_w(\omega)$. Relevant examples of this scenario are: (*i*) networks of diffusively coupled systems with a Laplacian connectivity matrix [21], i.e., $\mathbf{G} = -L_{\mathcal{D}}$, since Laplacian matrices always satisfy $L_{\mathcal{D}}\mathbf{1}_N = 0$; or (*ii*) k-regular networks [22], i.e., $\mathbf{G} = A_k$, since the adjacency matrix A_k satisfy $A_k\mathbf{1}_N = k$.

As stated in Problem 1, the PSD of the input noise $\mathbf{w}(t)$ is not available to us to perform the network reconstruction. The following lemma will allow us reconstruct this PSD when an eigenvalue-eigenvector pair of $\mathbf{G}$ is known *a priori*.

Lemma 5: Consider the continuous-time networked dynamical system (2). Then, under assumptions (A1)–(A2), the input PSD can be computed as

$$S_w(\omega) = \frac{\lambda^2 \left|h(\mathbf{j}\omega)\right|^2 - 2\lambda \mathrm{Re}\left\{h(\mathbf{j}\omega)\right\} + 1}{(\boldsymbol{u}^T\mathbf{S}^{-1}(\omega)\boldsymbol{u})\left|h(\mathbf{j}\omega)\right|^2} \qquad (7)$$

where $(\lambda, \boldsymbol{u})$ is an eigenvalue-eigenvector pair of $\mathbf{G}$, $h(\mathbf{j}\omega)$ is the nodal transfer function, and $\mathbf{S}(\omega) \triangleq [S_{y_iy_j}(\omega)]$ is the matrix of CPSD's.

Proof: From (3), we have

$$\mathbf{S}^{-1}(\omega)S_w(\omega) = \frac{I_N}{\left|h(\mathbf{j}\omega)\right|^2} + G^TG - \frac{G}{h^*(\mathbf{j}\omega)} - \frac{G^T}{h(\mathbf{j}\omega)}.$$

Pre- and post-multiplying by $\boldsymbol{u}^T$ and $\boldsymbol{u}$, respectively, we obtain

$$\left(\boldsymbol{u}^T\mathbf{S}^{-1}(\omega)\boldsymbol{u}\right)S_w(\omega) = \frac{1}{\left|h(\mathbf{j}\omega)\right|^2} + \lambda^2 - \frac{\lambda}{h(\mathbf{j}\omega)} - \frac{\lambda}{h^*(\mathbf{j}\omega)}.$$

Dividing by $\boldsymbol{u}^T\mathbf{S}^{-1}(\omega)\boldsymbol{u}$, we reach (7). ■

Lemma 5 shows that, given the eigenvalue-eigenvector pair $(\lambda, \boldsymbol{u})$, the PSD of the input noise can be reconstructed from the nodal transfer function and the matrix of CPSD's, $\mathbf{S}(\omega)$, which can be numerically approximated from the empirical cross-correlations between output signals.

IV. Reconstruction Methodologies

Based on the above results, we introduce several methodologies to reconstruct the structure of an unknown network following the dynamics in (2) when the PSD of the input noise is *unknown*. First, in Section IV-A, we present a technique to reconstruct the Boolean structure of an unknown (possibly weighted) directed network. Moreover, if an eigenvalue-eigenvector pair of $\mathbf{G}$ is known (for example, $\mathbf{G}$ is a Laplacian matrix), we show how to recover the weights of the directed edges, as well as the PSD of the input noise in Section IV-B. Finally, in Section IV-C and D, we provide reconstruction techniques to recover two special cases, namely, undirected networks and nonreciprocal directed networks, respectively.

Consider Problem 1, when $\mathbf{G}$ is an unknown connectivity matrix representing a weighted, directed network $\mathcal{D}$. We propose a reconstruction technique to recover the Boolean structure of $\mathcal{D}$ when the PSD of the input noise is unknown. Note that, in general, the result in Lemma 4 is not enough to extract the underlying structure of the network, even if the input noise PSD were known. In what follows, we propose a methodology to reconstruct a directed network of dynamical nodes by *grounding* the dynamics in a series of nodes, similar to the approach proposed in [15] to reconstruct undirected networks following a consensus dynamics.

