

Stationary Graph Processes and Spectral Estimation

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Abstract—Stationarity is a cornerstone property that facilitates the analysis and processing of random signals in the time domain. Although time-varying signals are abundant in nature, in many practical scenarios the information of interest resides in more irregular graph domains. This lack of regularity hampers the generalization of the classical notion of stationarity to graph signals. The contribution in this paper is twofold. Firstly, we propose a definition of weak stationarity for random graph signals that takes into account the structure of the graph where the random process takes place, while inheriting many of the meaningful properties of the classical definition in the time domain. Our definition requires that stationary graph processes can be modeled as the output of a linear graph filter applied to a white input. We will show that this is equivalent to requiring the correlation matrix to be diagonalized by the graph Fourier transform. Secondly, we analyze the properties of the power spectral density and propose a number of methods to estimate it. We start with nonparametric approaches, including periodograms, window-based average periodograms, and filter banks. We then shift the focus to parametric approaches, discussing the estimation of moving-average (MA), autoregressive (AR) and ARMA processes. Finally, we illustrate the power spectral density estimation in synthetic and real-world graphs.

Index Terms—Graph signal processing, Weak stationarity, Random graph process, Periodogram, Windowing, Power spectral density, Parametric estimation.

I. INTRODUCTION

Networks and graphs, which can be used to represent pairwise relationships between elements of a set, have often intrinsic value and are themselves the object of study. In other occasions, they define underlying notions of proximity or dependence, but the interest is in signals associated with the nodes of the graph. This is the matter addressed in the field of graph signal processing (GSP), where notions such as frequency and linear filtering are extended to signals supported on graphs [2], [3]. A plethora of graph signals exist in different fields, including gene-expression patterns defined on top of gene networks, the spread of epidemics over a social network, and the congestion level at the nodes of a communication network, to name a few. Transversal to the particular application, the question that arises is how to redesign tools originally conceived to study and process signals on regular domains to be used in the more complex graph domain.

This paper investigates the problem of generalizing the notion of stationary processes [4], [5] to the graph domain [6], [7]. We begin by proposing different equivalent definitions of weak stationarity for graph signals, all taking into account the structure of the graph where the random process takes place, while inheriting many of the meaningful properties of the classical definition for time-varying random processes. A straightforward generalization is not trivial because the shift (translation) operation in the graph domain is more involved, it changes the energy of the shifted signal (unless normalized [6]), and its effect in the frequency

domain is more difficult to analyze. With these considerations in mind, a random process in a graph is said to be stationary if either its correlation is invariant with respect to a constant number of applications of the graph shift operator or, alternatively, if it can be modeled as the output of a linear graph filter [2], [8]–[10] applied to a white input. This is shown to be equivalent to requiring the correlation matrix of the process and the graph-shift operator to be normal and simultaneously diagonalizable. Under these definitions, notions like the power spectral density (PSD) or results such as the spectral convolution theorem can be generalized to signals supported on graphs. After showing that stationary processes are easier to understand in the frequency domain, we propose and analyze different methods to estimate the PSD, which, if needed, can also be used to improve the estimate of the correlation matrix itself. We begin by looking at simple nonparametric methods for PSD estimation. We first extend the periodogram and the correlogram to the graph domain, and analyze their estimation performance. We then generalize more advanced estimators such as window-based average periodograms and filter banks [5, Chs. 2 and 5]. Differences relative to their time-domain counterparts are highlighted and open research problems are identified. After this, we shift the attention to parametric estimation. The focus is on estimating the PSD of autoregressive (AR), moving-average (MA) and ARMA graph processes, which are likely to arise in distributed setups driven by linear dynamics [11]–[13]. As in time, it turns out that the estimation of the ARMA parameters is a non-convex problem, although for certain particular cases –including that of positive semidefinite shifts– the optimization is tractable. Along with the proposed schemes, comparisons with traditional time-domain designs are provided.

Preliminary results generalizing the definition of stationarity to graph signals for Laplacian shifts were reported in [6] and [7]. Our contribution here is to draw a parallel between the fundamental properties of stationary stochastic processes in time and stationary processes in graphs. Specifically, we introduce the notions of shift-invariant correlations, responses of linear shift invariant systems to white inputs, and the existence of a PSD for graph processes as extensions of their analogous definitions for time signals. We show that while each of these extensions could lead to a different notion of stationarity in graphs, they all turn out equivalent. We also consider general normal shifts, identify properties hitherto unreported, establish connections with application settings such as diffusion dynamics, and formulate and evaluate different parametric and nonparametric approaches for PSD estimation.

Paper outline: Section II introduces the concepts of graph signals and filters. Section III presents the definition of weak stationarity and discusses some of its properties. Different nonparametric methods to estimate the PSD of a random graph process are presented in Section IV. Section V addresses the parametric estimation for AR, MA, and ARMA graph processes. Simulations and conclusions in Sections VI and VII wrap-up the paper.

Notation: Entries of a vector \mathbf{x} are written as x_i and entries of a matrix \mathbf{X} as X_{ij} . If needed for clarity we may alternatively write $[\mathbf{x}]_i$ and $[\mathbf{X}]_{ij}$. We use \mathbf{X}^* , \mathbf{X}^T , and \mathbf{X}^H to denote conjugate,

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transpose, and transpose conjugate, respectively. For a square matrix \mathbf{X} , we use $\text{tr}[\mathbf{X}]$ for its trace and $\text{diag}(\mathbf{X})$ for an operator returning a vector with the diagonal elements of \mathbf{X} . For a vector \mathbf{x} , we let $\text{diag}(\mathbf{x})$ denote a diagonal matrix with diagonal elements $\text{diag}[\text{diag}(\mathbf{x})] = \mathbf{x}$. The notation $\mathbf{x} \circ \mathbf{y}$ denotes the elementwise product of \mathbf{x} and \mathbf{y} . We use $\mathbf{0}$ and $\mathbf{1}$ for the all-zero and all-one vectors and \mathbf{e}_i for the i th element of the canonical basis of \mathbb{R}^N .

II. GRAPH SIGNALS AND FILTERS

Let $\mathcal{G} = (\mathcal{N}, \mathcal{E})$ be a directed graph or network with a set of N nodes \mathcal{N} and directed edges \mathcal{E} such that $(i, j) \in \mathcal{E}$ implies that node i is connected to node j . We associate with \mathcal{G} the graph shift operator \mathbf{S} , defined as an $N \times N$ matrix whose entry $S_{ji} \neq 0$ only if $i = j$ or if $(i, j) \in \mathcal{E}$ [3], [8]. The sparsity pattern of the matrix \mathbf{S} captures the local structure of \mathcal{G} , but we make no specific assumptions on the values of the nonzero entries of \mathbf{S} . Frequent choices for \mathbf{S} are the adjacency matrix of the graph [3], [8], its Laplacian [2], and their respective generalizations [14]. The intuition behind \mathbf{S} is to represent a linear transformation that can be computed locally at the nodes of the graph. More rigorously, if the set $\mathcal{N}_l(i)$ stands for the nodes within the l -hop neighborhood of node i and the signal \mathbf{y} is defined as $\mathbf{y} = \mathbf{S}\mathbf{x}$, then node i can compute y_i provided that it has access to the value of x_j at $j \in \mathcal{N}_l(i)$. We assume henceforth that \mathbf{S} is *normal*, so that there exists an $N \times N$ unitary matrix \mathbf{V} and an $N \times N$ diagonal matrix $\mathbf{\Lambda}$ that can be used to decompose \mathbf{S} as $\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^H$.

The focus of this paper is not on \mathcal{G} , but on graph signals defined on the set of nodes \mathcal{N} . Formally, each of these signals can be represented as a vector $\mathbf{x} = [x_1, \dots, x_N]^T \in \mathbb{R}^N$ where the i -th element represents the value of the signal at node i or, alternatively, as a function $f: \mathcal{N} \rightarrow \mathbb{R}$, defined on the vertices of the graph. Given a graph signal \mathbf{x} , we refer to $\tilde{\mathbf{x}} := \mathbf{V}^H \mathbf{x}$ as the frequency representation of \mathbf{x} , with \mathbf{V}^H being the graph Fourier transform (GFT) [8].

We further introduce the notion of a graph filter $\mathbf{H}: \mathbb{R}^N \rightarrow \mathbb{R}^N$ which is defined as a linear graph signal operator of the form

$$\mathbf{H} := \sum_{l=0}^{L-1} h_l \mathbf{S}^l, \quad (1)$$

where $\mathbf{h} = [h_0, \dots, h_{L-1}]^T$ is a vector of $L \leq N$ scalar coefficients. According to (1) graph filters are polynomials of degree $L - 1$ in the graph-shift operator \mathbf{S} [3], which due to the local structure of the shift can be implemented locally too [9], [10]. It is easy to see that graph filters are invariant to applications of the shift in the sense that if $\mathbf{y} = \mathbf{H}\mathbf{x}$, it must hold that $\mathbf{S}\mathbf{y} = \mathbf{H}(\mathbf{S}\mathbf{x})$. Using the factorization $\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^H$ the filter in (1) can be rewritten as $\mathbf{H} = \mathbf{V}(\sum_{l=0}^{L-1} h_l \mathbf{\Lambda}^l) \mathbf{V}^H$. The diagonal matrix $\sum_{l=0}^{L-1} h_l \mathbf{\Lambda}^l$ is termed the frequency response of the filter and extracted in the vector $\tilde{\mathbf{h}} := \text{diag}(\sum_{l=0}^{L-1} h_l \mathbf{\Lambda}^l)$.

