NETWORK TOPOLOGY INFERENCE FROM NON-STATIONARY GRAPH SIGNALS

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ABSTRACT

We address the problem of inferring a graph from nodal observations, which are modeled as *non-stationary* graph signals generated by local diffusion dynamics that depend on the structure of the sought network. Using the so-called graph-shift operator (GSO) as a matrix representation of the graph, we first identify the eigenvectors of the shift matrix from realizations of the diffused signals, and then we rely on these spectral templates to estimate the eigenvalues by imposing desirable properties on the graph to be recovered. Different from the stationary setting where the GSO and the covariance matrix of the observed signals are simultaneously diagonalizable, here they are not. Hence, estimating the eigenvectors requires first estimating the unknown *diffusion* (graph) *filter* – a polynomial in the GSO which does preserve the sought eigenbasis. To carry out this initial system identification step, we leverage different sources of information on the input signal driving the diffusion process on the graph. Numerical tests showcase the effectiveness of the proposed algorithms in recovering social and structural brain graphs.

***Index Terms*—** Network topology inference, graph signal processing, (non-)stationary graph processes, system identification.

1. INTRODUCTION

Consider a network represented as a weighted and undirected graph $\mathcal{G}$, consisting of a node set $\mathcal{N}$ of known cardinality N, an edge set $\mathcal{E}$ of unordered pairs of elements in $\mathcal{N}$, and edge weights $A_{ij} \in \mathbb{R}$ such that $A_{ij} = A_{ji} \neq 0$ for all $(i,j) \in \mathcal{E}$. The edge weights A_{ij} are collected in the symmetric adjacency matrix $\mathbf{A}$. More broadly, one can define a generic *graph-shift operator* (GSO) $\mathbf{S} \in \mathbb{R}^{N \times N}$ as any matrix having the same sparsity pattern than that of $\mathcal{G}$ [1]. Although the choice of $\mathbf{S}$ can be adapted to the problem at hand, most existing works set it to either $\mathbf{A}$, the combinatorial Laplacian $\mathbf{L}_c := \text{diag}(\mathbf{A1}) - \mathbf{A}$, or its normalized counterparts [2].

Our focus in this paper is on identifying graphs that explain the structure of a random signal. Formally, let $\mathbf{x} = [x_1, ..., x_N]^T \in \mathbb{R}^N$ be a graph signal in which the ith element x_i denotes the signal value at node i of an *unknown graph* $\mathcal{G}$ with shift operator $\mathbf{S}$. Further suppose that we are given a zero-mean signal $\mathbf{w}$ with covariance matrix $\mathbf{C_w} = \mathbb{E}\left[\mathbf{w}\mathbf{w}^T\right]$. We say that the graph $\mathbf{S}$ represents the structure of the signal $\mathbf{x}$ if there exists a diffusion process in the GSO $\mathbf{S}$ that produces the signal $\mathbf{x}$ from the input signal $\mathbf{w}$, that is

$$\mathbf{x} \;=\; \alpha_0 \textstyle\prod_{l=1}^{\infty}(\mathbf{I} - \alpha_l \mathbf{S})\mathbf{w} \;=\; \left(\sum_{l=0}^{\infty} \beta_l \mathbf{S}^l\right)\mathbf{w}. \qquad (1)$$

When $\mathbf{w}$ is white (i.e., $\mathbf{C_w} = \mathbf{I}$), (1) is equivalent to saying that the *graph* process $\mathbf{x}$ is stationary in $\mathbf{S}$; see [3] and Section 2.1 for further details. While $\mathbf{S}$ encodes only one-hop interactions, each successive application of the shift in (1) percolates $\mathbf{w}$ over $\mathcal{G}$; see e.g. [4]. The justification to say that $\mathbf{S}$ represents the structure of $\mathbf{x}$ is that we can think of the edges of $\mathbf{S}$ as direct (one-hop) relations between the elements of the signal. The diffusion described by (1) generates indirect relations. Our goal is to recover the fundamental relations described by $\mathbf{S}$ from a set $\mathcal{X} := \{\mathbf{x}^{(p)}\}_{p=1}^{P}$ of P independent samples of a non-stationary random signal $\mathbf{x}$, as well as realizations of $\mathbf{w}$, or, knowledge of $\mathbf{C_w}$. This additional information on the input $\mathbf{w}$ is the price paid to accommodate non-stationary $\mathbf{x}$, and is not needed when identifying the structure of stationary graph signals [5].

Relation to prior work. Since networks typically encode similarities between nodes, several topology inference approaches construct graphs whose edge weights correspond to nontrivial correlations or coherence measures between signal profiles at incident nodes [6, 7]. Going beyond pairwise interactions and acknowledging that the observed correlations can be due to latent network effects, alternative methods rely on partial correlations [6, 8], Gaussian graphical models [9–12], structural equation models [13–15], Granger causality [7, 16], or their nonlinear (kernelized) variants [17, 18]. Differently, recent graph signal processing (GSP)-based network inference frameworks postulate that the network exists as a latent underlying structure, and that observations are generated as a result of a network process defined in such graph [5, 19–22]. Different from [19–21] that operate on the graph domain, the goal here is to identify graphs that endow the given observations with desired spectral (frequency-domain) characteristics. Two works have recently explored this approach by identifying a GSO given its eigenvectors [5, 22], but both rely on observations of stationary graph signals.