Definition 6 (Grounded Dynamics): The dynamics of (2) grounded at node v_j takes the form

$$\begin{aligned}\dot{\widetilde{\mathbf{x}}}(t) &= (I_{N-1} \otimes A + \widetilde{\mathbf{G}}_j \otimes bc^T)\widetilde{\mathbf{x}}(t) + (I_{N-1} \otimes b)\widetilde{\mathbf{w}}(t),\\ \widetilde{\mathbf{y}}(t) &= (I_{N-1} \otimes c^T)\widetilde{\mathbf{x}}(t) \qquad (8)\end{aligned}$$

where $\widetilde{\mathbf{w}}(t)$ is obtained by eliminating the j-th entry from the input noise $\mathbf{w}(t)$, and $\widetilde{\mathbf{G}}_j \in \mathbb{R}^{(N-1)\times(N-1)}$ is obtained by eliminating the j-th row and column from $\mathbf{G}$.

The dynamics in (8) describes the evolution of (2) when we ground the state of node v_j to be $x_j(t) \equiv 0$. Applying Lemma 4 to the grounded dynamics (8), one obtains the following expression for the CPSD's:

$$\widetilde{\mathbf{S}}_j(\omega)=S_w(\omega)\left(\frac{I_{N-1}}{|h(\mathbf{j}\omega)|^2}+\widetilde{\mathbf{G}}_j^T\widetilde{\mathbf{G}}_j-\frac{\widetilde{\mathbf{G}}_j}{h^*(\mathbf{j}\omega)}-\frac{\widetilde{\mathbf{G}}_j^T}{h(\mathbf{j}\omega)}\right)^{-1}. \quad (9)$$

We will use the next Theorem to propose several reconstruction techniques in Section IV-A and B.

Theorem 7: Consider the networked dynamical system (2) with connectivity matrix $\mathbf{G} = [g_{ij}]$. Let us denote by $S_w(\omega)$ the PSD of the input noise, by $\mathbf{S}(\omega) = [S_{y_i y_j}(\omega)]$ the $N \times N$ matrix of CPSD's for the (ungrounded) dynamics (2), and by $\widetilde{\mathbf{S}}_j(\omega) = [\widetilde{S}_{y_i y_k}(\omega)]_{i,k\neq j}$ the $N-1 \times N-1$ matrix of CPSD's for the dynamics in (8) grounded at node v_j. Then, under assumptions (A1)–(A2), we have that, for $i < j$

$$g_{ji} = \left[S_w(\omega_0)\left(\left[\mathbf{S}^{-1}(\omega_0)\right]_{ii} - \left[\widetilde{\mathbf{S}}_j^{-1}(\omega_0)\right]_{ii}\right)\right]^{1/2}. \quad (10)$$

For $i > j$

$$g_{ji} = \left[S_w(\omega_0)\left(\left[\mathbf{S}^{-1}(\omega_0)\right]_{ii} - \left[\widetilde{\mathbf{S}}_j^{-1}(\omega_0)\right]_{i-1,i-1}\right)\right]^{1/2}. \quad (11)$$

Proof: Without loss of generality, we consider the case that $j = N$ (for any other $j \neq N$, we can transform the problem to the case $j = N$ via a simple reordering of rows and columns). Subtracting the diagonal elements of $\mathbf{S}^{-1}(\omega)$ in (9) from those of $\widetilde{\mathbf{S}}_j^{-1}(\omega)$ in (3), we obtain

$$\left[\mathbf{S}^{-1}(\omega)\right]_{ii} - \left[\widetilde{\mathbf{S}}_j^{-1}(\omega)\right]_{ii} = \frac{[\mathbf{G}^T\mathbf{G}]_{ii} - \left[\widetilde{\mathbf{G}}_N^T\widetilde{\mathbf{G}}_N\right]_{ii}}{S_w(\omega)}.$$