To relate the frequency response $\tilde{\mathbf{h}}$ with the filter coefficients \mathbf{h} let $\lambda_k = [\mathbf{\Lambda}]_{kk}$ be the k th eigenvalue of \mathbf{S} and define the $N \times N$ Vandermonde matrix $\mathbf{\Psi}$ with entries $\Psi_{kl} = \lambda_k^{l-1}$. Further define $\mathbf{\Psi}_L$ as a tall matrix containing the first L columns of $\mathbf{\Psi}$ to write $\tilde{\mathbf{h}} = \mathbf{\Psi}_L \mathbf{h}$ and conclude that the filter in (1) can be alternatively written as

$$\mathbf{H} = \sum_{l=0}^{L-1} h_l \mathbf{S}^l = \mathbf{V} \text{diag}(\tilde{\mathbf{h}}) \mathbf{V}^H = \mathbf{V} \text{diag}(\mathbf{\Psi}_L \mathbf{h}) \mathbf{V}^H. \quad (2)$$

Equation (2) implies that if \mathbf{y} is defined as $\mathbf{y} = \mathbf{H}\mathbf{x}$, its frequency representation $\tilde{\mathbf{y}} = \mathbf{V}^H \mathbf{y}$ satisfies

$$\tilde{\mathbf{y}} = \text{diag}(\mathbf{\Psi}_L \mathbf{h}) \mathbf{V}^H \mathbf{x} = \text{diag}(\tilde{\mathbf{h}}) \tilde{\mathbf{x}} = \tilde{\mathbf{h}} \circ \tilde{\mathbf{x}}, \quad (3)$$

which demonstrates that the output at a given frequency depends only on the value of the input and the filter response at that given frequency. Observe that when $L = N$ we have $\mathbf{\Psi}_N = \mathbf{\Psi}$ and that, if we are given a filter with order greater than $N - 1$, we can rewrite it as a different filter of order not larger than $N - 1$ due to the Cayley-Hamilton theorem.

III. WEAKLY STATIONARY RANDOM GRAPH PROCESSES

A stochastic process is said weakly stationary in finite discrete time if its correlation matrix is invariant to circular time shifts. Moreover, two important properties of time stationary processes are: (i) They can always be represented as the response of a linear time invariant filter to a white input. (ii) The correlation matrix can be represented with a power spectral density. Each of these three facts, can be used as a starting point to define graph stationary processes.

Commence then by considering the time invariance of correlation matrices. In the language of GSP, time invariance means that the correlation of a stationary signal \mathbf{x} and its shifted version $\mathbf{S}^l \mathbf{x}$ are the same. Save for a technical modification we adopt this as a definition that we formally state next.

Definition 1 Given a normal shift operator \mathbf{S} , a zero-mean random process \mathbf{x} is said to be weakly stationary with respect to \mathbf{S} if for any set of nonnegative integers a, b , and $c \leq b$ it holds

$$\mathbb{E}[(\mathbf{S}^a \mathbf{x})((\mathbf{S}^b \mathbf{x})^H)] = \mathbb{E}[(\mathbf{S}^{a+c} \mathbf{x})((\mathbf{S}^{b-c} \mathbf{x})^H)]. \quad (4)$$

In Definition 1 the constants a and b act as a reference and c as a shift that is applied backward and forward. The signal is said stationary if the application of these shifts does not alter the covariance matrix. In the particular case in which \mathbf{S} is a cyclic shift, the Hermitian $\mathbf{S}^H = \mathbf{S}^{-1}$ is a shift in the opposite direction. Then, if we set $a = 0$, $b = N$ and $c = l$ we recover $\mathbb{E}[\mathbf{x}\mathbf{x}^H] = \mathbb{E}[\mathbf{S}^l \mathbf{x}(\mathbf{S}^l \mathbf{x})^H]$, which is the definition of a stationary signal in time. The use of a reference shift in Definition 1 is necessary because the eigenvalues of the shift operator \mathbf{S} do not have unit magnitude and can change the energy of the signal; see [6] for an alternative approach and Remark 2 for further details.

A second definition follows from the representation of a stationary process as the response of a linear time-invariant filter to white noise. To define a stationary process in a graph it would suffice to consider processes that are outputs of linear shift-invariant filters. Formally, define a standard zero-mean white random process \mathbf{w} as one with mean $\mathbb{E}[\mathbf{w}] = \mathbf{0}$ and covariance $\mathbb{E}[\mathbf{w}\mathbf{w}^H] = \mathbf{I}$. We can then alternatively define a stationary graph process as follows:

Definition 2 Given a normal shift operator \mathbf{S} , a zero-mean random process \mathbf{x} is said to be weakly stationary with respect to \mathbf{S} if it can be written as the response of a linear shift-invariant filter $\mathbf{H} = \sum_{l=0}^{N-1} h_l \mathbf{S}^l$ to a zero-mean white input \mathbf{w} .

Definition 2 states that the process \mathbf{x} is stationary if we can write $\mathbf{x} = \mathbf{H}\mathbf{w}$ for some filter $\mathbf{H} = \sum_{l=0}^{N-1} h_l \mathbf{S}^l$ that we excite with a white input \mathbf{w} . Further observe that if we write $\mathbf{x} = \mathbf{H}\mathbf{w}$, the covariance matrix $\mathbf{C}_x := \mathbb{E}[\mathbf{x}\mathbf{x}^H]$ of the signal \mathbf{x} can be written as

$$\mathbf{C}_x = \mathbb{E}[(\mathbf{H}\mathbf{w})(\mathbf{H}\mathbf{w})^H] = \mathbf{H}\mathbb{E}[\mathbf{w}\mathbf{w}^H]\mathbf{H} = \mathbf{H}\mathbf{H}^H. \quad (5)$$

The statement in (5) implies that the color of the process is determined by the filter \mathbf{H} and that the rank of the covariance matrix is the rank of \mathbf{H} .

As a third alternative definition, we leverage the observation that in the case of time signals \mathbf{C}_x is characterizable with a

PSD. This latter property is a consequence of the fact that the correlation matrix \mathbf{C}_x of a stationary process is circulant and therefore diagonalized by the Fourier matrix. In the case of a graph signal the analogy is to have a covariance matrix \mathbf{C}_x that can be diagonalized by the GFT matrix \mathbf{V} as we formally state next.

Definition 3 Given a normal shift operator \mathbf{S} , a zero-mean random process \mathbf{x} is said to be weakly stationary with respect to \mathbf{S} if the matrices \mathbf{C}_x and \mathbf{S} are simultaneously diagonalizable.

We remark that the different definitions of stationarity that we state in Definitions 1, 2, and 3 are with respect to a graph-shift operator \mathbf{S} , which is required to be normal. We also emphasize that Definitions 1, 2, and 3 are equivalent for time signals by construction. As we shall see next, despite appearing possibly different, they are also equivalent for graph signals in most graphs.

Proposition 1 If the eigenvalues of \mathbf{S} are all distinct, Definitions 1, 2, and 3 are equivalent.

Proof: If Definition 1 holds, reorder terms in (4) to conclude that

$$\mathbf{S}^a \mathbf{C}_x \mathbf{S}^b = \mathbf{S}^{a+c} \mathbf{C}_x \mathbf{S}^{b-c}. \quad (6)$$

For (6) to be true, \mathbf{S}^c and \mathbf{C}_x must commute for all c . In turn, this can happen if and only if \mathbf{S} and \mathbf{C}_x are simultaneously diagonalizable [15], which implies Definition 3. Conversely, if Definition 3 holds we can write $\mathbf{C}_x = \mathbf{V} \text{diag}(\boldsymbol{\lambda}_c) \mathbf{V}^H$. Substituting this expression into (6) the equality checks and Definition 1 follows.

After proving that Definitions 1 and 3 are equivalent, we show that under the conditions in the proposition, Definition 2 is equivalent to 3. Assume first that Definition 2 holds. Since the graph filter \mathbf{H} in (5) is linear shift invariant, it is completely characterized by its frequency response $\tilde{\mathbf{h}} = \boldsymbol{\Psi} \mathbf{h}$ as stated in (2). Using this characterization we rewrite (5) as

$$\mathbf{C}_x = (\mathbf{V} \text{diag}(\tilde{\mathbf{h}}) \mathbf{V}^H) (\mathbf{V} \text{diag}(\tilde{\mathbf{h}}) \mathbf{V}^H)^H = \mathbf{V} \text{diag}^2(|\tilde{\mathbf{h}}|) \mathbf{V}^H. \quad (7)$$

This means that Definition 3 holds. Conversely, if Definition 3 holds it means that we can write $\mathbf{C}_x = \mathbf{V} \text{diag}(\boldsymbol{\lambda}_c) \mathbf{V}^H$ for some component-wise *nonnegative* vector $\boldsymbol{\lambda}_c$. Define now vector $\sqrt{\boldsymbol{\lambda}_c}$ where the square root is applied element-wise. Then, for Definition 2 to hold, there must exist a filter with coefficients \mathbf{h} satisfying $\tilde{\mathbf{h}} = \boldsymbol{\Psi} \mathbf{h} = \sqrt{\boldsymbol{\lambda}_c}$. Since $\boldsymbol{\Psi}$ is Vandermonde, the system is guaranteed to have a solution with respect to \mathbf{h} provided that all modes of $\boldsymbol{\Psi}$ (the eigenvalues of \mathbf{S}) are distinct, as required in the proposition. ■

As seen from the proof of Proposition 1, Definitions 1 and 3 are equivalent, while Definition 2 implies Definitions 1 and 3. The shift \mathbf{S} having distinct eigenvalues is required for Definitions 1 and 3 to imply Definition 2. Note that if for the shift \mathbf{S} one has that $\lambda_k = \lambda_{k'}$, then the frequency response of a graph filter satisfies $\tilde{h}_k = \tilde{h}_{k'}$, which implies that the generated covariance, besides being simultaneously diagonalizable, must have repeated eigenvalues too.

