DIRECTED NETWORK TOPOLOGY INFERENCE VIA GRAPH FILTER IDENTIFICATION

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ABSTRACT

We address the problem of inferring a *directed* network from nodal observations of graph signals generated by linear diffusion dynamics on the sought graph. Observations are modeled as the outputs of a linear graph filter (i.e., a polynomial on a local diffusion graph-shift operator encoding the unknown graph topology), excited with an ensemble of independent graph signals with arbitrarily-correlated nodal components. In this context, we first rely on observations of the output signals along with prior statistical information on the inputs to identify the diffusion filter. Such problem entails solving a system of quadratic matrix equations, which we recast as a smooth quadratic minimization subject to Stiefel manifold constraints. Subsequent identification of the network topology given the graph filter estimate boils down to finding a sparse and structurally admissible shift that commutes with the given filter, thus forcing the latter to be a polynomial in the sought graph-shift operator. Preliminary numerical tests corroborating the effectiveness of the proposed algorithms in recovering synthetic and real-world digraphs are provided.

Index Terms— Network topology inference, graph signal processing, directed networks, network diffusion, system identification.

1. INTRODUCTION

Consider a network represented as a weighted and directed (di)graph $\mathcal{G}$, with a node set $\mathcal{N}$ of known cardinality N, an edge set $\mathcal{E}$ of ordered pairs of elements in $\mathcal{N}$. The edge weights $A_{ij} \in \mathbb{R}$ such that $A_{ij} \neq 0$ for all $(i,j) \in \mathcal{E}$ are collected in the (generally non-symmetric) adjacency matrix $\mathbf{A}$. As a more general algebraic descriptor of network structure, one can define a *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]. Accordingly, $\mathbf{S}$ can be viewed as a local diffusion operator. Common choices for digraphs are to set it to either $\mathbf{A}$ (and its normalized counterparts) or variations of adjacency matrices [2].

Our focus in this paper is on identifying graphs that explain the structure of a random signal. Formally, let $\mathbf{y} = [y_1, ..., y_N]^T \in \mathbb{R}^N$ be a graph signal in which the ith element y_i denotes the signal value at node i of an *unknown digraph* $\mathcal{G}$ with shift operator $\mathbf{S}$. Further suppose that we are given a zero-mean signal $\mathbf{x}$ with covariance matrix $\mathbf{C_x} = \mathbb{E}\left[\mathbf{xx}^T\right]$. We say that the sparse digraph $\mathbf{S}$ represents the structure of the signal $\mathbf{y}$ if there exists a diffusion process in the GSO $\mathbf{S}$ – formalized as a polynomial graph filter – that generates the observed signal $\mathbf{y}$ from the input signal $\mathbf{x}$ via linear filtering, that is

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

for some set of parameters $\{\alpha_l\}$, or equivalently $\{\beta_l\}$. While $\mathbf{S}$ encodes only one-hop interactions, each successive application of

the shift in (1) percolates $\mathbf{x}$ over $\mathcal{G}$; see e.g. [3]. The justification to say that $\mathbf{S}$ represents the structure of $\mathbf{y}$ 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. Alternatively, one can view the input-output relationship in (1) as encompassing all possible smooth (analytic) functions of the sparse matrix $\mathbf{S}$. Our goal is then to exploit this model to recover the fundamental relations described by $\mathbf{S}$ from a set $\mathcal{Y}$ of independent realizations of a random signal $\mathbf{y}$ along with prior knowledge of $\mathbf{C_x}$. This additional statistical information on the input is the price paid to accommodate non-stationary processes $\mathbf{y}$ with respect to (possibly) asymmetric GSOs [4–7].

Relation to prior work. Workhorse topology inference approaches construct (mostly symmetric) graphs whose edge weights correspond to nontrivial correlations between signals at incident nodes [8, 9]. Acknowledging that the observed correlations can be due to latent network effects, alternative statistical methods rely on inference of partial correlations [8, Ch. 7.3.2]. Under Gaussianity assumptions, this line of work has well-documented connections with covariance selection [10] and sparse precision matrix estimation [11–14], as well as high-dimensional sparse linear regression [15]. Extensions to digraphs include structural equation models (SEMs) [16–18], Granger causality [9,19], or their nonlinear (e.g., kernelized) variants [20, 21]. 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 a graph [22–27]. Different from [22, 24, 28, 29] that infer structure from signals assumed to be smooth over the sought undirected graph, here the measurements are assumed related to the graph via filtering. Few works have recently explored this approach by identifying a symmetric GSO given its eigenvectors, either assuming that the input is white [25, 26] – equivalently implying $\mathbf{y}$ is graph stationary [4–6]; or, colored as in the present paper [7, 30]. Here instead, we distinctly address the general case of digraphs. Relative to [18] that relies on a single-pole graph filter [31], the filter structure underlying (1) can be arbitrary (subsuming correlation networks, Gaussian graphical models, and SEMs [25, Remark 2]), but the focus here is on learning time-invariant graphs.