Also, since $[\mathbf{G}^T\mathbf{G}]_{ii} = \sum_k g_{ki}^2$ and $[\widetilde{\mathbf{G}}_N^T\widetilde{\mathbf{G}}_N]_{ii} = \sum_{k\neq N} g_{ki}^2$, we have that

$$[\mathbf{G}^T\mathbf{G}]_{ii} - \left[\widetilde{\mathbf{G}}_N^T\widetilde{\mathbf{G}}_N\right]_{ii} = g_{Ni}^2$$

for any $i < N$. The same analysis holds for $j \neq N$. Hence, we can recover the entries g_{ji}, for $i < j$, as stated in our theorem. Notice also that, for $j \neq N$ and $i > j$, we must use the entry $[\widetilde{\mathbf{S}}_j^{-1}(\omega)]_{i-1,i-1}$ in (11), to take into account that $\widetilde{\mathbf{S}}_j(\omega)$ is an $(N-1)\times(N-1)$ matrix associated to the dynamics grounded at node v_j. ■

A. Boolean Reconstruction of Directed Networks

Theorem 7 allows us to reconstruct the Boolean structure of an unknown directed network if we have access to the matrices of CPSD's, $\mathbf{S}(\omega_0)$ and $\widetilde{\mathbf{S}}_j(\omega_0)$, for any ω_0 in the excitation frequency interval $(-\Omega, \Omega)$. In particular, one can verify the existence of a directed edge (i, j) by checking the condition $g_{ji} > 0$, where g_{ji} is computed from Theorem 7. In practice, the CPSD's $\mathbf{S}(\omega_0)$ and $\widetilde{\mathbf{S}}_j(\omega_0)$ are empirically computed from the stochastic outputs of the network, $\mathbf{y}(t)$ and $\widetilde{\mathbf{y}}(t)$; therefore, they are subject to numerical errors. Hence, in the implementation, one should relax the condition $g_{ji} > 0$ to $g_{ji} > \tau$, where τ is a small threshold used to account for numerical precision.

Based on Theorem 7, we propose Algorithm 1 to find the Boolean representation of $\mathbf{G}$, denoted by $\mathbf{B}(\mathbf{G})$, when a directed dynamical network is excited by an input noise of unknown PSD.

Algorithm 1 Boolean reconstruction of directed networks

Require: $h(\mathbf{j}\omega)$, $\mathbf{y}(t)$ from (2), $\widetilde{\mathbf{y}}(t)$ from (8), and any $\omega_0 \in (-\Omega, \Omega)$;
Compute $\mathbf{S}(\omega_0)$ from $\mathbf{y}(\mathbf{t})$;
for $j = 1 : N$ **do**
  Compute $\widetilde{\mathbf{S}}_j(\omega_0)$ from $\widetilde{\mathbf{y}}(t)$;
  for $i = 1 : j-1$ **do**
    if $[\mathbf{S}^{-1}(\omega_0)]_{ii} - [\widetilde{\mathbf{S}}_j^{-1}(\omega_0)]_{ii} > \tau$ **then** $b_{ji} = 1$;
    if $[\mathbf{S}^{-1}(\omega_0)]_{ii} - [\widetilde{\mathbf{S}}_j^{-1}(\omega_0)]_{ii} < \tau$ **then** $b_{ji} = 0$;
  end for
  for $i = j+1 : N$ **do**
    if $[\mathbf{S}^{-1}(\omega_0)]_{ii} - [\widetilde{\mathbf{S}}_j^{-1}(\omega_0)]_{i-,1i-1} > \tau$ **then** $b_{ji} = 1$;
    if $[\mathbf{S}^{-1}(\omega_0)]_{ii} - [\widetilde{\mathbf{S}}_j^{-1}(\omega_0)]_{i-1,i-1} < \tau$ **then** $b_{ji} = 0$;
  end for
end for