Paper outline. In Sec. 2 we formulate the problem of identifying a GSO that explains the fundamental structure of a random signal diffused on a graph. When $\mathbf{w}$ is white, such a problem was shown in [5] to be underdetermined and related to the concept of stationarity of graph signals [3, 23]. While for stationary $\mathbf{x}$ the sought GSO shares its eigenvectors with the signal's covariance matrix, in the general (non-stationary) setting dealt with here this no longer holds. Still, the graph's eigenvectors are preserved by the polynomial graph filter that governs the underlying diffusion dynamics. This motivates a novel two-step network topology inference approach whereby we: i) identify the GSO's eigenbasis from a judicious graph filter estimate; and ii) rely on these *spectral templates* (ST) to recover the GSO by estimating its eigenvalues. Different from [5], the additional system identification step requires extra information on the excitation signal $\mathbf{w}$ (Sec. 3). Numerical tests in Sec. 4 show the effectiveness of this approach in recovering the topology of social and brain networks.

2. PROBLEM STATEMENT

Consider identifying graphs that explain the structure of a random signal $\mathbf{x}$, meaning that there exists a diffusion process in the GSO that can generate the observed signal. Alternatively, we can say that the goal is to recover the GSO which encodes direct relationships between the elements of $\mathbf{x}$ from observable indirect relationships generated by a diffusion process. To formally state the problem, start by

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assuming that $\mathbf{S}$ is symmetric. Define the eigenvector matrix $\mathbf{V} := [\mathbf{v}_1, \ldots, \mathbf{v}_N]$ and the eigenvalue matrix $\mathbf{\Lambda} := \text{diag}(\lambda_1, \ldots, \lambda_N)$ to write $\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$. Now observe that while the diffusion expressions in (1) are polynomials on the GSO of possibly infinite degree, the Cayley-Hamilton theorem implies they are equivalent to polynomials of degree smaller than N. Upon defining the vector of coefficients $\mathbf{h} := [h_0, \ldots, h_{L-1}]^T$ and the graph filter $\mathbf{H} := \sum_{l=0}^{L-1} h_l \mathbf{S}^l$, the generative model in (1) can be rewritten as

$$\mathbf{x} = \left(\sum_{l=0}^{L-1} h_l \mathbf{S}^l\right) \mathbf{w} = \mathbf{H}\mathbf{w} \tag{2}$$

for some particular $\mathbf{h}$ and $L \leq N$. Fundamental for the present paper is to note that since $\mathbf{H}$ is a polynomial on $\mathbf{S}$ [1]: 1) all graph filters have the *same eigenvectors*, and 2) such eigenvectors are the same than those of the shift. In other words, while the diffusion implicit in $\mathbf{H}$ obscures the eigenvalues of the GSO, the eigenvectors $\mathbf{V}$ remain as ST of the underlying network topology. Next, Sec. 2.1 describes how to leverage (2) to obtain the ST from a set of nodal observations. Sec. 2.2 outlines how to use the ST to recover the desired GSO.

2.1. Stationary versus non-stationary observations

In this section we suppose that the set of observations $\mathcal{X} := \{\mathbf{x}^{(p)}\}_{p=1}^P$ correspond to random realizations of a process $\mathbf{x}$ adhering to the generative model in (2). The ultimate goal is to use the available observations to estimate the ST of the filter (hence the eigenvectors of the GSO) that governs the diffusion in (2).

To that end, suppose first that $\mathbf{w}$ is white (i.e., $\mathbf{C}_\mathbf{w} = \mathbf{I}$). Then the covariance matrix of $\mathbf{x}$ is $\mathbf{C}_\mathbf{x} := \mathbb{E}[\mathbf{x}\mathbf{x}^T] = \mathbb{E}[\mathbf{H}\mathbf{w}(\mathbf{H}\mathbf{w})^T] = \mathbf{H}\mathbb{E}[\mathbf{w}\mathbf{w}^T]\mathbf{H} = \mathbf{H}\mathbf{H}$. Using the spectral decomposition of $\mathbf{S}$ to express the filter as $\mathbf{H} = \sum_{l=0}^{L-1} h_l (\mathbf{V}\mathbf{\Lambda}\mathbf{V}^T)^l = \mathbf{V}(\sum_{l=0}^{L-1} h_l \mathbf{\Lambda}^l)\mathbf{V}^T$, we can write the covariance matrix as $\mathbf{C}_\mathbf{x} = \mathbf{V}\left|\sum_{l=0}^{L-1} h_l \mathbf{\Lambda}^l\right|^2 \mathbf{V}^T$, where the squared-modulus operator $|\cdot|^2$ is applied entrywise. Such covariance expression is precisely the requirement for a graph signal to be stationary on $\mathbf{S}$ [3, Def. 3]. Remarkably, if $\mathbf{x}$ is stationary or equivalently, if $\mathbf{w}$ is white, the *eigenvectors* of the shift $\mathbf{S}$, the filter $\mathbf{H}$ and the covariance $\mathbf{C}_\mathbf{x}$ are *all the same*. As a result, a simple method to estimate $\mathbf{V}$ from the observations $\{\mathbf{x}^{(p)}\}_{p=1}^P$ is to form the *sample covariance* $\hat{\mathbf{C}}_\mathbf{x}$ and use its eigenvectors as ST [5].