Paper outline and contributions. In Section 2 we formulate the problem of identifying a GSO that explains the fundamental structure of a random signal diffused on a digraph. We advocate an innovative bilevel approach whereby: i) given independent output observations and prior information on the input statistics we identify the graph filter; and ii) given the filter estimate along with structural constraints on the GSO we recover the topology of the digraph. In Section 3 we address the problem of identifying the diffusion filter [cf. i)], which entails solving a system of *quadratic* matrix equations formed using the available information on the input along with output signal measurements. We show that the set of feasible filters is related to the square roots of the observations' covariance matrix,

and that such a set is markedly larger that its counterpart for symmetric filters (Section 3.1). Building on these insights, in Section 3.2 we recast the filter-inference problem as a smooth quadratic minimization subject to Stiefel manifold constraints. Such non-convex problem can be tackled leveraging recent advances for orthogonality-constrained optimization; see e.g., [32]. Subsequent identification of a directed GSO given the diffusion filter estimate [cf. ii)] is addressed in Section 4. The focus is on finding a *sparse* and structurally admissible shift that commutes with the given filter, thus forcing the latter to be a polynomial in the GSO as in (1). Preliminary numerical tests corroborate the effectiveness of the proposed approach in recovering both synthetic and social networks are given in Section 5.

2. PRELIMINARIES AND PROBLEM STATEMENT

Suppose we observe realizations of a random signal $\mathbf{y}$ generated through diffusion on $\mathcal{G}$ of an input $\mathbf{x}$, namely via successive applications of a GSO $\mathbf{S}$ as in (1). Since the (statistical) properties of the signal $\mathbf{y}$ depend on $\mathbf{S}$, our goal is to use a set of observations together with available information on the excitation input to infer the digraph topology. In other words, we aim to recover the GSO which encodes pairwise influence between graph nodes, given observable indirect relationships generated by a diffusion process. To formally state the problem, we elaborate on the diffusion model in (1) as well as on the available information from the graph signals.

Network diffusion as graph filtering. While the diffusion expressions in (1) entail (possibly) infinite-degree polynomials in $\mathbf{S} \in \mathbb{R}^{N \times N}$, the Cayley-Hamilton theorem asserts that 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 $\mathbf{H} := \sum_{l=0}^{L-1} h_l \mathbf{S}^l$ [1], the model in (1) can thus be rewritten as

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

for some particular $\mathbf{h}$ and $L \leq N$. Central to the present paper is to note that since $\mathbf{H}$ is a polynomial in $\mathbf{S}$, if $\mathbf{S}$ is diagonalizable and all its eigenvalues are simple then $\mathbf{H}$ and $\mathbf{S}$ commute, i.e., $\mathbf{HS} = \mathbf{SH}$ [33, Prop. 2.3]. We will exploit this identity in Section 4, which can be interpreted to imply that graph filters are shift invariant. Another upshot of the polynomial relationship is that the eigenvectors of $\mathbf{H}$ and $\mathbf{S}$ coincide. Hence, while the diffusion implicit in $\mathbf{H}$ obscures part of the structure of $\mathbf{S}$ (its eigenvalues), its eigenvectors remain as templates of the underlying network topology [7, 25, 26].

Observations and prior information on the input signals. We observe M network processes $\{\mathbf{y}_m\}_{m=1}^M$ on $\mathcal{G}$, each one corresponding to a different input random signal $\mathbf{x}_m$ that is diffused via a common filter $\mathbf{H}$. The multiplicity and statistical diversity of input processes will be instrumental towards identifying (uniquely) the diffusion filter. Let $\mathcal{Y}_m := \{\mathbf{y}_m^{(p)}\}_{p=1}^{P_m}$ capture the observed output signal realizations associated with the mth process, and likewise let $\mathcal{Y} := \bigcup_{m=1}^M \mathcal{Y}_m$ collect all available observations. Regarding the mth input process, one could conceivably assume its mean vector $\boldsymbol{\mu}_{\mathbf{x},m} := \mathbb{E}[\mathbf{x}_m]$, its covariance matrix $\mathbf{C}_{\mathbf{x},m}$, or even realizations of the signal $\{\mathbf{x}_m^{(p)}\}_{p=1}^{P_m}$ are given. Henceforth the focus will be on the most pragmatic setting whereby only second-order statistics are available, but other scenarios will be briefly outlined in Section 3.3.

Problem statement. Given observations $\mathcal{Y} = \bigcup_{m=1}^M \mathcal{Y}_m$ adhering to the generative model (2), where a common filter $\mathbf{H} := \sum_{l=0}^{L-1} h_l \mathbf{S}^l$ diffuses M zero-mean inputs $\mathbf{x}_m$ with known covariance matrices $\mathbf{C}_{\mathbf{x},m} = \mathbb{E}[\mathbf{x}_m \mathbf{x}_m^T]$, $m = 1, \ldots, M$, find the sparsest shift $\mathbf{S}$ with desirable topological properties (e.g., it is a valid adjacency matrix) that is consistent with the available observations.

Motivated by the discussion following (2), our bilevel network topology inference approach is to: i) first use realizations of observed signals in $\mathcal{Y}$ together with side information on the excitation inputs $\{\mathbf{x}_m\}_{m=1}^M$ to *identify the diffusion filter* $\mathbf{H}$; and ii) then use the estimated filter along with prior information on the network topology to *infer the GSO* $\mathbf{S}$. Step i) is addressed in Section 3, while ii) is discussed in Section 4.