Algorithm 1 incurs the following computational cost:

i) It computes the cross-correlation functions for all the N^2 pairs of outputs in (2). For each one of the N grounded dynamics in (8), the algorithm also computes $(N-1)^2$ pairs of cross-correlation functions, resulting in a total of $\mathcal{O}(N^3)$ computations. To compute these cross-correlations we use time series of length L. Since each each cross-correlation takes $\mathcal{O}(L^2)$ operations, we have a total of $\mathcal{O}(N^3L^2)$ operations to compute all the required cross-correlations.
ii) Algorithm 1 evaluates the DFT of all $(N+1)N^2$ cross-correlation functions of length L in (*i*) at a particular frequency $\omega_0 \in (-\Omega, \Omega)$. Since evaluating the DFT at a single frequency takes $\mathcal{O}(L)$ operations, we have a total of $\mathcal{O}(N^3L)$ operations to compute the CPSD's matrices $\mathbf{S}(\omega_0)$ and $\widetilde{\mathbf{S}}_j(\omega_0)$, for all $j = 1, \ldots, N$.
iii) Our algorithm also needs to compute the inverse of $\mathbf{S}(\omega)$ and $\widetilde{\mathbf{S}}_j(\omega)$. Since each inversion takes $\mathcal{O}(N^3)$, we have a total of $\mathcal{O}(N^4)$ operations to compute the inverses of all the $N+1$ matrices involved in our computations.

Therefore, the total computational cost of our algorithm is $\mathcal{O}(N^4 + N^3L^2)$. In the next subsection, we extend Algorithm 1 to reconstruct the exact connectivity matrix $\mathbf{G}$.

B. Exact Reconstruction of Directed Networks

Apart from a Boolean reconstruction of $\mathbf{G}$, we can also compute the weights of the edges in the network if we know one eigenvalue-eigenvector pair $(\lambda, \mathbf{u})$ of $\mathbf{G}$, as follows. This can be the case of $\mathbf{G}$ being, for example, a Laplacian matrix (since $\mathbf{G}\mathbf{1}_N = 0$, in this case), or the adjacency matrix of a d-regular graph (since $\mathbf{G}\mathbf{1}_N = d\mathbf{1}_N$). In these cases, we use Lemma 7 to find the value of $S_w(\omega_0)$ at a particular frequency $\omega_0 \in (-\Omega, \Omega)$. For example, in the case of $\mathbf{G}$ being a Laplacian, we have the following result:

Corollary 8: Consider the networked dynamical system in (2), when $\mathbf{G} = -L_{\mathcal{D}}$, where $L_{\mathcal{G}}$ is the Laplacian matrix of a directed graph $\mathcal{D}$. Then, under assumptions (A1)–(A2), the PSD of the input noise, $S_w(\omega)$, can be computed as

$$S_w(\omega) = \frac{N}{\left(\mathbf{1}^T\mathbf{S}^{-1}(\omega)\mathbf{1}\right)|h(\mathbf{j}\omega)|^2}.$$

Proof: This result can be directly obtained from Lemma 5 taking into account that the eigenpair $(\lambda, \boldsymbol{u})$ for the Laplacian matrix is $(0, \mathbf{1}_N)$. ■

In general, we can reconstruct the weights of directed edges in a dynamical network using Algorithm 2.

Algorithm 2 Exact reconstruction of directed networks

Require: $h(\mathbf{j}\omega)$, $\mathbf{y}(t)$ from (2), $\widetilde{\mathbf{y}}(t)$ from (8), and any $\omega_0 \in (-\Omega, \Omega)$;
Compute $\mathbf{S}(\omega_0)$ from $\mathbf{y}(\mathbf{t})$ and $S_w(\omega_0)$ using (7);
for $j = 1 : N$ **do**
  Compute $\widetilde{\mathbf{S}}_j(\omega_0)$ from $\widetilde{\mathbf{y}}(t)$;
  for $i = 1 : j - 1$ **do**
    $g_{ji} = [S_w(\omega_0)([\mathbf{S}^{-1}(\omega_0)]_{ii} - [\widetilde{\mathbf{S}}_j^{-1}(\omega_0)]_{ii})]^{1/2}$;
  end for
  for $i = j + 1 : N$ **do**
    $g_{ji} = [S_w(\omega_0)([\mathbf{S}^{-1}(\omega_0)]_{ii} - [\widetilde{\mathbf{S}}_j^{-1}(\omega_0)]_{i-1,i-1})]^{1/2}$;
  end for
end for

Remark 9: It is worth remarking that the reconstruction methods proposed in the technical note do not require the entire power spectra for $\mathbf{S}(\omega)$ or $S_w(\omega)$, but only the values of these spectral densities at any frequency $\omega_0 \in (-\Omega, \Omega)$. This dramatically reduces the computational complexity of the reconstruction.