In this context, the broader focus of the present paper is on identifying the GSO $\mathbf{S}$ that is considered to be the best possible description of the structure of a *non-stationary* signal $\mathbf{x} = \mathbf{H}\mathbf{w}$ [cf. (2), where $\mathbf{w}$ is not white]. For generic (non-identity) input covariance matrix $\mathbf{C}_\mathbf{w}$, we face the challenge that *the signal covariance* $\mathbf{C}_\mathbf{x} = \mathbf{H}\mathbf{C}_\mathbf{w}\mathbf{H}$ *is no longer simultaneously diagonalizable with* $\mathbf{S}$. This rules out using the eigenvectors of the sample covariance $\hat{\mathbf{C}}_\mathbf{x}$ as ST of $\mathbf{S}$. Still, as argued following (2) the eigenvectors of the GSO coincide with those of the graph filter $\mathbf{H}$ that governs the underlying diffusion dynamics. This motivates using realizations of observed signals together with additional information on the excitation inputs $\mathbf{w}_m$ (either realizations of the graph signals or their covariance matrices $\mathbf{C}_{\mathbf{w},m}$ [15]) to *identify the filter* $\mathbf{H}$, with the ultimate goal of estimating its eigenvectors $\mathbf{V}$. This is the subject dealt with in Sec. 3, but before we close the loop showing how to find $\mathbf{S}$ given its ST.

2.2. Using the spectral templates to recover the shift

If the ST of the GSO are known, recovery of $\mathbf{S}$ amounts to selecting its eigenvalues. Since the problem is underdetermined (there are as many GSO as eigenvalues), we say that the GSO of interest is optimal in some sense. To be more precise, we can introduce criteria in the form of generic cost functions $f(\mathbf{S}, \mathbf{\lambda})$ and find the GSO as

$$\mathbf{S}^* := \underset{\{\mathbf{S},\mathbf{\lambda}\}}{\text{argmin}}\ f(\mathbf{S}, \mathbf{\lambda}), \quad \text{s. to } \mathbf{S} = \sum_{k=1}^N \lambda_k \mathbf{v}_k \mathbf{v}_k^T, \quad \mathbf{S} \in \mathcal{S}, \tag{3}$$

where $\mathbf{\lambda} = [\lambda_1, ..., \lambda_N]^T$, and $\mathcal{S}$ is a convex set that specifies the type of GSO we want to identify [5]. Also, we wrote $\mathbf{V}\mathbf{\Lambda}\mathbf{V}^T = \sum_{k=1}^N \lambda_k \mathbf{v}_k \mathbf{v}_k^T$ to emphasize that since the $\mathbf{v}_k$ are known, the equality constraints in (3) are linear on the unknown eigenvalues λ_k.

Criteria. Possible choices for the criteria in (3) are to: (i) Adopt $f(\mathbf{S}, \mathbf{\lambda}) = \|\mathbf{S}\|_F$, which finds a GSO minimizing the total energy stored in the weights of the edges. (ii) Make $f(\mathbf{S}, \mathbf{\lambda}) = \|\mathbf{S}\|_\infty$, which yields GSOs for graphs with uniformly low edge weights. This can be meaningful, e.g., when identifying graphs subject to capacity constraints. (iii) Minimize the ℓ_0 norm $f(\mathbf{S}, \mathbf{\lambda}) = \|\mathbf{S}\|_0$ which is non-convex, but of widespread interest in identifying sparse graphs (e.g., of direct relations among signal elements).

Constraints. The constraint $\mathbf{S} \in \mathcal{S}$ in (3) incorporates a priori knowledge about $\mathbf{S}$. If we let $\mathbf{S} = \mathbf{A}$ represent the adjacency matrix of an undirected graph with non-negative weights and no self-loops, we can explicitly write $\mathcal{S}$ as follows

$$\mathcal{S}_\text{A} := \{\mathbf{S} \,|\, S_{ij} \geq 0,\ \mathbf{S} \in \mathcal{H}_N,\ S_{ii} = 0,\ \textstyle\sum_j S_{j1} = 1\}. \tag{4}$$

The first condition in $\mathcal{S}_\text{A}$ encodes the non-negativity of the weights whereas the second condition incorporates that $\mathcal{G}$ is undirected, hence, $\mathbf{S}$ must belong to the set $\mathcal{H}_N$ of real and symmetric $N \times N$ matrices. The third condition encodes the absence of self-loops, thus, each diagonal entry of $\mathbf{S}$ must be null. Finally, the last condition fixes the scale of the admissible graphs by setting the weighted degree of the first node to 1, and rules out the trivial solution $\mathbf{S} = \mathbf{0}$. Other GSOs (e.g., $\mathbf{L}_c$ and its normalized variants) can be accommodated in our framework via minor adaptations to $\mathcal{S}$; see [5].