3. ASYMMETRIC DIFFUSION FILTER IDENTIFICATION

In a number of applications, realizations of the excitation input $\mathbf{x}_m$ may be challenging to acquire, but information about the *statistical* description of $\mathbf{x}_m$ could still be available. As in our statement of the problem, assume for now that the excitation inputs are zero mean and their covariance matrices $\mathbf{C}_{\mathbf{x},m}$ are known. As explained in Section 2, suppose also that for each $m = 1, \ldots, M$ we acquire a set of observations $\mathcal{Y}_m = \{\mathbf{y}_m^{(p)}\}_{p=1}^{P_m}$, which are then used to estimate the output covariance $\mathbf{C}_{\mathbf{y},m} = \mathbb{E}[\mathbf{y}_m \mathbf{y}_m^T]$ via sample averaging, that is

$$\hat{\mathbf{C}}_{\mathbf{y},m} = \frac{1}{P_m} \sum_{p=1}^{P_m} \mathbf{y}_m^{(p)} (\mathbf{y}_m^{(p)})^T. \qquad (3)$$

Since under (2) the ensemble output covariance is given by $\mathbf{C}_{\mathbf{y},m} = \mathbf{H}\mathbf{C}_{\mathbf{x},m}\mathbf{H}^T$, the aim is to identify a filter $\mathbf{H}$ such that matrices $\hat{\mathbf{C}}_{\mathbf{y},m}$ and $\mathbf{H}\mathbf{C}_{\mathbf{x},m}\mathbf{H}^T$ are close in some sense.

3.1. Solving matrix quadratic equations for filter identification

Assuming for now perfect knowledge of the signal covariances, the above rationale suggests studying the solutions of the following system of matrix quadratic equations

$$\mathbf{C}_{\mathbf{y},m} = \mathbf{H}\mathbf{C}_{\mathbf{x},m}\mathbf{H}^T, \quad m = 1, \ldots, M \qquad (4)$$

for real-valued and possibly asymmetric $\mathbf{H}$. To gain insights on the solutions to (4), consider first the case where $M = 1$ and henceforth drop the subindex m to focus on the square roots of $\mathbf{C_y} = \mathbf{H}\mathbf{C_x}\mathbf{H}^T$.

To that end, recall first that the principal square root of $\mathbf{C_y}$ is the only symmetric and positive semidefinite (PSD) matrix $\mathbf{C_y}^{1/2}$ which satisfies $\mathbf{C_y} = \mathbf{C_y}^{1/2}\mathbf{C_y}^{1/2}$. Such a matrix is given by $\mathbf{C_y}^{1/2} = \mathbf{V_y}\boldsymbol{\Lambda_y}^{1/2}\mathbf{V_y}^T$, where $\mathbf{V_y}$ are the eigenvectors of $\mathbf{C_y}$ and $\boldsymbol{\Lambda_y}^{1/2}$ stands for a diagonal matrix with the square roots of the (non-negative) eigenvalues of $\mathbf{C_y}$. With $\mathbf{U}$ denoting an *orthogonal* matrix (such that $\mathbf{U}\mathbf{U}^T = \mathbf{I}$), one can show that any square matrix $\mathbf{H_x}$ such that $\mathbf{C_y} = \mathbf{H_x}\mathbf{H_x}^T$ is of the form $\mathbf{H_x} = \mathbf{C_y}^{1/2}\mathbf{U}$. This observation can be leveraged to establish the following result, which characterizes the solution set of each individual equation in (4).

Lemma 1 If $\mathbf{C}_{\mathbf{x},m}$ and $\mathbf{C}_{\mathbf{y},m}$ are full rank, the set $\mathcal{H}_m$ containing all the (possibly asymmetric) matrices $\mathbf{H}$ that solve (4) for a particular m is given by

$$\mathcal{H}_m = \{\mathbf{H} \,|\, \mathbf{H} = \mathbf{C}_{\mathbf{y},m}^{1/2}\mathbf{U}\mathbf{C}_{\mathbf{x},m}^{-1/2} \text{ and } \mathbf{U}\mathbf{U}^T = \mathbf{I}\}. \qquad (5)$$

A simple substitution suffices to show that every $\mathbf{H}$ of the form in (5) solves the corresponding mth equation in (4). Conversely, given an $\mathbf{H}$ that solves (4), form the matrix $\mathbf{U} = \mathbf{C}_{\mathbf{y},m}^{-1/2}\mathbf{H}\mathbf{C}_{\mathbf{x},m}^{1/2}$ and observe that if $\mathbf{U}$ is orthogonal, then $\mathbf{H} \in \mathcal{H}_m$. Orthogonality of $\mathbf{U}$ follows since $\mathbf{U}\mathbf{U}^T = \mathbf{C}_{\mathbf{y},m}^{-1/2}\mathbf{H}\mathbf{C}_{\mathbf{x},m}\mathbf{H}^T\mathbf{C}_{\mathbf{y},m}^{-1/2} = \mathbf{I}$, where the last equality comes from the fact that $\mathbf{H}$ solves (4).