The fact of \mathbf{C}_x being diagonalized by the GFT matrix motivates the following definition.

Definition 4 The power spectral density (PSD) of a random process \mathbf{x} that is stationary with respect to the normal graph shift $\mathbf{S} = \mathbf{V} \boldsymbol{\Lambda} \mathbf{V}^H$ is the nonnegative $N \times 1$ vector \mathbf{p}

$$\mathbf{p} := \text{diag}(\mathbf{V}^H \mathbf{C}_x \mathbf{V}). \quad (8)$$

Since \mathbf{C}_x is diagonalized by \mathbf{V} [cf. (3)] the matrix $\mathbf{V}^H \mathbf{C}_x \mathbf{V}$ is diagonal and it follows that the PSD in (8) corresponds to the

eigenvalues of the positive semidefinite correlation matrix \mathbf{C}_x . Thus, (8) is equivalent to

$$\mathbf{C}_x = \mathbf{V} \text{diag}(\mathbf{p}) \mathbf{V}^H. \quad (9)$$

Further note that if we interpret \mathbf{x} as the output of a graph filter applied to a white input with unitary variance [cf. (3)], it follows from comparing (7) and (8) that the PSD is given by the squared magnitude of the filter's frequency response, i.e., $\mathbf{p} = |\tilde{\mathbf{h}}|^2$. This latter observation is consistent with the interpretation that the color of a process is determined by the frequency response $\tilde{\mathbf{h}}$ of the filter \mathbf{H} . We give representative examples below and move on to study properties of the PSD \mathbf{p} and the correlation \mathbf{C}_x .

Example 1 (White noise) Zero-mean white noise is stationary in any graph shift \mathbf{S} . The PSD of white noise with covariance $\mathbb{E}[\mathbf{w} \mathbf{w}^H] = \sigma^2 \mathbf{I}$ is $\mathbf{p} = \sigma^2 \mathbf{1}$.

Example 2 (Covariance matrix graph) Any random process is stationary with respect to the graph shift $\mathbf{S} = \mathbf{C}_x^a$ defined as the a -th power of the covariance matrix, with $a < 0$ only if the inverse exists. The PSD in this case is $\mathbf{p} = \text{diag}(\boldsymbol{\Lambda})^{1/a}$. Two examples of particular interest are setting $\mathbf{S} = \mathbf{C}_x$ (the covariance matrix graph) and $\mathbf{S} = \mathbf{C}_x^{-1}$ (the precision matrix graph).

Example 3 (Heat diffusion process) Suppose that a zero-mean white input \mathbf{w} diffuses through a graph with Laplacian $\mathbf{L} = \mathbf{V} \boldsymbol{\Lambda} \mathbf{V}^H$ to generate the signal $\mathbf{x} = \alpha_0 \sum_{l=0}^{\infty} (\alpha \mathbf{L})^l \mathbf{w} = \alpha_0 (\mathbf{I} - \alpha \mathbf{L})^{-1} \mathbf{w}$. The process \mathbf{x} is stationary in the shift $\mathbf{S} = \mathbf{L}$ with PSD $\mathbf{p} = \text{diag}[\alpha_0^2 (\mathbf{I} - \alpha \boldsymbol{\Lambda})^{-2}]$ because we can write the covariance matrix as $\mathbf{C}_x = \alpha_0^2 (\mathbf{I} - \alpha \mathbf{L})^{-2} = \mathbf{V} \alpha_0^2 (\mathbf{I} - \alpha \boldsymbol{\Lambda})^{-2} \mathbf{V}^H$ [cf. (9)]. This is a particular case of a more general category that we discuss in Sections III-B and V-B.

A. Properties of Graph Stationary Processes

We start by analyzing the effect of a linear graph filter on the covariance matrix and the PSD of a stationary graph random process.

Property 1 Let \mathbf{x} be a stationary process in \mathbf{S} with covariance matrix \mathbf{C}_x and PSD \mathbf{p}_x . Consider a filter \mathbf{H} with coefficients \mathbf{h} and frequency response $\tilde{\mathbf{h}}$ and define $\mathbf{y} := \mathbf{H} \mathbf{x}$ as the response of \mathbf{H} to input \mathbf{x} . Then, the process \mathbf{y} :

- (a) Is stationary in \mathbf{S} with covariance $\mathbf{C}_y = \mathbf{H} \mathbf{C}_x \mathbf{H}^H$.
- (b) Has a PSD given by $\mathbf{p}_y = |\tilde{\mathbf{h}}|^2 \circ \mathbf{p}_x$.

Proof: Use the definition $\mathbf{y} := \mathbf{H} \mathbf{x}$ to compute the covariance

$$\mathbf{C}_y = \mathbb{E}[\mathbf{y} \mathbf{y}^H] = \mathbf{H} \mathbb{E}[\mathbf{x} \mathbf{x}^H] \mathbf{H}^H = \mathbf{H} \mathbf{C}_x \mathbf{H}^H. \quad (10)$$

Since the process \mathbf{x} is stationary with PSD \mathbf{p}_x we use (9) to write $\mathbf{C}_x = \mathbf{V} \text{diag}(\mathbf{p}_x) \mathbf{V}^H$. We attempt to diagonalize \mathbf{C}_y with \mathbf{V} and use this expression along with the expression in (10) to write

$$\mathbf{V}^H \mathbf{C}_y \mathbf{V} = \mathbf{V}^H \mathbf{H} (\mathbf{V} \text{diag}(\mathbf{p}_x) \mathbf{V}^H) \mathbf{H}^H \mathbf{V}^H. \quad (11)$$

Regrouping factors in (11) and observing that the filter's graph frequency response is $\tilde{\mathbf{h}} = \text{diag}(\mathbf{V}^H \mathbf{H} \mathbf{V})$ we can reduce (11) to

$$\mathbf{V}^H \mathbf{C}_y \mathbf{V} = \text{diag}(\tilde{\mathbf{h}}) \text{diag}(\mathbf{p}_x) \text{diag}(\tilde{\mathbf{h}})^H. \quad (12)$$

Since matrices in the right hand side of (12) are diagonal, \mathbf{C}_y is diagonalized by \mathbf{V} . This means \mathbf{y} is stationary in \mathbf{S} with \mathbf{C}_y as in (10) and (a) follows. Since diagonal matrices commute in (12), (b) follows from the PSD definition in (8). ■

Property 1 is a statement of the spectral convolution theorem for stationary graph signals. When filtering stationary graph processes, the PSD of the output can be found as the product of the PSD of the input with the squared magnitude of the frequency response of the filter. Property 1 is also a generalization of Definition 2 for inputs that are not necessarily white.

In time signals the correlation matrix often conveys a notion of locality as the significant values of \mathbf{C}_x accumulate close to the diagonal. To prove a similar result for graph signals, recall that $\mathcal{N}_l(i)$ denotes the l -hop neighborhood of a node i . Formally, this set can be written as $\mathcal{N}_l(i) := \{j : [\mathbf{S}^l]_{ij} \neq 0 \text{ for some } l' \leq l\}$. The following proposition shows that the correlation between l -hop neighbors depends on the order L of the filter that generates \mathbf{x} from white noise.

Property 2 Let $\mathbf{x} = \mathbf{H}\mathbf{w}$ be a process written as the response of a linear graph filter $\mathbf{H} = \sum_{l=0}^{L-1} h_l \mathbf{S}^l$ of degree $L-1$ to a white input. Then, $[\mathbf{C}_x]_{ij} = 0$ for all $j \notin \mathcal{N}_{2(L-1)}(i)$.

Proof : Using (5) the covariance of \mathbf{x} is $\mathbf{C}_x = \mathbf{H}\mathbf{H}^H = (\sum_{l=0}^{L-1} h_l \mathbf{S}^l)(\sum_{l=0}^{L-1} h_l (\mathbf{S}^H)^l)$. Hence, \mathbf{C}_x is a polynomial of \mathbf{S} and \mathbf{S}^H , with the highest degree monomial being $(\mathbf{S}\mathbf{S}^H)^{L-1}$. All of these monomials have zero (i, j) entries if $j \notin \mathcal{N}_{2(L-1)}(i)$. ■

Property 2 puts a limit on the spatial extent of the components x_j of a graph signal that can be correlated with a given element x_i . Only those elements that are in the $2(L-1)$ -hop neighborhood – i.e., elements x_j with indices $j \in \mathcal{N}_{2(L-1)}(i)$ – can be correlated with x_i . This spatial limitation of correlations can be used to design windows for spectral estimation as we explain in Section IV-B.