Robust formulations. While (3) assumes perfect information on the ST, modified formulations that can accommodate noisy observations and model mismatches are of interest. Tractable relaxations of (3) to estimate $\mathbf{\lambda}$ while being robust to errors stemming from the eigenvector estimation step are proposed in [24]; see also Sec. 4.

3. INFERRING ST FROM NON-STATIONARY SIGNALS

For $m = 1, \ldots, M$ diffusion processes on $\mathcal{G}$, we assume that the observed non-stationary signal $\mathbf{x}_m$ corresponds to an input $\mathbf{w}_m$ diffused by an unknown graph filter $\mathbf{H} = \sum_{l=0}^{L-1} h_l \mathbf{S}^l$ (which encodes the structure of the network via $\mathbf{S}$). In this section we show how additional information about the excitation $\mathbf{w}_m$ can be used to identify $\mathbf{H}$ and, as byproduct, its eigenvectors $\mathbf{V}$.

3.1. Input-output graph signal realization pairs

Suppose first that realizations of M output-input pairs $\{\mathbf{x}_m, \mathbf{w}_m\}_{m=1}^M$ are available. The goal is to identify a filter $\mathbf{H}$ such that the observed signal $\mathbf{x}_m$ and the predicted one $\mathbf{H}\mathbf{w}_m$ are close in some sense. Using the workhorse least-squares (LS) cost $\varepsilon_m(\mathbf{H}) = \|\mathbf{x}_m - \mathbf{H}\mathbf{w}_m\|_2^2$, the filter can then be estimated as

$$\mathbf{H}^* = \underset{\mathbf{H} \in \mathcal{H}_N}{\text{argmin}} \sum_{m=1}^M \varepsilon_m(\mathbf{H}), \text{ where } \varepsilon_m(\mathbf{H}) = \|\mathbf{x}_m - \mathbf{H}\mathbf{w}_m\|_2^2. \tag{5}$$

Several properties of the solution $\mathbf{H}^*$ of (5) are stated next [1].

Proposition 1 *Define the matrices* $\mathbf{W} = [\mathbf{w}_1, ..., \mathbf{w}_M]$ *and* $\mathbf{X} = [\mathbf{x}_1, ..., \mathbf{x}_M]$. *Then the filter* $\mathbf{H}^*$ *that solves* (5) *can be found as*

$$\text{vec}(\mathbf{H}^*) = \left((\mathbf{W}^T)^\dagger \otimes \mathbf{I}_N\right) \text{vec}(\mathbf{X}). \tag{6}$$

Moreover, if $M \geq N$ *and* $\mathbf{W}$ *is full rank, the minimizer* $\mathbf{H}^*$ *is unique.*

[1] Prop. 1 is agnostic to the symmetry in $\mathbf{H}$. Although leveraging symmetry is straightforward, it overloads notation and hinders clarity of exposition.

Proof: First, note that the cost in (5) can be compactly rewritten as $\|\mathbf{X}-\mathbf{H}\mathbf{W}\|_F^2$. Using the Kronecker product and the vec operator, we can further rewrite it as $\|\mathbf{X}-\mathbf{H}\mathbf{W}\|_F^2 = \|\operatorname{vec}(\mathbf{X}) - \big(\mathbf{W}^T \otimes \mathbf{I}_N\big)\operatorname{vec}(\mathbf{H})\|_2^2$. This LS cost can be minimized using the Moore-Penrose pseudoinverse as $\operatorname{vec}(\mathbf{H}^*) = \big((\mathbf{W}^T)\otimes\mathbf{I}_N\big)^\dagger \operatorname{vec}(\mathbf{X})$. Noting that $\big((\mathbf{W}^T)\otimes\mathbf{I}_{N\times N}\big)^\dagger = \big((\mathbf{W}^T)^\dagger\otimes\mathbf{I}_N^\dagger\big)$, (6) follows. Regarding uniqueness, it holds that if $(\mathbf{W}^T)\otimes\mathbf{I}_{N\times N}$ has rank at least N^2, then the $N^2\times 1$ vector $\operatorname{vec}(\mathbf{H}^*)$ minimizing $\|\operatorname{vec}(\mathbf{X}) - \big(\mathbf{W}^T\otimes\mathbf{I}_N\big)\operatorname{vec}(\mathbf{H})\|_2^2$ is unique. Since $\operatorname{rank}(\mathbf{I}_N)=N$, this is guaranteed if $\operatorname{rank}(\mathbf{W}^T)=\operatorname{rank}(\mathbf{W})=N$. ■

Proposition 1 asserts that if the excitation input set $\{\mathbf{x}_m\}_{m=1}^M$ is sufficiently rich – i.e., if $M\geq N$ and the excitation signals are linearly independent –, the entries of the generating filter $\mathbf{H}$ can be found as the solution of an LS problem. As explained at the beginning of Sec. 3, once $\mathbf{H}^*$ is estimated using (6), the next step is to factorize the filter as $\mathbf{H}^* = \mathbf{V}_{H^*}\mathbf{\Lambda}_{H^*}\mathbf{V}_{H^*}^T$ and use $\mathbf{V}=\mathbf{V}_{H^*}$ as input for the GSO identification problem (3), or its robust variant in Sec. 4.