We now turn to two particular types of networks, namely, undirected and nonreciprocal networks, in which the computational cost of reconstruction can be drastically reduced.

C. Exact Reconstruction of Undirected Networks

Consider Problem 1, when the connectivity matrix $\mathbf{G}$ is an unknown (possibly weighted) symmetric matrix. Then, when an eigenpair $(\lambda, \boldsymbol{u})$ is known, we can find the exact structure of the network from the matrix of CPSD's, $\mathbf{S}(\omega) = [S_{y_i y_j}(\omega)]_{1 \le i,j \le N}$, and the nodal transfer function, $h(\mathbf{j}\omega) = c^T(\mathbf{j}\omega I_n - A)^{-1} b$, using the following result:

Theorem 10: Consider the networked dynamical system (2), when $\mathbf{G} = \mathbf{G}^T$. Then, under assumptions (A1)–(A2), we have that

$$\mathbf{G} = \left(\mathbf{S}^{-1}(\omega_0) S_w(\omega_0) - \mathrm{Im}^2\left\{h^{-1}(\mathbf{j}\omega_0)\right\} I_N\right)^{1/2} + \mathrm{Re}\left\{h^{-1}(\mathbf{j}\omega_0)\right\} I_N. \quad (12)$$

for any $\omega_0 \in (-\Omega, \Omega)$.

Proof: From Lemma 4, we obtain the following for $\mathbf{G}^T = \mathbf{G}$:

$$\begin{aligned}
&\mathbf{S}^{-1}(\omega) S_w(\omega) \\
&= \frac{I_N}{|h(\mathbf{j}\omega)|^2} + \mathbf{G}^2 - \frac{\mathbf{G}}{h^*(\mathbf{j}\omega)} - \frac{\mathbf{G}}{h(\mathbf{j}\omega)} \\
&= \mathbf{G}^2 - 2\mathrm{Re}\left\{h^{-1}(\mathbf{j}\omega)\right\}\mathbf{G} \\
&\quad + I_N\left(\mathrm{Im}^2\left\{h^{-1}(\mathbf{j}\omega)\right\} + \mathrm{Re}^2\left\{h^{-1}(\mathbf{j}\omega)\right\}\right) \\
&= \left(\mathbf{G} - \mathrm{Re}\left\{h^{-1}(\mathbf{j}\omega)\right\} I_N\right)^2 + \mathrm{Im}^2\left\{h^{-1}(\mathbf{j}\omega)\right\} I_N
\end{aligned}$$

thereby completing the proof. ■

Based on Theorem 10, we can reconstruct the connectivity matrix $\mathbf{G} = \mathbf{G}^T$ when we know an eigenpair of $\mathbf{G}$. The input PSD in (12) can be computed using Lemma 5. Notice that this algorithm does not require grounding the dynamics of the network, resulting in a reduced computational cost. In particular, the computational cost is dominated by the computation of $\mathbf{S}(\omega_0)$, which requires $\mathcal{O}(N^2 L^2)$ operations, and its inversion, which requires $\mathcal{O}(N^3)$, resulting in a total cost of $\mathcal{O}(N^2 L^2 + N^3)$.

D. Reconstruction of Non-Reciprocal Networks

Another particular network structure that does not require grounding in the reconstruction method is the so-called nonreciprocal directed networks. In a *nonreciprocal network*, having an edge $(v_j, v_i) \in \mathcal{E}_d$ implies that $(v_i, v_j) \notin \mathcal{E}_d$. In other words, the connectivity matrix of a purely unidirectional network satisfies $\mathrm{Tr}(\mathbf{G}^2) = \sum_i \sum_j g_{ij} g_{ji} = 0$, since, if $g_{ij} \neq 0$, then $g_{ij} = 0$ (and assuming there are no self-loops in the network).

The following theorem allows the Boolean reconstructing of a nonreciprocal network. Moreover, if we have access to an eigenpair of $\mathbf{G}$, this theorem could be used to perform an exact reconstruction without grounding the dynamics of the network.