We close by considering the covariance matrix associated with the GFT of a graph stationary process.

Property 3 Given a process \mathbf{x} that is stationary in $\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^H$ with PSD \mathbf{p} , define the GFT process as $\tilde{\mathbf{x}} = \mathbf{V}^H \mathbf{x}$. The covariance matrix of $\tilde{\mathbf{x}}$ is

$$\mathbf{C}_{\tilde{\mathbf{x}}} := \mathbb{E}[\tilde{\mathbf{x}}\tilde{\mathbf{x}}^H] := \mathbb{E}[(\mathbf{V}^H \mathbf{x})(\mathbf{V}^H \mathbf{x})^H] = \text{diag}(\mathbf{p}). \quad (13)$$

Proof : The proof is by direct computation. Indeed, using definitions we have $\mathbf{C}_{\tilde{\mathbf{x}}} := \mathbb{E}[\tilde{\mathbf{x}}\tilde{\mathbf{x}}^H] = \mathbb{E}[\mathbf{V}^H \mathbf{x} \mathbf{x}^H \mathbf{V}] = \mathbf{V}^H \mathbb{E}[\mathbf{x} \mathbf{x}^H] \mathbf{V} = \mathbf{V}^H \mathbf{C}_x \mathbf{V}$. To conclude, just observe that $\mathbf{V}^H \mathbf{C}_x \mathbf{V}$ is diagonal for a stationary process \mathbf{x} (cf. Definition 3) and that $\mathbf{p} = \text{diag}(\mathbf{V}^H \mathbf{C}_x \mathbf{V})$ as per Definition 4. ■

An important consequence of Property 3 is that the elements of $\tilde{\mathbf{x}}$ are uncorrelated. This provides motivation for the analysis and modeling of stationary graph processes in the frequency domain which we undertake in ensuing sections. It also shows that if a process \mathbf{x} is stationary in the shift $\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^H$, then the GFT \mathbf{V}^H provides the Karhunen-Loève expansion of the process. This is as it should be because \mathbf{C}_x is diagonalized by \mathbf{V} .

Remark 1 Definitions 1, 2, and 3 assumed that the random process \mathbf{x} has mean $\bar{\mathbf{x}} := \mathbb{E}[\mathbf{x}] = \mathbf{0}$. In time processes, stationarity implies that the mean must be constant. This restriction can be incorporated into our definitions by requiring $\bar{\mathbf{x}} = \bar{x}\mathbf{1}$ for some scalar \bar{x} . This is possible but it is not difficult to see that for a generic \mathbf{S} this restriction invalidates (the desirable) Property 1. Alternatively, we can require $\bar{\mathbf{x}} = \bar{x}\mathbf{v}_k$ where \mathbf{v}_k is an arbitrary eigenvector of \mathbf{S} . This choice maintains validity of Property 1. If \mathbf{S} is either the adjacency matrix of the directed cycle or the Laplacian of any graph and we set $\mathbf{v}_k = \mathbf{1}$, the choices coincide. The selection of $\mathbf{v}_k = \mathbf{1}$ is further justified because $\mathbf{1}$ is the

Laplacian eigenvector associated with smallest total variation [16] and therefore a natural choice for the notion of DC component.

Remark 2 Definitions 2 and 3 are straightforward extensions of time properties but Definition 1 makes use of reference shifts \mathbf{S}^a and \mathbf{S}^b from which we move forward and backward with the shift \mathbf{S}^c . This is a more contrived definition of the more natural requirement of making $\mathbb{E}[\mathbf{S}^l \mathbf{x} (\mathbf{S}^l \mathbf{x})^H]$ equal to $\mathbb{E}[\mathbf{x} \mathbf{x}^H]$. To understand the justification of this choice write $\mathbf{S}^l = \mathbf{V}\mathbf{\Lambda}^l \mathbf{V}^H$ and utilize the PSD definition in (8) to write the covariance of the shifted signal $\mathbf{S}^l \mathbf{x}$ as

$$\mathbb{E}[\mathbf{S}^l \mathbf{x} (\mathbf{S}^l \mathbf{x})^H] = \mathbf{V}\mathbf{\Lambda}^l \text{diag}(\mathbf{p})(\mathbf{\Lambda}^l)^H \mathbf{V}^H. \quad (14)$$

The expression in (14) implies that the shifted signal $\mathbf{S}^l \mathbf{x}$ is also stationary. However, when the eigenvalues of the shift operator are different from the identity, the PSD of $\mathbf{S}^l \mathbf{x}$ is scaled by the eigenvalue norms $|\mathbf{\Lambda}|^{2l}$. This issue is circumvented in [6], which defines stationarity based on the novel translation operator introduced in [17]. However, such an operator is not local and thus hard to implement in a distributed fashion. The use of reference shifts in Definition 1 avoids the need of defining this new operator.

B. Stationarity in Network Diffusion Processes

Many graph processes are characterized by local interactions between nodes of a (sparse) graph that can be approximated as linear [12], [13]. This implies that we can track the evolution of the signal at the i th node through a local recursion of the form $x_i^{(l+1)} = x_i^{(l)} - \gamma^{(l)} \sum_j s_{ij} x_j^{(l)}$ where the system is seeded with an initial condition $x_i^{(0)}$, s_{ij} are elements of the graph shift operator, and $\gamma^{(l)}$ are time varying diffusion coefficients. The diffusion halts after L iterations – which can be possibly infinite – to produce the output $y_i = x_i^{(L)}$. Diffusion dynamics appear in, e.g., network control systems [18], opinion formation [12], brain networks [19], and molecular communications [20].

Utilizing the graph shift operator, diffusion dynamics can be written as $\mathbf{x}^{(l+1)} = (\mathbf{I} - \gamma^{(l)} \mathbf{S}) \mathbf{x}^{(l)}$ and the output $\mathbf{y} = \mathbf{x}^{(L)}$ can be written in terms of the input as

$$\mathbf{y} = \mathbf{x}^{(L)} = \prod_{l=0}^{L-1} (\mathbf{I} - \gamma^{(l)} \mathbf{S}^l) \mathbf{x}. \quad (15)$$

Regardless of whether L is finite or infinite, the Cayley-Hamilton theorem guarantees that the mapping can always be expressed as a polynomial of \mathbf{S} with degree less than N . Hence, we can construe \mathbf{y} as the output of a graph filter $\mathbf{H} = \sum_{l=0}^{N-1} h_l \mathbf{S}^l$ applied to the initial condition \mathbf{x} . If we now think of \mathbf{x} as a process that is stationary in \mathbf{S} it follows that the process \mathbf{y} – which filters realizations of \mathbf{x} according to (15) – is also stationary. This is a corollary to Property 3 that we state below for future reference.

Corollary 1 A process \mathbf{y} is obtained by the linear diffusion dynamics in (15) in response to an input process \mathbf{x} . If \mathbf{x} is stationary in \mathbf{S} , so is \mathbf{y} .

Proof: Property 1 applies because $\prod_{l=0}^{L-1} (\mathbf{I} - \gamma^{(l)} \mathbf{S}^l)$ is a linear shift-invariant filter. ■

The corollary includes white seeds \mathbf{x} as a particular input model and the heat diffusion dynamics in Example 3 as a particular case with $\gamma^{(l)} = \gamma$ for all l and $L = \infty$.

IV. NONPARAMETRIC PSD ESTIMATION

The interest in this and the following section is in estimating the PSD of a random process \mathbf{x} that is stationary with respect to \mathbf{S} using as input either one or a few realizations $\{\mathbf{x}_r\}_{r=1}^R$ of \mathbf{x} . In this section we consider nonparametric methods that do not assume a particular model for \mathbf{x} . We generalize to graph signals the periodogram, correlogram, windowing, and filter bank techniques that are used for PSD estimation in the time domain. Parametric methods are analyzed in Section V.

A. Periodogram and Correlogram

Since Property 3 implies that $\mathbf{C}_{\tilde{\mathbf{x}}}$ is diagonal, we can rewrite (13) to conclude that the PSD can be written as $\mathbf{p} = \mathbb{E} [|\mathbf{V}^H \mathbf{x}|^2]$. This yields a natural approach to estimate \mathbf{p} with the GFT of realizations of \mathbf{x} . Thus, compute the GFTs $\tilde{\mathbf{x}}_r = \mathbf{V}^H \mathbf{x}_r$ of each of the samples \mathbf{x}_r in the training set and estimate \mathbf{p} as

$$\hat{\mathbf{p}}_{\text{pg}} := \frac{1}{R} \sum_{r=1}^R |\tilde{\mathbf{x}}_r|^2 = \frac{1}{R} \sum_{r=1}^R |\mathbf{V}^H \mathbf{x}_r|^2. \quad (16)$$

The estimator in (16) is the analogous of the *periodogram* of time signals and is referred as such from now on. Its intuitive appeal is that it writes the PSD of the process \mathbf{x} as the average of the squared magnitudes of the GFTs of realizations of \mathbf{x} .