If the GSO $\mathbf{S}$ (and hence the filter $\mathbf{H}$) is symmetric, then $\mathbf{U}$ must be of the form $\mathbf{U} = \text{diag}(\mathbf{b})$, with $\mathbf{b} = \{-1, 1\}^N$. This additional structure reduces considerably the size of the feasible set

in (5); see [7] for details. Still, even in this case it is apparent that for $M = 1$ **H** is non-identifiable (up to an unavoidable sign ambiguity).

For the general case of $M > 1$, the set of solutions to the system of quadratic equations (4) is just given by the intersection of (5) for all diffusion processes, i.e., $\mathcal{H}_{1:M} := \bigcap_{m=1}^{M} \mathcal{H}_m$. Studying the structure of $\mathcal{H}_{1:M}$ to obtain identifiability conditions for (4) is of interest, but out of the scope of this short paper. The role of M on the identification of **H** is briefly discussed at the end on the next section.

3.2. Orthogonality-constrained least-squares estimator

In practice, only empirical covariances (3) are available and the equalities in (4) must be relaxed. Given estimates $\{\hat{\mathbf{C}}_{\mathbf{y},m}\}_{m=1}^{M}$ obtained with enough samples to ensure full-rankness, our filter identification approach is to rely on (5) to solve the manifold-constrained least-squares (LS) problem

$$\min_{\{\mathbf{U}_m\}_{m=1}^{M}} \sum_{m,m'} \|\hat{\mathbf{C}}_{\mathbf{y},m}^{1/2}\mathbf{U}_m\mathbf{C}_{\mathbf{x},m}^{-1/2} - \hat{\mathbf{C}}_{\mathbf{y},m'}^{1/2}\mathbf{U}_{m'}\mathbf{C}_{\mathbf{x},m'}^{-1/2}\|_F^2 \quad (6)$$

$$\text{s. to } \mathbf{U}_m \in \mathcal{U}_N, \ m = 1, \ldots, M,$$

where $\mathcal{U}_N$ denotes the Stiefel manifold of $N \times N$ real orthogonal matrices. Note that both terms within the Frobenius norm in (6) should equal **H** in a noiseless setting. Thus, (6) minimizes this discrepancy across the M processes considered. Accordingly, given a solution $\{\hat{\mathbf{U}}_m\}_{m=1}^{M}$ of (6), the diffusion filter **H** can be estimated as

$$\hat{\mathbf{H}} = \frac{1}{M} \sum_{m=1}^{M} \hat{\mathbf{C}}_{\mathbf{y},m}^{1/2}\hat{\mathbf{U}}_m\mathbf{C}_{\mathbf{x},m}^{-1/2}. \quad (7)$$

Even though the objective in (6) is convex in the unknowns $\{\mathbf{U}_m\}_{m=1}^{M}$, the constraint set $\mathcal{U}_N$ is not. For the numerical tests in Section 5, we solve (6) using a provably-convergent feasible method for optimization of differentiable functions over the Stiefel manifold [32].

As the number M of observed processes increases, recoverability of (6) improves. Notice that in the absence of noise we would be effectively intersecting more sets $\mathcal{H}_m$ [cf. (5)], thus necessarily aiding identifiability, which is necessary for recoverability. Intuitively, each m provides a new set of observations that reduces the original N^2 degrees of freedom in **H**, to $N(N-1)/2$ in the manifold-constrained $\mathbf{U}_m$. As a result, assuming that the input covariances $\mathbf{C}_{\mathbf{x},m}$ provide sufficiently rich information, the problem could become identifiable even for $M = 2$. Simulations in Section 5 assess recovery as M increases.

3.3. Combining quadratic and linear observations

There may be scenarios where the system of matrix quadratic equations in (4) can be augmented with some matrix linear equations. That is the case if both input covariances and pairs of input-output realizations $\{\mathbf{y}_m, \mathbf{x}_m\}_{m=1}^{M}$ are available. It is also relevant when the inputs are not zero-mean but both their first and second-order moments are known. Defining $\hat{\boldsymbol{\mu}}_{\mathbf{y},m} := (1/P_m)\sum_{p=1}^{P_m}\mathbf{y}_m^{(p)}$ and recalling that $\boldsymbol{\mu}_{\mathbf{x},m} = \mathbb{E}[\mathbf{x}_m]$, a natural criterion is

$$\min_{\mathbf{H},\{\mathbf{U}_m\}_{m=1}^{M}} \sum_m \|\mathbf{H} - \hat{\mathbf{C}}_{\mathbf{y},m}^{1/2}\mathbf{U}_m\mathbf{C}_{\mathbf{x},m}^{-1/2}\|_F^2 + \beta\|\hat{\boldsymbol{\mu}}_{\mathbf{y},m} - \mathbf{H}\boldsymbol{\mu}_{\mathbf{x},m}\|_2^2$$

$$\text{s. to } \mathbf{U}_m \in \mathcal{U}_N, \ m = 1, \ldots, M, \quad (8)$$

where β is a tuning constant. The cost in (8) is again smooth, and the only source of non-convexity is the manifold constraint. Note also that if $\beta = 0$ the optimization (8) serves as an alternative formulation to (6), with the additional variable **H**.