Theorem 11: Consider the networked dynamical system (2), with a connectivity matrix satisfying $\mathbf{G} \ge 0$ (nonnegativity) and $\mathrm{Tr}(\mathbf{G}^2) = 0$ (nonreciprocity). Then, under assumptions (A1)–(A2), we have that

$$g_{ij} = \max\left\{S_w(\omega)\left(\frac{[\mathrm{Im}\left\{\mathbf{S}^{-1}(\omega)\right\}]_{ij}}{\mathrm{Im}\left\{h^{-1}(\mathbf{j}\omega)\right\}}\right), 0\right\} \quad (13)$$

for $1 \le i \neq j \le N$.

Proof: Under purview of Lemma 4, we obtain

$$\mathbf{S}^{-1}(\omega) S_w(\omega) = \frac{I_N}{|h(\mathbf{j}\omega)|^2} + \mathbf{G}^T\mathbf{G} - \frac{\mathbf{G}}{h^*(\mathbf{j}\omega)} - \frac{\mathbf{G}^T}{h(\mathbf{j}\omega)}.$$

Taking the imaginary parts, we obtain

$$\begin{aligned}
\mathrm{Im}\left\{\mathbf{S}^{-1}(\omega) S_w(\omega)\right\} &= \mathrm{Im}\left\{-\frac{\mathbf{G}}{h^*(\mathbf{j}\omega)} - \frac{\mathbf{G}^T}{h(\mathbf{j}\omega)}\right\} \\
&= \mathrm{Im}\left\{h^{-1}(\mathbf{j}\omega)\right\}(\mathbf{G} - \mathbf{G}^T)
\end{aligned}$$

which entails

$$\mathbf{G} - \mathbf{G}^T = \frac{S_w(\omega)}{\mathrm{Im}\left\{h^{-1}(\mathbf{j}\omega)\right\}} \mathrm{Im}\left\{\mathbf{S}^{-1}(\omega)\right\}.$$

Given that $\mathbf{G} \ge 0$ and the network is nonreciprocal, if $[\mathbf{G} - \mathbf{G}^T]_{ij} > 0$, then $g_{ij} > 0$ and $g_{ji} = 0$. If $[\mathbf{G} - \mathbf{G}^T]_{ij} < 0$, then $g_{ij} = 0$ and $g_{ji} > 0$. Finally, if $[\mathbf{G} - \mathbf{G}^T]_{ij} = 0$, then no directed edge between v_i and v_j exists. These three conditional statements can be condensed into (13). ■

Using this theorem, we can find the the Boolean representation of $\mathbf{G}$, $\mathbf{B}(\mathbf{G}) = [b_{ij}]$, as follows:

$$b_{ij} = \begin{cases} 1, & \text{if } \frac{[\mathrm{Im}\{\mathbf{S}^{-1}(\omega_0)\}]_{ij}}{\mathrm{Im}\{h^{-1}(\mathbf{j}\omega_0)\}} > 0 \\ 0, & \text{otherwise} \end{cases}$$

where $\omega_0 \in (-\Omega, \Omega)$. Moreover, if an eigenvalue eigenvector pair of $\mathbf{G}$ is known, we can recover $S_w(\omega_0)$ using Lemma 5, which allows us to recover the value of g_{ij} directly from (13). Following the analysis of previous algorithms, the computational cost of the reconstruction of a nonreciprocal directed network is $\mathcal{O}(N^2 L^2 + N^3)$.

V. Conclusion

In this technical note, we have addressed the problem of identifying the topology of an unknown directed network of LTI systems stimulated by wide-sense stationary noises of an unknown power spectral density. We have proposed several reconstruction algorithms based on the power spectral properties of the network response to the input noise. Our first algorithm reconstructs the Boolean structure of a directed network based on a series of grounded dynamical responses. Our second algorithm recovers the exact structure of the network (including edge weights) when an eigenvalue-eigenvector pair of the connectivity matrix is known. This algorithm is useful, for example, when the connectivity matrix is a Laplacian matrix or the adjacency matrix of a regular graph. Apart from general directed networks, we have also proposed more computationally efficient algorithms for reconstruction of both directed nonreciprocal networks and undirected networks.

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