Alternatively, one can replace \mathbf{C}_x in (8) by its empirical estimate $\hat{\mathbf{C}}_x = (1/R) \sum_{r=1}^R \mathbf{x}_r \mathbf{x}_r^H$ and propose the PSD estimate

$$\hat{\mathbf{p}}_{\text{cg}} := \text{diag} \left(\mathbf{V}^H \hat{\mathbf{C}}_x \mathbf{V} \right) := \text{diag} \left[\mathbf{V}^H \left[\frac{1}{R} \sum_{r=1}^R \mathbf{x}_r \mathbf{x}_r^H \right] \mathbf{V} \right]. \quad (17)$$

An important observation in the correlogram definition in (17) is that the empirical covariance $\hat{\mathbf{C}}_x$ is not necessarily diagonalized by \mathbf{V} . However, since we know that the actual covariance \mathbf{C}_x is diagonal, we retain only the diagonal elements of $\mathbf{V}^H \hat{\mathbf{C}}_x \mathbf{V}$ to estimate the PSD of \mathbf{x} . The expression in (17) is the analogous of the time *correlogram*. Its intuitive appeal is that it estimates the PSD with a double GFT transformation of the empirical covariance matrix.

Although different in genesis, it is apparent from their respective expressions that the periodogram in (16) and the correlogram in (17) are identical estimates as we prove next.

Proposition 2 Given observations $\{\mathbf{x}_r\}_{r=1}^R$, the periodogram in (16) and the correlogram in (17) are equivalent, i.e.,

$$\hat{\mathbf{p}}_{\text{pg}} := \frac{1}{R} \sum_{r=1}^R |\mathbf{V}^H \mathbf{x}_r|^2 = \text{diag} \left[\mathbf{V}^H \left[\frac{1}{R} \sum_{r=1}^R \mathbf{x}_r \mathbf{x}_r^H \right] \mathbf{V} \right] := \hat{\mathbf{p}}_{\text{cg}}. \quad (18)$$

Proof: Move matrices \mathbf{V}^H and \mathbf{V} into the empirical covariance sum in the correlogram definition in (18). Observe that the summands end up being of the form $(\mathbf{V}^H \mathbf{x}_r)(\mathbf{V}^H \mathbf{x}_r)^H$. The diagonal elements of these outer products are $|\mathbf{V}^H \mathbf{x}_r|^2$, which are the summands in the periodogram definition in (18). ■

The result in Proposition 2 is consistent with the equivalence of correlograms and periodograms in time signals. Henceforth, we choose to call $\hat{\mathbf{p}}_{\text{pg}} = \hat{\mathbf{p}}_{\text{cg}}$ the periodogram estimate of \mathbf{p} .

To evaluate the performance of the periodogram estimator in (16) we assess its mean and variance. The estimator is unbiased by design and, as we shall prove next, this is easy to establish formally. To study the estimator's variance we need the additional hypothesis of the process having a Gaussian distribution. Expressions for means and variances of periodogram estimators are given in the following proposition.

Proposition 3 Let \mathbf{p} be the PSD of a process \mathbf{x} that is stationary with respect to the shift $\mathbf{S} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^H$. Independent samples $\{\mathbf{x}_r\}_{r=1}^R$ are drawn from the distribution of the process \mathbf{x} and the periodogram $\hat{\mathbf{p}}_{\text{pg}}$ is computed as in (16). The bias \mathbf{b}_{pg} of the estimator is zero,

$$\mathbf{b}_{\text{pg}} := \mathbb{E} [\hat{\mathbf{p}}_{\text{pg}}] - \mathbf{p} = \mathbf{0}. \quad (19)$$

Further define the covariance matrix of the periodogram estimator as $\Sigma_{\text{pg}} := \mathbb{E} [(\hat{\mathbf{p}}_{\text{pg}} - \mathbf{p})(\hat{\mathbf{p}}_{\text{pg}} - \mathbf{p})^H]$. If the process \mathbf{x} is assumed Gaussian and \mathbf{S} is symmetric, the covariance matrix can be written as

$$\Sigma_{\text{pg}} := \mathbb{E} [(\hat{\mathbf{p}}_{\text{pg}} - \mathbf{p})(\hat{\mathbf{p}}_{\text{pg}} - \mathbf{p})^H] = (2/R) \text{diag}^2(\mathbf{p}). \quad (20)$$

Proof: See Appendix A. ■

The expression in (19) states that the bias of the periodogram is $\mathbf{b}_{\text{pg}} = \mathbf{0}$, or, equivalently, that the expectation of the periodogram estimator is the PSD itself, i.e., $\mathbb{E} [\hat{\mathbf{p}}_{\text{pg}}] = \mathbf{p}$. The expression for the covariance matrix of Σ_{pg} holds true only when the process \mathbf{x} has a Gaussian distribution. The reason for this limitation is that the determination of this covariance involves operations with the fourth order moments of the process \mathbf{x} . This necessity and associated limitation also arise in time signals [4, Sec. 8.2]. To help readability and intuition, the covariance Σ_{pg} in (20) is stated for a symmetric \mathbf{S} , however, in Appendix A the proof is done for a generic normal, not necessarily symmetric, \mathbf{S} .

The variance expression in (20) is analogous to the periodogram variances of PSDs of time domain signals in that: (i) Estimates of different frequencies are uncorrelated – because Σ_{pg} is diagonal. (ii) The variance of the periodogram is proportional to the square of the PSD. The latter fact is more often expressed in terms of the mean squared error (MSE), which we define as $\text{MSE}(\hat{\mathbf{p}}_{\text{pg}}) := \mathbb{E} [\|(\hat{\mathbf{p}}_{\text{pg}} - \mathbf{p})\|_2^2]$ and write as [cf. (19) and (20)]

$$\text{MSE}(\hat{\mathbf{p}}_{\text{pg}}) = \|\mathbf{b}_{\text{pg}}\|_2^2 + \text{tr}[\Sigma_{\text{pg}}] = (2/R) \|\mathbf{p}\|_2^2. \quad (21)$$

As it happens in time signals, the MSE in (21) is large and results in estimation errors that are on the order of the magnitude of the frequency component itself. Two of the workarounds to reduce the MSE in (21) are the use of windows and filterbanks. Both tradeoff bias for variance as we explain in the following sections.

B. Windowed Average Periodogram

The Bartlett and Welch methods for PSD estimation of time signals utilize windows to, in effect, generate multiple samples of the process even if only a single realization is given [5, Sec. 2.7]. These methods reduce variances of PSD estimates but introduce some distortion (bias). The purpose of this section is to define counterparts of windowing methods for PSD estimation of graph signals.

To understand the use of windows in estimating a PSD let us begin by defining windows for graph signals and understanding their effect on the graph frequency domain. We say that a signal \mathbf{w} is a window if its energy is $\|\mathbf{w}\|_2^2 = \|\mathbf{1}\|_2^2 = N$. Applying the window \mathbf{w} to a signal¹ \mathbf{x} entails componentwise multiplication to produce the signal $\mathbf{x}_{\mathbf{w}} = \text{diag}(\mathbf{w})\mathbf{x}$. In the graph frequency domain we can use the definition of the GFT $\tilde{\mathbf{x}}_{\mathbf{w}} = \mathbf{V}^H \mathbf{x}_{\mathbf{w}}$, the definition of the windowed signal $\mathbf{x}_{\mathbf{w}} = \text{diag}(\mathbf{w})\mathbf{x}$, and the definition of the iGFT to write

$$\tilde{\mathbf{x}}_{\mathbf{w}} = \mathbf{V}^H \mathbf{x}_{\mathbf{w}} = \mathbf{V}^H \text{diag}(\mathbf{w})\mathbf{x} = \mathbf{V}^H \text{diag}(\mathbf{w})\mathbf{V}\tilde{\mathbf{x}} := \tilde{\mathbf{W}}\tilde{\mathbf{x}}, \quad (22)$$

where in the last equality we defined the dual of the windowing operator $\text{diag}(\mathbf{w})$ in the frequency domain as the matrix $\tilde{\mathbf{W}} :=$

¹To keep notation simple, we use \mathbf{x} to denote a realization of process \mathbf{x} .

$\mathbf{V}^H \text{diag}(\mathbf{w}) \mathbf{V}$. In time signals the frequency representation of a window is its Fourier transform and dual operator of windowing is the convolution between the spectra of the window and the signal. This decoupled explanation is lost in graph signals. Nonetheless, (22) can be used to design windows with small spectral distortion. Ideal windows are such that $\tilde{\mathbf{W}} = \mathbf{I}$ which can be achieved by setting $\mathbf{w} = \mathbf{1}$, although this is unlikely to be of any use. More interestingly, (22) implies that good windows for spectral estimation must have $\tilde{\mathbf{W}} \approx \mathbf{I}$ or can allow nonzero values in columns k where the components \tilde{x}_k of $\tilde{\mathbf{x}}$ are known or expected to be small.