By viewing the new terms in the objective of (8) as a Lagrangian penalty, one would expect these additional constraints relative to (6) would result in improved recovery performance. Equally important, availability of linear observations will also aid identifiability in the noise-free case. In fact, one can show that if the number of linear equations grows large and we have that rank$([\boldsymbol{\mu}_{\mathbf{x},1}, ..., \boldsymbol{\mu}_{\mathbf{x},M}]) \geq N$, then the problem becomes identifiable (see, [30] for a related argument for symmetric filters).

4. DIGRAPH TOPOLOGY INFERENCE

Given the graph filter **H**, our approach to infer the topology of the underlying graph is to find a GSO **S** that satisfies certain desirable topological properties and is compatible with **H**. Focusing on recovery of the sparsest shift operator (i.e., the graph that minimizes the number of direct interactions among nodes), one can solve

$$\hat{\mathbf{S}} := \underset{\mathbf{S}}{\operatorname{argmin}} \ \|\mathbf{S}\|_0, \quad \text{s. to } \mathbf{S} \in \mathcal{S}, \quad \mathbf{HS} = \mathbf{SH}, \quad (9)$$

where $\|\mathbf{S}\|_0$ counts the number of non-zero entries of **S**, $\mathcal{S}$ is a convex set specifying the type of GSO we want to identify [25], and the constraint $\mathbf{HS} = \mathbf{SH}$ forces the filter **H** to be a polynomial in **S**; see [23, 34] and the discussion following (2). Imposing this last constraint offers an important departure from the (undirected) graph learning algorithms in [25, 26, 30]. These approaches first estimate the *eigenvectors* of **H**, and then constrain **S** to be diagonalized by those eigenvectors in a convex problem to recover the unknown eigenvalues. While the approaches in [25, 26, 30] search over a lower-dimensional space, the formulation (9) avoids computing an eigendecomposition and, more importantly, solving a problem over complex-valued variables. This was not an issue in [25, 26, 30], since the focus therein was on symmetric shifts with real-valued spectrum.

The sparsity-inducing ℓ_0 pseudo-norm (or its convex ℓ_1-norm surrogate) in the objective of (9) can be replaced with a generic cost $f(\mathbf{S})$. Possible choices for such a cost include setting $f(\mathbf{S}) = \|\mathbf{S}\|_F$, which finds a GSO minimizing the total energy stored in the weights of the edges; or, $f(\mathbf{S}) = \|\mathbf{S}\|_\infty$, which yields GSOs for graphs with uniformly low edge weights [25]. The constraint $\mathbf{S} \in \mathcal{S}$ in (9) incorporates a priori knowledge about **S**. If we let $\mathbf{S} = \mathbf{A}$ represent the adjacency matrix of a digraph with non-negative weights and no self-loops, we can explicitly write the set of feasible shifts as $\mathcal{S} := \{\mathbf{S} \mid S_{ij} \geq 0, \ S_{ii} = 0, \ \sum_j S_{j1} = 1\}$. The first condition in $\mathcal{S}$ encodes the non-negativity of the weights whereas the second condition encodes the absence of self-loops, thus, each diagonal entry of **S** must be null. The last condition fixes the scale of the admissible graphs by setting the weighted in-degree of the first node to 1, and rules out the trivial solution $\mathbf{S} = \mathbf{0}$. Other GSOs can be accommodated in our framework with minor adaptations to $\mathcal{S}$; see [25].

Robust formulations. While (9) assumes perfect information on **H**, the formulation should be modified to account for imperfect estimates $\hat{\mathbf{H}}$ [e.g., obtained via (7)] and model mismatches. This entails relaxing the linear matrix equality constraint in (9), with some bounded measure of the residual error $\hat{\mathbf{H}}\mathbf{S} - \mathbf{S}\hat{\mathbf{H}}$. Naturally, the specific form of the error measure should be selected based on the source of imperfections. For the numerical tests in Section 5, we adopt a Frobenius-norm error measure and solve the convex ℓ_1-norm minimization problem

$$\hat{\mathbf{S}} := \underset{\mathbf{S}}{\operatorname{argmin}} \ \|\mathbf{S}\|_1, \quad \text{s. to } \mathbf{S} \in \mathcal{S}, \quad \|\hat{\mathbf{H}}\mathbf{S} - \mathbf{S}\hat{\mathbf{H}}\|_F \leq \epsilon, \quad (10)$$

which focuses on the similarities between the entries of $\hat{\mathbf{H}}\mathbf{S}$ and $\mathbf{S}\hat{\mathbf{H}}$. The bound ϵ can also be selected based on the priori knowledge we may have on the effectiveness of the prior filter identification step.