3.2. Input covariance and positive semidefinite filters

In a number of applications, realizations of the excitation input $\mathbf{w}_m$ may be challenging to acquire, but information about the *statistical* description of $\mathbf{w}_m$ could still be available. To be specific, assume that the excitation inputs are zero mean and their covariance $\mathbf{C}_{\mathbf{w},m} = \mathbb{E}[\mathbf{w}_m\mathbf{w}_m^T]$ is known. Further suppose that for each input $\mathbf{w}_m$, we have access to a set of observations $\{\mathbf{x}_m^{(p)}\}_{p=1}^{P_m}$, which are then used to *estimate the output covariance* as $\hat{\mathbf{C}}_{\mathbf{x},m} = \frac{1}{P_m}\sum_{p=1}^{P_m}\mathbf{x}_m^{(p)}(\mathbf{x}_m^{(p)})^T$. Since under (2) the *ensemble covariance* is $\mathbf{C}_{\mathbf{x},m} = \mathbb{E}[\mathbf{x}_m\mathbf{x}_m^T] = \mathbf{H}\mathbf{C}_{\mathbf{w},m}\mathbf{H}$, the aim is to identify a filter $\mathbf{H}$ such that matrices $\hat{\mathbf{C}}_{\mathbf{x},m}$ and $\mathbf{H}\mathbf{C}_{\mathbf{w},m}\mathbf{H}$ are close.

In this section, we investigate the more favorable case where the filter $\mathbf{H}$ is a positive semidefinite (PSD) matrix. Such filters arise, for example, in Laplacian diffusion processes of the form $\mathbf{x} = (\sum_{l=0}^\infty \beta^l\mathbf{L}_c^l)\mathbf{w}$ with $\beta>0$, where the shift $\mathbf{L}_c$ is PSD and the filter coefficients $h_l=\beta^l$ are all positive. To select a convenient distance, note that matching covariance matrices $\hat{\mathbf{C}}_{\mathbf{x},m}$ and $\mathbf{H}\mathbf{C}_{\mathbf{w},m}\mathbf{H}$ using an LS metric is not trivial because the resultant cost is a fourth order polynomial on the entries of $\mathbf{H}$. For that reason, we leverage the fact that the square root of symmetric PD matrices is well defined and consider the matching error $\bar{\varepsilon}_m(\mathbf{H}) := \|(\mathbf{C}_{\mathbf{w},m}^{1/2}\hat{\mathbf{C}}_{\mathbf{x},m}\mathbf{C}_{\mathbf{w}}^{1/2})^{1/2} - \mathbf{C}_{\mathbf{w},m}^{1/2}\mathbf{H}\mathbf{C}_{\mathbf{w},m}^{1/2}\|_F^2$, where $(\cdot)^{1/2}$, when applied to matrices, denotes the *principal* square root. This matching error is convex in $\mathbf{H}$ and the filter can be thus identified as

$$\mathbf{H}^* = \operatorname*{argmin}_{\mathbf{H}\in\mathcal{H}_N^{++}} \sum_{m=1}^M \bar{\varepsilon}_m(\mathbf{H}),\ \text{where} \tag{7}$$
$$\bar{\varepsilon}_m(\mathbf{H}) = \|(\mathbf{C}_{\mathbf{w},m}^{1/2}\hat{\mathbf{C}}_{\mathbf{x},m}\mathbf{C}_{\mathbf{w}}^{1/2})^{1/2} - \mathbf{C}_{\mathbf{w},m}^{1/2}\mathbf{H}\mathbf{C}_{\mathbf{w},m}^{1/2}\|_F^2,$$

with $\mathcal{H}_N^{++}$ standing for the set of symmetric and PSD matrices. The following proposition offers insights on the solution to (7).

Proposition 2 *From the matrices* $\mathbf{W} = [\mathbf{W}_1,...,\mathbf{W}_M]^T$ *and* $\mathbf{X} = [\mathbf{X}_1,...,\mathbf{X}_M]^T$, *where* $\mathbf{W}_m := \mathbf{C}_{\mathbf{w},m}^{1/2}\otimes\mathbf{C}_{\mathbf{w},m}^{1/2}$ *and* $\mathbf{X}_m := (\mathbf{C}_{\mathbf{w},m}^{1/2}\hat{\mathbf{C}}_{\mathbf{x},m}\mathbf{C}_{\mathbf{w}}^{1/2})^{1/2}$. *Then, the filter* $\mathbf{H}^*$ *that solves* (7) *can be found as*

$$\operatorname{vec}(\mathbf{H}^*) = \mathbf{W}^\dagger\operatorname{vec}(\mathbf{X}^T). \tag{8}$$