Turning now to the problem of PSD estimation, consider the estimate $\hat{\mathbf{p}}$ obtained after computing the periodogram in (16) using a *single* realization \mathbf{x} , so that we have that $\hat{\mathbf{p}} = |\mathbf{V}^H \mathbf{x}|^2$. Suppose now that we window the realization \mathbf{x} to produce $\mathbf{x}_w = \text{diag}(\mathbf{w})\mathbf{x}$ and compute the *windowed periodogram* $\hat{\mathbf{p}}_w := |\mathbf{V}^H \mathbf{x}_w|^2$. Utilizing the definition of the window's frequency representation, we can write this windowed periodogram as

$$\hat{\mathbf{p}}_w := |\mathbf{V}^H \mathbf{x}_w|^2 = |\mathbf{V}^H \text{diag}(\mathbf{w})\mathbf{x}|^2 = |\tilde{\mathbf{W}} \mathbf{V}^H \mathbf{x}|^2. \quad (23)$$

The expression in (23) can be used to compute the expectation of the windowed periodogram that we report in the following proposition.

Proposition 4 Let \mathbf{p} be the PSD of a process \mathbf{x} that is stationary with respect to the shift $\mathbf{S} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^H$. The expectation of the windowed periodogram $\hat{\mathbf{p}}_w$ in (23) is,

$$\mathbb{E}[\hat{\mathbf{p}}_w] = (\tilde{\mathbf{W}} \circ \tilde{\mathbf{W}}^*) \mathbf{p}. \quad (24)$$

Proof : Write $\hat{\mathbf{p}}_w = |\tilde{\mathbf{W}} \mathbf{V}^H \mathbf{x}|^2 = \text{diag}(\tilde{\mathbf{W}} \mathbf{V}^H \mathbf{x} \mathbf{x}^H \mathbf{V} \tilde{\mathbf{W}})$. Take expectation and use $\mathbb{E}[\mathbf{x} \mathbf{x}^H] = \mathbf{C}_x$ to write $\mathbb{E}[\hat{\mathbf{p}}_w] = \text{diag}(\tilde{\mathbf{W}} \mathbf{V}^H \mathbf{C}_x \mathbf{V} \tilde{\mathbf{W}})$. Further observe that $\mathbf{V}^H \mathbf{C}_x \mathbf{V} = \text{diag}(\mathbf{p})$ to conclude that $\hat{\mathbf{p}}_w = \text{diag}(\tilde{\mathbf{W}} \text{diag}(\mathbf{p}) \tilde{\mathbf{W}}^H)$. This latter expression is identical to (24). ■

Proposition 4 implies that the windowed periodogram in (25) is a biased estimate of the PSD \mathbf{p} and that the bias is determined by the dual of the windowing operator in the frequency domain $\tilde{\mathbf{W}}$.

Multiple windows yield, in general, better estimates than single windows. Consider then a bank of M windows $\mathcal{W} = \{\mathbf{w}_m\}_{m=1}^M$ and use each of the windows \mathbf{w}_m to construct the windowed signal $\mathbf{x}_m := \text{diag}(\mathbf{w}_m)\mathbf{x}$. We estimate the PSD \mathbf{p} with the *windowed average periodogram*

$$\hat{\mathbf{p}}_{\mathcal{W}} := \frac{1}{M} \sum_{m=1}^M |\mathbf{V}^H \mathbf{x}_m|^2 = \frac{1}{M} \sum_{m=1}^M |\mathbf{V}^H \text{diag}(\mathbf{w}_m)\mathbf{x}|^2. \quad (25)$$

The estimator $\hat{\mathbf{p}}_{\mathcal{W}}$ is an average of the windowed periodograms in (25) but is also reminiscent of the periodogram in (16). The difference is that in (16) the samples $\{\mathbf{x}_r\}_{r=1}^R$ are independent observations whereas in (25) the samples $\{\mathbf{x}_m\}_{m=1}^M$ are all generated through multiplications with the window bank \mathcal{W} . This means that: (i) There is some distortion in the windowed periodogram estimate because the windowed signals \mathbf{x}_m are used in lieu of \mathbf{x} . (ii) The different signals \mathbf{x}_m are correlated with each other and the reduction in variance resulting from the averaging operation in (25) is less significant than the reduction of variance that we observe in Proposition 3.

To study these effects, given the windowing operation $\text{diag}(\mathbf{w}_m)$, we obtain its dual in the frequency domain as $\tilde{\mathbf{W}}_m := \mathbf{V}^H \text{diag}(\mathbf{w}_m) \mathbf{V}$ [cf. (22)], and use those to define the power *spectrum mixing* matrix of windows m and m' as the componentwise

product

$$\tilde{\mathbf{W}}_{mm'} := \tilde{\mathbf{W}}_m \circ \tilde{\mathbf{W}}_{m'}^*. \quad (26)$$

We use these matrices to give expressions for the bias and covariance of the estimator in (25) in the following proposition.

Proposition 5 Let \mathbf{p} be the PSD of a process \mathbf{x} that is stationary with respect to the shift $\mathbf{S} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^H$. A single observation \mathbf{x} is given along with the window bank $\mathcal{W} = \{\mathbf{w}_m\}_{m=1}^M$ and the windowed average periodogram $\hat{\mathbf{p}}_{\mathcal{W}}$ is computed as in (25). The expectation of the estimator $\hat{\mathbf{p}}_{\mathcal{W}}$ is

$$\mathbb{E}[\hat{\mathbf{p}}_{\mathcal{W}}] = \frac{1}{M} \sum_{m=1}^M \tilde{\mathbf{W}}_{mm} \mathbf{p}. \quad (27)$$

Equivalently, $\hat{\mathbf{p}}_{\mathcal{W}}$ is biased with bias $\mathbf{b}_{\mathcal{W}} := \mathbb{E}[\hat{\mathbf{p}}_{\mathcal{W}}] - \mathbf{p}$. Further define the covariance matrix of the windowed periodogram as $\Sigma_{\mathcal{W}} := \mathbb{E}[(\hat{\mathbf{p}}_{\mathcal{W}} - \mathbb{E}[\hat{\mathbf{p}}_{\mathcal{W}}])(\hat{\mathbf{p}}_{\mathcal{W}} - \mathbb{E}[\hat{\mathbf{p}}_{\mathcal{W}}])^H]$. If the process \mathbf{x} is assumed Gaussian and \mathbf{S} is symmetric, the trace of the covariance matrix can be written as

$$\text{tr}[\Sigma_{\mathcal{W}}] = \frac{2}{M^2} \sum_{m=1, m' \neq m}^M \text{tr}[(\tilde{\mathbf{W}}_{mm'} \mathbf{p})(\tilde{\mathbf{W}}_{mm'} \mathbf{p})^H]. \quad (28)$$

Proof : See Appendix B, where the expression of $\text{tr}[\Sigma_{\mathcal{W}}]$ for nonsymmetric normal shifts is given too [cf. (64)]. ■

The first claim of Proposition 5 is a generalization of the bias expression for the bias of windowed periodograms in (24). It states that the estimator $\hat{\mathbf{p}}_{\mathcal{W}}$ is biased with a bias determined by the average of the spectrum mixing matrices $\tilde{\mathbf{W}}_{mm} = \tilde{\mathbf{W}}_m \circ \tilde{\mathbf{W}}_m^*$. The form of these mixing matrices depends on the design of the window bank $\mathcal{W} = \{\mathbf{w}_m\}_{m=1}^M$ and on the topology of the graph \mathcal{G} . Observe that even if the individual spectrum mixing matrices $\tilde{\mathbf{W}}_{mm}$ are not close to identity we can still have small bias by making their weighted sum $M^{-1} \sum_m \tilde{\mathbf{W}}_{mm} \approx \mathbf{I}$.

The second claim in Proposition 5 is a characterization of the trace of the covariance matrix $\Sigma_{\mathcal{W}}$. To interpret the expression in (28) it is convenient to separate the summands with $m = m'$ from the rest to write

$$\begin{aligned} \text{tr}[\Sigma_{\mathcal{W}}] &= \frac{2}{M^2} \sum_{m=1}^M \text{tr}[(\tilde{\mathbf{W}}_{mm} \mathbf{p})(\tilde{\mathbf{W}}_{mm} \mathbf{p})^H] \\ &+ \frac{2}{M^2} \sum_{m=1, m' \neq m}^M \text{tr}[(\tilde{\mathbf{W}}_{mm'} \mathbf{p})(\tilde{\mathbf{W}}_{mm'} \mathbf{p})^H] \end{aligned} \quad (29)$$

Comparing (29) with (24), we see that the terms in the first summand are $\text{tr}[(\tilde{\mathbf{W}}_{mm} \mathbf{p})(\tilde{\mathbf{W}}_{mm} \mathbf{p})^H] = \|\mathbb{E}[\hat{\mathbf{p}}_{\mathbf{w}_m}]\|_2^2$. Given that the windows have energy $\|\mathbf{w}_m\|_2^2 = \|\mathbf{1}\|_2^2 = N$ we expect $\|\mathbb{E}[\hat{\mathbf{p}}_{\mathbf{w}_m}]\|_2 \approx \|\mathbb{E}[\hat{\mathbf{p}}_{\mathbf{x}}]\|_2 = \|\mathbf{p}\|_2$. This implies that the first sum in (29) is approximately proportional to $2\|\mathbf{p}\|_2^2/M$. Thus, this first term behaves as if the different windows in the bank \mathcal{W} were generating independent samples [cf. (21)].