(a)　　　　　　　　　　　(b)　　　　　　　　　　　(c)
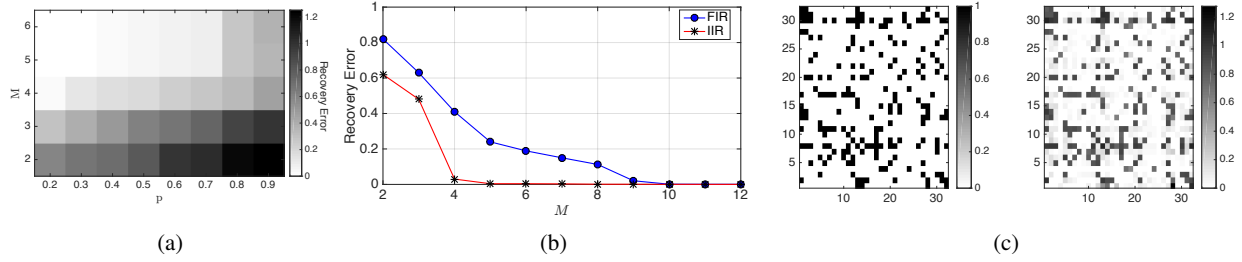
Fig. 1: (a) Recovery error as a function of the number of covariance pairs (M) and edge formation probabilities (p) in Erdős-Rényi digraphs. (b) Error in recovering a social network as a function of the number of covariance pairs (M) of signals generated according to FIR and IIR diffusion filters. (c) True adjacency matrix (left) and corresponding estimate (right) attained from $M = 5$ covariance pairs, where each output covariance is estimated from $P = 10^4$ signals.

Stationary observations. To have a better understanding of the proposed approach, it is instructive to compare our scenario with the one in [25], where the input is white and the shift is undirected. In the context of GSP, those two assumptions imply that the output $\mathbf{y}$ is graph stationary in $\mathbf{S}$ [4–6]. Regardless of the terminology, for that case it follows from (2) that $\mathbf{C_y} = \mathbb{E}[\mathbf{yy}^T] = \mathbf{H}\mathbb{E}[\mathbf{xx}^T]\mathbf{H}^T = \mathbf{HH}^T = \mathbf{H}^2$. Such identity reveals that the output covariance is itself a polynomial on the GSO. Hence, there is no need to estimate the filter $\mathbf{H}$ as in Section 3, since one can directly solve (9) using $\mathbf{C_y}$ (or $\hat{\mathbf{C}}_\mathbf{y}$) in lieu of $\mathbf{H}$ [25].

5. PRELIMINARY NUMERICAL TESTS

To gain insights on the behavior of the proposed network topology inference algorithm, here we evaluate the recovery performance on some synthetic and real-world digraphs. Throughout, we let $\mathbf{S} = \mathbf{A}$ be the adjacency matrix of the digraph under study. Moreover, we define the FIR and IIR graph filters $\mathbf{H}_1 = \sum_{l=0}^2 h_l \mathbf{S}^l$ and $\mathbf{H}_2 = (\mathbf{I} + \alpha\mathbf{S})^{-1}$, respectively, where the coefficients $\{h_l\}$ and α are drawn uniformly on $[0, 1]$. Finally, denoting by $\hat{\mathbf{S}}$ the GSO estimate, we characterize the recovery error as $\|\hat{\mathbf{S}} - \mathbf{S}\|_F/\|\mathbf{S}\|_F$.

Perfect knowledge of second-order statistics. Consider Erdős-Rényi random digraphs with $N = 20$ nodes, where edges are formed independently with probability p. We generate M random input-output covariance pairs $\{\mathbf{C}_{\mathbf{x},m}, \mathbf{C}_{\mathbf{y},m}\}_{m=1}^M$, where: i) the input covariances were generated as $\mathbf{C}_{\mathbf{x},m} = \mathbf{B}_m \mathbf{B}_m^T$, with the entries of $\mathbf{B}_m$ drawn independently from a standard normal distribution; and ii) the corresponding output covariances were computed as $\mathbf{C}_{\mathbf{y},m} = \mathbf{H}_1 \mathbf{C}_{\mathbf{x},m} \mathbf{H}_1^T$ [cf. (4)]. To recover the GSO, we first estimate the FIR filter $\mathbf{H}_1$ by solving (6) using the algorithm in [32]. We then use $\hat{\mathbf{H}}_1$ in (10) with $\epsilon = 10^{-3}$ to obtain $\hat{\mathbf{S}}$; the convex problem (10) is solved with CVX [35]. In Fig. 1(a) we plot the GSO recovery error as a function of M and p averaged over 10 realizations. First, notice that as M increases, the recovery error of the proposed method decreases monotonically, due to improved filter identification [cf. (6)]. Second, for smaller p and hence sparser digraphs, we can better recover the underlying network topology by solving the ℓ_1-norm minimization problem (10).

Imperfect covariance information. We consider the social network $\mathcal{G}$ of $N = 32$ students in a class at the University of Ljubljana[1], where directed edges between students represent perceived friendships. More precisely, students were asked with whom they would like to share seats in a bus so that an edge from node i to j exists if student i selected student j in the questionnaire. A signal $\mathbf{x}$ in this graph can be regarded as a unidimensional opinion of each stu-

dent regarding a specific topic and the filtering operators $\mathbf{H}_1$ and $\mathbf{H}_2$ represent different opinion dynamics in the network. Our goal is to recover $\mathbf{S}$ – hence, the social structure of the students – 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 $\mathbf{y}_m$ is generated by the diffusion through the network of an initial signal $\mathbf{x}_m$. More precisely, for each topic $m = 1, \ldots, M$, we model $\mathbf{x}_m$ as a zero-mean Gaussian random vector with known covariance $\mathbf{C}_{\mathbf{x},m}$ generated as in the previous experiment. We then observe a set $\{\mathbf{y}_m^{(p)}\}_{p=1}^P$ of opinion profiles generated from different sources $\{\mathbf{x}_m^{(p)}\}_{p=1}^P$ diffused either through $\mathbf{H}_1$ or $\mathbf{H}_2$. From these P opinion profiles we estimate $\hat{\mathbf{C}}_{\mathbf{y},m}$ as in (3), and identify the diffusion filter by solving (6). Lastly, we use the estimated $\hat{\mathbf{H}}_1$ or $\hat{\mathbf{H}}_2$ to solve (10) and obtain our GSO estimate $\hat{\mathbf{S}}$.