Moreover, if $M=1$ *and matrix* $\mathbf{C}_{\mathbf{w},1}$ *is full rank, the minimizer* $\mathbf{H}^*$ *is unique and can be found as*

$$\mathbf{H}^* = \mathbf{C}_{\mathbf{w},1}^{-1/2}\big(\mathbf{C}_{\mathbf{w},1}^{1/2}\hat{\mathbf{C}}_{\mathbf{x},1}\mathbf{C}_{\mathbf{w},1}^{1/2}\big)^{1/2}\mathbf{C}_{\mathbf{w},1}^{-1/2}. \tag{9}$$

Proof: To show (8) one can follow steps similar to those for (6) in Proposition 1. To show the identifiability result for $M=1$, note that the cost $\bar{\varepsilon}_1(\mathbf{H})$ is minimum if $\mathbf{H}$ can be selected to satisfy $(\mathbf{C}_{\mathbf{w},1}^{1/2}\hat{\mathbf{C}}_{\mathbf{x},1}\mathbf{C}_{\mathbf{w},1}^{1/2})^{1/2} = \mathbf{C}_{\mathbf{w},1}^{1/2}\mathbf{H}\mathbf{C}_{\mathbf{w},1}^{1/2}$, so that $\bar{\varepsilon}_1(\mathbf{H})$ is zero. Left and right multiplying both sides by $\mathbf{C}_{\mathbf{w},m}^{-1/2}$ yields (9). ■

Proposition 2 demonstrates that the assumption of $\mathbf{H}\in\mathcal{H}_N^{++}$ gives rise to a strong identifiability result. Indeed, if $\{\mathbf{C}_{\mathbf{x},m}\}_{m=1}^M$ are known perfectly, identifiability and consistency are attained even for $M=1$. The reason is that although the inverse mapping from $\mathbf{C}_{\mathbf{x},m}$ to $\mathbf{H}$ requires finding a square root (this is a problem because multiple roots exist), only one of them is symmetric and PSD.

3.3. Input covariance and generic filters

Here we investigate the filter identification problem for a generic symmetric $\mathbf{H}$. As in Sec. 3.2, the problem is to identify a filter $\mathbf{H}$ that drives the observed covariances $\{\mathbf{C}_{\mathbf{x},m}\}_{m=1}^M$ close to $\{\mathbf{H}\mathbf{C}_{\mathbf{w},m}\mathbf{H}\}_{m=1}^M$, the latter which can be formed using input covariance information. Since the filter is not PSD, using square roots is not prudent here. Hence, one can instead adopt the ordinary LS cost $\tilde{\varepsilon}_m(\mathbf{H}) = \|\hat{\mathbf{C}}_{\mathbf{x},m} - \mathbf{H}\mathbf{C}_{\mathbf{w},m}\mathbf{H}\|_F^2$ and estimate the filter as

$$\mathbf{H}^* = \operatorname*{argmin}_{\mathbf{H}\in\mathcal{H}_N} \sum_{m=1}^M \tilde{\varepsilon}_m(\mathbf{H}), \tag{10}$$
$$\text{where}\ \ \tilde{\varepsilon}_m(\mathbf{H}) = \|\hat{\mathbf{C}}_{\mathbf{x},m} - \mathbf{H}\mathbf{C}_{\mathbf{w},m}\mathbf{H}\|_F^2.$$

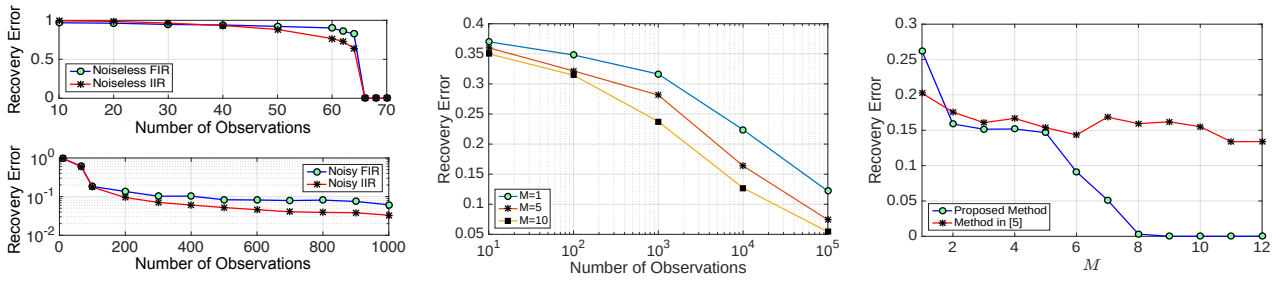
The above problem is a non-convex fourth order polynomial optimization, which can potentially have multiple solutions. Since finding $\mathbf{H}^*$ is challenging, we seek efficient algorithms able to find stationary solutions. To that end, we introduce the auxiliary variables $\mathbf{H}_L$ and $\mathbf{H}_R$ and reformulate (10) as a bi-convex problem with linear constraints $\mathbf{H}_L=\mathbf{H}_R=\mathbf{H}$, namely

$$\{\mathbf{H}_L^*,\mathbf{H}_R^*\} = \operatorname*{arg\,min}_{\mathbf{H}_L\in\mathcal{H}_N,\mathbf{H}_R\in\mathcal{H}_N} \sum_{m=1}^M \|\hat{\mathbf{C}}_{\mathbf{x},m} - \mathbf{H}_L\mathbf{C}_{\mathbf{w},m}\mathbf{H}_R\|_F^2 \tag{11}$$
$$\text{s. to}\ \ \mathbf{H}_L=\mathbf{H}_R$$