The effect of the correlation between different windowed signals appears in the cross terms of the second sum, which can be viewed as the price to pay for the signals $\{\mathbf{x}_m\}_{m=1}^M$ being generated from the same realization \mathbf{x} instead of actually being independent. We explain in the following section that the price we pay in this second sum is smaller than the gain we get in the first term.

Window design. The overall MSE is given by the squared bias norm summed to the trace of the covariance matrix,

$$\text{MSE}(\hat{\mathbf{p}}_{\mathcal{W}}) = \|\mathbf{b}_{\mathcal{W}}\|_2^2 + \text{tr}[\Sigma_{\mathcal{W}}]. \quad (30)$$

The expression in (30) can be used to design (optimal) windows with minimum MSE. Do notice that the bias in (30) depends on the unknown PSD \mathbf{p} . This problem can be circumvented by making $\mathbf{p} = \mathbf{1}$ in the bias and trace expressions in Proposition 5. This choice implies that the PSD is assumed white a priori. If some other knowledge of the PSD is available, it can be used as an alternative prior. Irrespectively of the choice of prior, finding windows that minimize the MSE is computationally challenging.

An alternative approach to design the window bank $\mathcal{W} = \{\mathbf{w}_m\}_{m=1}^M$ is to exploit the local properties of the random process \mathbf{x} . As stated in Property 2, some stationary processes are expected to have correlations with local structure. It is then reasonable to expect that windows without overlap capture independent information that results in a reduction of the cross-terms in (29). This intuition is formalized in the following proposition.

Proposition 6 Consider two windows \mathbf{w}_m and $\mathbf{w}_{m'}$ and assume that the distance between any node in \mathbf{w}_m and any node in $\mathbf{w}_{m'}$ is larger than $2L$ hops. If the process \mathbf{x} can be modeled as the output of an L -degree filter, then it holds that $\text{tr}[\tilde{\mathbf{W}}_{mm'}\mathbf{p}(\tilde{\mathbf{W}}_{mm'}\mathbf{p})^H] = 0$.

Proof : Let $\mathcal{N}(\mathbf{w}_m) = \{i : [\mathbf{w}_m]_i \neq 0\}$ be the set of nodes in the support of \mathbf{w}_m , and $\mathcal{N}(\mathbf{w}_{m'})$ the ones in the support of $\mathbf{w}_{m'}$. We know that the distance between any $i \in \mathcal{N}(\mathbf{w}_m)$ and any $i' \in \mathcal{N}(\mathbf{w}_{m'})$ is greater than $2L$. Invoking Property 2, this implies that $[\mathbf{C}_x]_{ii'} = 0$, which allows us to write $\text{diag}(\mathbf{e}_i)\mathbf{C}_x\text{diag}(\mathbf{e}_{i'}) = \mathbf{0}$. Since this is true for any pair (i, i') with $i \in \mathcal{N}(\mathbf{w}_m)$ and $i' \in \mathcal{N}(\mathbf{w}_{m'})$, we have that: *f1*) $\text{diag}(\mathbf{w}_m)\mathbf{C}_x\text{diag}(\mathbf{w}_{m'}) = \mathbf{0}$. Note now that $\tilde{\mathbf{W}}_{mm'}\mathbf{p} = \tilde{\mathbf{W}}_m \circ \mathbf{W}_{m'}^*\mathbf{p} = \tilde{\mathbf{W}}_m\text{diag}(\mathbf{p})\tilde{\mathbf{W}}_{m'}^*$, which using the definitions $\tilde{\mathbf{W}}_m = \mathbf{V}^H\text{diag}(\mathbf{w}_m)\mathbf{V}$ and $\mathbf{C}_x = \mathbf{V}\text{diag}(\mathbf{p})\mathbf{V}^H$ can be written as: *f2*) $\tilde{\mathbf{W}}_{mm'}\mathbf{p} = \mathbf{V}^H\text{diag}(\mathbf{w}_m)\mathbf{C}_x\text{diag}(\mathbf{w}_{m'}^*)\mathbf{V}$. Substituting *f1*) into *f2*) yields $\tilde{\mathbf{W}}_{mm'}\mathbf{p} = \mathbf{V}^H\mathbf{0}\mathbf{V} = \mathbf{0}$. ■

The result in Proposition 6 implies that if we use windows without overlap, the second sum in (29) is null. This means that the covariance matrix $\Sigma_{\mathcal{W}}$ of the PSD estimator in (25) behaves as if the separate windowed samples were independent samples. We emphasize that Proposition 6 provides a lax bound for a rather stringent correlation model. The purpose of the result is to illustrate the reasons why local windows are expected to reduce estimation MSE. In practice, we expect local windows to reduce MSE as long as the correlation decreases with the hop distance between nodes. Windowing design can then be related to clustering (if the windows are non-overlapping) and covering (if they overlap) with the goal of keeping the diameter of the window large enough so that most of the correlation of the process is preserved. Section VI evaluates the estimation performance when estimating the PSD of a graph process for different types of windows.

C. Filter Banks

Windows reduce the MSE of periodograms by exploiting the locality of correlations. Filter banks reduce MSE by exploiting the locality of the PSD [5, Sec. 5]. To define filter bank PSD estimators for graph processes, suppose that we are given a filter bank $\mathcal{Q} := \{\mathbf{Q}_k\}_{k=1}^N$ with N filters (as many as frequencies). The filters \mathbf{Q}_k are assumed linear shift invariant with frequency responses $\tilde{\mathbf{q}}_k$, so that we can write $\mathbf{Q}_k = \mathbf{V}\text{diag}(\tilde{\mathbf{q}}_k)\mathbf{V}^H$. We further assume that their energies are normalized $\|\tilde{\mathbf{q}}_k\|_2^2 = 1$. The k th (bandpass) filter is intended to estimate the k th component of the PSD $\mathbf{p} = [p_1, \dots, p_N]^T$ through the energy of the output

signal $\mathbf{x}_k := \mathbf{Q}_k\mathbf{x}$, i.e.,

$$\hat{p}_{\tilde{\mathbf{q}}_k} := \|\mathbf{x}_k\|_2^2 = \|\mathbf{Q}_k\mathbf{x}\|_2^2. \quad (31)$$

The filter bank PSD estimate is given by the concatenation of the individual estimates in (31) into the vector $\hat{\mathbf{p}}_{\mathcal{Q}} := [\hat{p}_{\tilde{\mathbf{q}}_1}, \dots, \hat{p}_{\tilde{\mathbf{q}}_N}]^T$. We emphasize that we can think of filter banks as an alternative approach to generate multiple virtual realizations \mathbf{x}_k from a single actual realization \mathbf{x} . In the case of windowing, realizations \mathbf{x}_m correspond to different pieces of \mathbf{x} . In the case of filter banks, realizations \mathbf{x}_k correspond to different filtered versions of \mathbf{x} .

Using Parseval's theorem and the frequency representations $\tilde{\mathbf{q}}_k$ and $\tilde{\mathbf{x}}$ of the filter \mathbf{Q}_k and the realization \mathbf{x} , respectively, the estimate in (31) is equivalent to

$$\hat{p}_{\tilde{\mathbf{q}}_k} = \|\tilde{\mathbf{x}}_k\|_2^2 = \|\text{diag}(\tilde{\mathbf{q}}_k)\tilde{\mathbf{x}}\|_2^2. \quad (32)$$

The expression in (32) guides the selection of the response $\tilde{\mathbf{q}}_k$. E.g., if the PSD values at frequencies k and k' are expected to be similar, i.e., if $p_k \approx p_{k'}$ we can make $[\tilde{\mathbf{q}}_k]_k = [\tilde{\mathbf{q}}_k]_{k'} = (1/\sqrt{2})$ so that the PSD components $[\|\mathbf{V}^H\mathbf{x}\|_2^2]_k$ and $[\|\mathbf{V}^H\mathbf{x}\|_2^2]_{k'}$ are averaged. More generically, the design of the filter $\tilde{\mathbf{q}}_k$ can be guided by the bias and variance expressions that we present in the following proposition.