In Fig. 1(b) we plot the shift recovery error averaged over 10 realizations as a function of the number of covariance pairs M for two types of filters and for sufficiently large $P = 10^6$. As expected, the estimate $\hat{\mathbf{S}}$ becomes more reliable for larger M as argued following (7). Moreover, notice that performance when considering the IIR filter $\mathbf{H}_2$ is consistently better than for the FIR filter $\mathbf{H}_1$. Finally, we study the case of $M = 5$ processes filtered by $\mathbf{H}_1$ where the output covariances are estimated by observing $P = 10^4$ signals. Fig. 1-(c) depicts the heat maps of the ground-truth (left) and inferred (right) adjacency matrices. Although the procedure results in a modestly high recovery error (> 0.2), it still reveals the underlying support of $\mathbf{A}$ with reasonable accuracy.

6. CONCLUSIONS

We studied the problem of inferring the topology of a digraph from observations of signals diffusing on the network. Modeling the mapping between the (arbitrarily correlated) excitation inputs and the observed outputs as a polynomial graph filter, enabled a two-step topology inference approach whereby: i) we first use (statistical) information on the inputs and outputs to infer the said diffusion filter; and ii) we then combine the filter estimate along with prior structural information on the digraph to recover the network topology. For the first step, the focus was on the most pragmatic case where only second-order statistical information on the inputs were available. While such a problem can be naturally formulated as a non-convex fourth order optimization, we recast it as a smooth quadratic minimization subject to Stiefel manifold constraints. Modifications to handle linear observations and their effect on identifiability and recovery performance were briefly discussed as well. Regarding the second step, the focus was on finding the sparsest graph-shift (diffusing) operator compatible with the estimated filter, namely that both operators commute. The overall network topology inference pipeline was evaluated on synthetic and social networks.

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[1]http://vladowiki.fmf.uni-lj.si/doku.php?id=pajek:data:pajek:students

7. REFERENCES

[1] A. Sandryhaila and J.M.F. Moura, "Discrete signal processing on graphs," *IEEE Trans. Signal Process.*, vol. 61, no. 7, pp. 1644–1656, Apr. 2013.

[2] A. Gavili and X. P. Zhang, "On the shift operator, graph frequency, and optimal filtering in graph signal processing," *IEEE Trans. Signal Process.*, vol. 65, no. 23, pp. 6303–6318, Dec 2017.

[3] S. Segarra, A. G. Marques, and A. Ribeiro, "Optimal graph-filter design and applications to distributed linear network operators," *IEEE Trans. Signal Process.*, vol. 65, no. 15, pp. 4117–4131, Aug 2017.

[4] B. Girault, "Stationary graph signals using an isometric graph translation," in *European Signal Process. Conf. (EUSIPCO)*, Aug. 2015, pp. 1516–1520.

[5] A. G. Marques, S. Segarra, G. Leus, and A. Ribeiro, "Stationary graph processes and spectral estimation," *IEEE Trans. Signal Process.*, vol. 65, pp. 467 – 483, Nov. 2017.

[6] N. Perraudin and P. Vandergheynst, "Stationary signal processing on graphs," *IEEE Trans. Signal Process.*, vol. 65, no. 13, pp. 3462–3477, Jul. 2017.

[7] R. Shafipour, S. Segarra, A. G. Marques, and G. Mateos, "Identifying the topology of undirected networks from diffused non-stationary graph signals," *IEEE Trans. Signal Process.*, 2017, (submitted; see also arXiv:1801.03862 [eess.SP]).

[8] E. D. Kolaczyk, *Statistical Analysis of Network Data: Methods and Models*, Springer, New York, NY, 2009.

[9] O. Sporns, *Discovering the Human Connectome*, MIT Press, Boston, MA, 2012.

[10] A. P. Dempster, "Covariance selection," *Biometrics*, vol. 28, no. 1, pp. 157–175, 1972.

[11] J. Friedman, T. Hastie, and R. Tibshirani, "Sparse inverse covariance estimation with the graphical lasso," *Biostatistics*, vol. 9, no. 3, pp. 432–441, 2008.

[12] B. M. Lake and J. B. Tenenbaum, "Discovering structure by learning sparse graph," in *Annual Cognitive Sc. Conf.*, 2010, pp. 778 – 783.

[13] M. Slawski and M. Hein, "Estimation of positive definite M-matrices and structure learning for attractive gaussian markov random fields," *Linear Algebra and its Applications*, vol. 473, pp. 145–179, 2015.

[14] H. E. Egilmez, E. Pavez, and A. Ortega, "Graph learning from data under laplacian and structural constraints," *IEEE J. Sel. Topics Signal Process.*, vol. 11, no. 6, pp. 825–841, Sept. 2017.