Problem (11) can be tackled using the Alternating Direction Method of Multipliers (ADMM) [25], which has been applied to a wide variety of linearly constrained convex and non-convex problems. Since multiple local optima exist, we run the algorithm for I random initializations and among the I estimated filters we select the one whose eigenvectors lead to the sparsest graph shift $\mathbf{S}$; see also Sec. 4.

Since (11) is non-convex, in general identifiability and consistency cannot be guaranteed. As discussed in Sec. 3.2, this is somehow expected since the mapping from $\mathbf{H}$ to the observed covariance is quadratic and hence, multiple feasible solutions (as many as square roots) exist. Conceivably, as M increases the number of feasible solutions will decrease and the problem can become identifiable. Formalizing this requires imposing conditions on the eigenspace of the input covariance matrices $\{\mathbf{H}\mathbf{C}_{\mathbf{w},m}\mathbf{H}\}_{m=1}^M$. For example, one can show that if all *covariances* have the *same eigenvectors*, the problem remains non identifiable even for high values of M. Last but not least, defining error metrics tailored to the quadratic mapping between $\mathbf{H}$ and $\mathbf{C}_{\mathbf{x}}$ and giving rise to a more tractable optimization is also of interest, but left as future work.

Remark 1 The formulations in Secs. 3.1 and 3.3 can be combined to exploit multiple sources of information. This can be useful if both input covariances and pairs of input-output realizations are available. It is also relevant in scenarios where the inputs are not zero-mean but their first and second moments are known. Defining $\hat{\boldsymbol{\mu}}_{\mathbf{x},m} := \frac{1}{P_m}\sum_{p=1}^{P_m}\mathbf{x}_m^{(p)}$ and $\boldsymbol{\mu}_{\mathbf{w},m} := \mathbb{E}[\mathbf{w}_m]$, a natural cost would be



(a) (b) (c)

Fig. 1: (a) Recovery error for FIR and IIR filters versus number of observed signals in noiseless (top) and noisy (bottom) settings. (b) Error in recovering a social network as a function of the number of opinion profiles observed and parametrized by the number of topics M. (c) Recovery error for the proposed method and the algorithm in [5] as a function of M, the number of observed sample covariance matrices.

$\breve{\varepsilon}(\mathbf{H}) = \beta_1 \sum_{m=1}^{M} \|\hat{\boldsymbol{\mu}}_{\mathbf{x},m} - \mathbf{H}\boldsymbol{\mu}_{\mathbf{w},m}\|_2^2 + \beta_2 \sum_{m=1}^{M} \tilde{\varepsilon}_m(\mathbf{H})$, where β_1 and β_2 are tuning constants and $\tilde{\varepsilon}_m(\mathbf{H})$ is defined in (10).

4. NUMERICAL TESTS

We study the recovery of two real-world graphs to assess the performance of the proposed network topology inference algorithms. We first obtain estimates $\hat{\mathbf{V}}$ of the GSO eigenvectors under the three settings described in Secs. 3.1-3.3. Given those ST we form $\mathbf{S}' := \sum_{k=1}^{N} \lambda_k \hat{\mathbf{v}}_k \hat{\mathbf{v}}_k^T$ and search for a *sparse* shift $\mathbf{S}$ that is close to $\mathbf{S}'$, namely we solve the convex problem

$$\hat{\mathbf{S}}^* := \underset{\{\mathbf{S},\boldsymbol{\lambda},\mathbf{S}'\}}{\operatorname{argmin}} \ \|\mathbf{S}\|_1 \qquad (12)$$
$$\text{s. to } \ \mathbf{S}' = \textstyle\sum_{k=1}^{N} \lambda_k \hat{\mathbf{v}}_k \hat{\mathbf{v}}_k^T, \ \ \mathbf{S} \in \mathcal{S}, \ \ \|\mathbf{S} - \mathbf{S}'\|_F \leq \epsilon.$$

Brain graph. Consider a brain graph $\mathcal{G}$ with $N = 66$ nodes or neural regions and edge weights given by the density of anatomical connections between regions [26]. Denoting by $\mathbf{S} = \mathbf{A}$ the weighted adjacency of the brain graph, we consider two types of filters $\mathbf{H}_1 = \sum_{l=0}^{2} h_l \mathbf{A}^l$ and $\mathbf{H}_2 = (\mathbf{I} + \alpha\mathbf{A})^{-1}$, where the coefficients h_l and α are drawn uniformly on $[0, 1]$. We then generate M random input-output pairs $\{\mathbf{w}_m, \mathbf{x}_m\}_{m=1}^{M}$ (cf. Sec. 3.1), where signals are filtered by either $\mathbf{H}_1$ or $\mathbf{H}_2$, and estimate the filter using (6). Problem (12) with $\hat{\mathbf{V}}$ given by the eigenvectors of the estimated filter is then solved in order to infer the brain graph. In Fig. 1-(a) (top) we plot the recovery error $\|\hat{\mathbf{S}}^* - \mathbf{S}\|_F / \|\mathbf{S}\|_F$ as a function of M for both types of filters. First, notice that the performance is independent of the filter type. More importantly, for $M \geq N$, the optimal filter estimation is unique (cf. Proposition 1) and leads to perfect recovery. We also consider the case where the observation of the output signals $\mathbf{x}_m$ is noisy; see Fig. 1-(a) (bottom). For this latter case, even though the estimation improves with increasing M, a larger number of observations is needed to guarantee successful recovery of the brain graph.