[15] N. Meinshausen and P. Buhlmann, "High-dimensional graphs and variable selection with the lasso," *Ann. Stat.*, vol. 34, pp. 1436–1462, 2006.

[16] X. Cai, J. A. Bazerque, and G. B. Giannakis, "Sparse structural equation modeling for inference of gene regulatory networks exploiting genetic perturbations," *PLoS, Computational Biology*, June 2013.

[17] B. Baingana, G. Mateos, and G. B. Giannakis, "Proximal-gradient algorithms for tracking cascades over social networks," *IEEE J. Sel. Topics Signal Process.*, vol. 8, pp. 563–575, Aug. 2014.

[18] Y. Shen, B. Baingana, and G. B. Giannakis, "Tensor decompositions for identifying directed graph topologies and tracking dynamic networks," *IEEE Trans. Signal Process.*, vol. 65, no. 14, pp. 3675–3687, Jul. 2017.

[19] A. Brovelli, M. Ding, A. Ledberg, Y. Chen, R. Nakamura, and S. L. Bressler, "Beta oscillations in a large-scale sensorimotor cortical network: directional influences revealed by granger causality," *PNAS*, vol. 101, pp. 98499854, 2004.

[20] G. V. Karanikolas, G. B. Giannakis, K. Slavakis, and R. M. Leahy, "Multi-kernel based nonlinear models for connectivity identification of brain networks," in *IEEE Intl. Conf. Acoust., Speech and Signal Process. (ICASSP)*, Shanghai, China, Mar. 20-25, 2016.

[21] Y. Shen, B. Baingana, and G. B. Giannakis, "Kernel-based structural equation models for topology identification of directed networks," *IEEE Trans. Signal Process.*, vol. 65, no. 10, pp. 2503–2516, Feb. 2017.

[22] X. Dong, D. Thanou, P. Frossard, and P. Vandergheynst, "Learning Laplacian matrix in smooth graph signal representations," *IEEE Trans. Signal Process.*, vol. 64, no. 23, pp. 6160–6173, Dec 2016.

[23] J. Mei and J.M.F. Moura, "Signal processing on graphs: Estimating the structure of a graph," in *IEEE Intl. Conf. Acoust., Speech and Signal Process. (ICASSP)*, 2015, pp. 5495–5499.

[24] V. Kalofolias, "How to learn a graph from smooth signals," in *Intl. Conf. Artif. Intel. Stat. (AISTATS)*. J Mach. Learn. Res., 2016, pp. 920–929.

[25] S. Segarra, A.G. Marques, G. Mateos, and A. Ribeiro, "Network topology inference from spectral templates," *IEEE Trans. Signal Inf. Process. Netw.*, vol. 3, pp. 5911 – 5926, Sept. 2017.

[26] B. Pasdeloup, V. Gripon, G. Mercier, D. Pastor, and M. G. Rabbat, "Characterization and inference of graph diffusion processes from observations of stationary signals," *IEEE Trans. Signal Inf. Process. Netw.*, vol. PP, no. 99, pp. 1–1, 2017.

[27] D. Thanou, X. Dong, D. Kressner, and P. Frossard, "Learning heat diffusion graphs," *IEEE Trans. Signal Inf. Process. Netw.*, vol. 3, no. 3, pp. 484–499, Sept 2017.

[28] S. P. Chepuri, S. Liu, G. Leus, and A. O. Hero, "Learning sparse graphs under smoothness prior," in *IEEE Intl. Conf. Acoust., Speech and Signal Process. (ICASSP)*, New Orleans, LA, Mar. 5-9, 2017, pp. 6508–6512.

[29] M. G. Rabbat, "Inferring sparse graphs from smooth signals with theoretical guarantees," in *IEEE Intl. Conf. Acoust., Speech and Signal Process. (ICASSP)*, New Orleans, LA, Mar. 5-9, 2017, pp. 6533–6537.

[30] R. Shafipour, S. Segarra, A. G. Marques, and G. Mateos, "Network topology inference from non-stationary graph signals," in *IEEE Intl. Conf. Acoust., Speech and Signal Process. (ICASSP)*, New Orleans, LA, Mar. 5-9, 2017.

[31] E. Isufi, A. Loukas, A. Simonetto, and G. Leus, "Autoregressive moving average graph filtering," *IEEE Trans. Signal Process.*, vol. 65, no. 2, pp. 274–288, Jan. 2017.

[32] Z. Wen and W. Yin, "A feasible method for optimization with orthogonality constraints," *Mathematical Programming*, vol. 142, no. 1-2, pp. 397–434, 2013.

[33] N. Tremblay, P. Gonçalves, and P. Borgnat, "Design of graph filters and filterbanks," *arXiv preprint arXiv:1711.02046*, 2017.

[34] S. Segarra, Y. Wang, C. Uhler, and A. G. Marques, "Joint inference of networks from stationary graph signals," in *Asilomar Conf. on Signals, Systems, and Computers*, Pacific Grove, CA, Oct. 29 - Nov. 1,, 2017.

[35] M. Grant, S. Boyd, and Y. Ye, "CVX: Matlab software for disciplined convex programming," 2008.