Social network. We consider the social network of Zachary's karate club [27] represented by a graph $\mathcal{G}$ consisting of $N = 34$ nodes or members of the club and undirected edges symbolizing friendships among them. Denoting by $\mathbf{L}$ the normalized Laplacian of $\mathcal{G}$, we define the graph shift operator $\mathbf{S} = \mathbf{I} - \alpha\mathbf{L}$ with $\alpha = 1/\lambda_{\max}(\mathbf{L})$, modeling the diffusion of opinions between the members of the club. A signal $\mathbf{x}$ can be regarded as a unidimensional opinion of each club member regarding a specific topic, and each application of $\mathbf{S}$ can be seen as an opinion update. Our goal is to recover $\mathbf{L}$ – hence, the social structure of the Karate club – from the observations of opinion profiles. We consider M different processes in the graph – corresponding, e.g., to opinions on M different topics – and assume that an opinion profile $\mathbf{x}_m$ is generated by the diffusion through the network of an initial signal $\mathbf{w}_m$. More precisely, for each topic $m = 1, \ldots, M$, we model $\mathbf{w}_m$ as a zero-mean process with known covariance $\mathbf{C}_{\mathbf{w},m}$. We are then given a set $\{\mathbf{x}_m^{(p)}\}_{p=1}^{P}$ of opinion profiles generated from different sources $\{\mathbf{w}_m^{(p)}\}_{p=1}^{P}$ diffused through a filter of unknown nonnegative coefficients $\boldsymbol{\beta}$. From these P opinion profiles we build an estimate $\hat{\mathbf{C}}_{\mathbf{x},m}$ of the output covariance and, leveraging the fact that $\mathbf{S}$ is PSD and $\boldsymbol{\beta} \geq 0$ (cf. Sec. 3.2), we estimate the unknown filter $\mathbf{H}^*$ as in (9). Lastly, we use the eigenvectors $\hat{\mathbf{V}}$ of $\mathbf{H}^*$ to solve (12), where $\mathcal{S}$ is modified accordingly for the recovery of a normalized Laplacian; see [24]. In Fig. 1-(b) we plot the shift recovery error as a function of the number of observations P and for three different values of M. As P increases, the estimate $\hat{\mathbf{C}}_{\mathbf{x},m}$ becomes more reliable entailing a better estimation of the underlying filter and, ultimately, leading to more accurate eigenvectors $\hat{\mathbf{V}}$. Hence, we observe a decreasing error with increasing P. Moreover, for a fixed P, the error in the estimation of $\hat{\mathbf{C}}_{\mathbf{x},m}$ can be partially overcome by observing multiple processes, thus, larger values of M lead to smaller errors.

Finally, we use the same graph to generate input-output covariance pairs $\{\mathbf{C}_{\mathbf{w},m}, \mathbf{C}_{\mathbf{x},m}\}_{m=1}^{M}$ and evaluate the performance of the method in Sec. 3.3. Signals are generated using the filter $\mathbf{H}_1 = \sum_{l=0}^{2} h_l \mathbf{A}^l$, where the coefficients are drawn randomly on $[0, 1]$. We first estimate the ST by solving (11), and then use (12) to recover the GSO. Fig. 1-(c) depicts the recovery error versus M for two different approaches – the proposed one and its counterpart in [5] for stationary signals. First, we notice that as M increases, for the proposed method the recovery error decreases monotonically. For instance, we can successfully recover almost all the edges with 9 observed covariances. As expected, for $M > 1$ the proposed method outperforms the algorithm in [5] which uses the output covariance eigenvectors as ST.

5. CONCLUSIONS

We studied the problem of inferring a network from *non-stationary* signals diffused on the unknown graph. Relative to the stationary setting, the main challenge is that the GSO eigenvectors differ from those of the signal covariance matrix. To overcome this hurdle, we leverage that the sought eigenbasis is preserved by the polynomial graph filter that governs the diffusion process. As a result, the novel approach is to first identify the GSO eigenvectors from a judicious graph filter estimate, and then we rely on these spectral templates to estimate the eigenvalues by imposing desirable properties on the graph to be recovered; e.g., edge sparsity. We propose different estimators of the diffusion filter depending on whether realizations, or, second-order statistical information is available from the input-output graph signal pair. The overall network topology inference pipeline is validated on social and structural brain networks.

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