Proposition 7 Let $\mathbf{p} = [p_1, \dots, p_N]^T$ be the PSD of a process \mathbf{x} that is stationary with respect to the shift $\mathbf{S} = \mathbf{V}\mathbf{A}\mathbf{V}^H$. A single observation \mathbf{x} is given along with the filter bank $\mathcal{Q} = \{\tilde{\mathbf{q}}_k\}_{k=1}^N$ and the filter bank PSD estimates $\hat{\mathbf{p}}_{\mathcal{Q}}$ are computed as in (32). The expectation of the k entry of $\hat{\mathbf{p}}_{\mathcal{Q}}$ is,

$$\mathbb{E}[\hat{p}_{\tilde{\mathbf{q}}_k}] := (|\tilde{\mathbf{q}}_k|^2)^T \mathbf{p}. \quad (33)$$

Equivalently, $\hat{p}_{\tilde{\mathbf{q}}_k}$ is biased with bias $b_{\tilde{\mathbf{q}}_k} := \mathbb{E}[\hat{p}_{\tilde{\mathbf{q}}_k}] - p_k$. Further define the variance of the k th entry of the filter bank estimate $\hat{\mathbf{p}}_{\mathcal{Q}}$ as $\text{var}[\hat{p}_{\tilde{\mathbf{q}}_k}] := \mathbb{E}[(\hat{p}_{\tilde{\mathbf{q}}_k} - \mathbb{E}[\hat{p}_{\tilde{\mathbf{q}}_k}])^2]$. If the process \mathbf{x} is assumed Gaussian and \mathbf{S} is symmetric, the variance can be written as

$$\text{var}[\hat{p}_{\tilde{\mathbf{q}}_k}] := \mathbb{E}[(\hat{p}_{\tilde{\mathbf{q}}_k} - \mathbb{E}[\hat{p}_{\tilde{\mathbf{q}}_k}])^2] = 2 \|\text{diag}(|\tilde{\mathbf{q}}_k|^2) \mathbf{p}\|_2^2. \quad (34)$$

Proof : See Appendix C, where the expression of $\text{var}[\hat{p}_{\tilde{\mathbf{q}}_k}]$ for nonsymmetric normal shifts is given too [cf. (69)]. ■

The variance expression in (33) shows that the estimation accuracy of a filter bank benefits from an averaging effect – recall that the filter is normalized to have unit energy $\|\tilde{\mathbf{q}}_k\|_2^2 = 1$. This averaging advantage manifests only if the bias in (33) is made small so that the overall MSE, given by $\text{MSE}(\hat{\mathbf{p}}_{\mathcal{Q}}) = \sum_{k=1}^N b_{\tilde{\mathbf{q}}_k}^2 + \text{var}[\hat{p}_{\tilde{\mathbf{q}}_k}]$, decreases. In time signals the bias is made small by exploiting the fact that the PSD of nearby frequencies are similar. In graph signals, some extra information is necessary to identify frequency components with similar PSD values. If, e.g., the process \mathbf{x} is a diffusion process as the one in Example 3, the PSD components p_k and $p_{k'}$ are similar – irrespectively of α – if the eigenvalues λ_k and $\lambda_{k'}$ of the Laplacian \mathbf{L} are similar. If the eigenvalues of the Laplacian are further ordered, averaging of nearby PSD estimates can be interpreted as the use of a bandpass filter.

A generic approach to designing bandpass filters for PSD estimation is to exploit (FIR) filters, which are attractive due their ability to be implemented distributedly [9]. Formally, write $\mathbf{Q}_k = \sum_{l=1}^L q_k^l \mathbf{S}^l$, denote as $\mathbf{q}_k = [q_k^1, \dots, q_k^L]^T$ the vector of filter coefficients, and as $\tilde{\mathbf{q}}_k = \Psi_L \mathbf{q}_k$ its frequency response, where we recall that Ψ_L stands for the first L columns of Ψ . The coefficients \mathbf{q}_k could be designed upon substituting $\tilde{\mathbf{q}}_k = \Psi_L \mathbf{q}_k$ into both (33) and (34) and minimizing the resultant MSE. This

can be challenging because it involves fourth-order polynomials and requires some prior knowledge on \mathbf{p} . For the purpose of PSD estimation in time, a traditional approach for suboptimal FIR design is to select coefficients guaranteeing that $[\tilde{\mathbf{q}}_k]_k = 1$ while minimizing the out-of-band power [4]. Defining $\psi_{k,L}^T$ as the k th row of Ψ_L , this can be formalized as

$$\mathbf{q}_k := \underset{\mathbf{q}_L}{\operatorname{argmin}} \|\Psi_L \mathbf{q}_L\|_2^2, \quad \text{s. t. } \psi_{k,L}^T \mathbf{q}_L = 1, \quad (35)$$

with the constraint forcing $[\tilde{\mathbf{q}}_k]_k = 1$ and the objective attempting to minimize the contribution to $\hat{p}_{\tilde{\mathbf{q}}_k}$ from frequencies other than k . If we make $L \geq N$ the solution to (35) is $[\tilde{\mathbf{q}}_k]_{k'} = 0$ for all $k' \neq k$. For $L < N$, the filter \mathbf{q}_k has a response in which nonzero coefficients $[\tilde{\mathbf{q}}_k]_{k'}$ are clustered at frequencies k' that are similar to k – in the sense of being associated with multipliers $\lambda_{k'} \approx \lambda_k$. We further observe that (35) has the additional advantage of being solved in closed form as

$$\mathbf{q}_k = (\psi_{k,L}^T \Psi_L^H \Psi_L \psi_{k,L}^*)^{-1} (\Psi_L^H \Psi_L)^{-1} \psi_{k,L}, \quad (36)$$

which does not have unit energy but can be normalized.

V. PARAMETRIC PSD ESTIMATION

We address PSD estimation assuming that the graph process \mathbf{x} can be well approximated by a parametric model in which \mathbf{x} is the response of a graph filter \mathbf{H} to a white input. As per Definition 2, this is always possible if the filter's order is sufficiently large. The goal here is to devise filter representations of an order (much) smaller than the number of signal elements N . Mimicking time processes, we devise moving average (MA), autoregressive (AR), and ARMA models.

A. Moving Average Graph Processes

Consider a vector of coefficients $\boldsymbol{\beta} = [\beta_0, \dots, \beta_{L-1}]^T$ and assume that \mathbf{x} is stationary in the graph \mathbf{S} and generated by the FIR filter $\mathbf{H}(\boldsymbol{\beta}) = \sum_{l=0}^{L-1} \beta_l \mathbf{S}^l$. The degree of the filter is less than $N - 1$ although we want in practice to have $L \ll N$. If the process is indeed generated as the response of $\mathbf{H}(\boldsymbol{\beta})$ to a white input, the covariance matrix of the process can be written as

$$\mathbf{C}_x(\boldsymbol{\beta}) = \mathbf{H}(\boldsymbol{\beta}) \mathbf{H}^H(\boldsymbol{\beta}) = \sum_{l=0, l'=0}^{L-1} (\beta_l \mathbf{S}^l) (\beta_{l'} \mathbf{S}^{l'})^H. \quad (37)$$

The PSD corresponding to the covariance in (37) is the magnitude squared of the frequency representation of the filter. To see this formally, notice that it follows from the definition in (8) that $\mathbf{p}(\boldsymbol{\beta}) = \operatorname{diag}(\mathbf{V}^H \mathbf{C}_x(\boldsymbol{\beta}) \mathbf{V})$. Writing the covariance matrix as $\mathbf{C}_x(\boldsymbol{\beta}) = \mathbf{H}(\boldsymbol{\beta}) \mathbf{H}^H(\boldsymbol{\beta})$ and the frequency representation of the filter as $\tilde{\mathbf{h}}(\boldsymbol{\beta}) = \operatorname{diag}(\mathbf{V} \mathbf{H}(\boldsymbol{\beta}) \mathbf{V}^H)$, it follows readily that $\mathbf{p}(\boldsymbol{\beta}) = |\tilde{\mathbf{h}}(\boldsymbol{\beta})|^2$. For the purposes of this section it is convenient to write the latter explicitly in terms of $\boldsymbol{\beta}$ as [cf. (3)]

$$\mathbf{p}(\boldsymbol{\beta}) = |\tilde{\mathbf{h}}(\boldsymbol{\beta})|^2 = |\Psi_L \boldsymbol{\beta}|^2. \quad (38)$$

The covariance and PSD expressions in (37) and (38) are graph counterparts of MA time processes generated by FIR filters – see Section III-B for a discussion on their practical relevance.

The estimation of the coefficients $\boldsymbol{\beta}$ can be addressed in either the graph or graph frequency domain. In the graph domain we compute the sample covariance $\hat{\mathbf{C}}_x = \mathbf{x} \mathbf{x}^H$ and introduce a distortion function $D_{\mathbf{C}}(\hat{\mathbf{C}}_x, \mathbf{C}_x(\boldsymbol{\beta}))$ to measure the similarity of $\hat{\mathbf{C}}_x$ and $\mathbf{C}_x(\boldsymbol{\beta})$. The filter coefficients $\boldsymbol{\beta}$ are then selected as the ones with minimal distortion,

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} D_{\mathbf{C}}(\hat{\mathbf{C}}_x, \mathbf{C}_x(\boldsymbol{\beta})). \quad (39)$$

The expression for $\mathbf{C}_x(\boldsymbol{\beta})$ in (37) is a quadratic function of $\boldsymbol{\beta}$ that is generally indefinite. The optimization problem in (39) will therefore be not convex in general.

To perform estimation in the frequency domain we first compute the periodogram $\hat{\mathbf{p}}_{\text{pg}}$ defined in (16). We then introduce a distortion measure $D_{\mathbf{P}}(\hat{\mathbf{p}}_{\text{pg}}, |\Psi_L \boldsymbol{\beta}|^2)$ to compare the periodogram $\hat{\mathbf{p}}_{\text{pg}}$ with the PSD $|\Psi_L \boldsymbol{\beta}|^2$ and select the coefficients $\boldsymbol{\beta}$ that solve the following optimization

$$\hat{\boldsymbol{\beta}} := \underset{\boldsymbol{\beta}}{\operatorname{argmin}} D_{\mathbf{P}}(\hat{\mathbf{p}}_{\text{pg}}, |\Psi_L \boldsymbol{\beta}|^2). \quad (40)$$

We observe that although we use the periodogram in (40), any of the nonparametric methods of Section IV-A can be used instead. Since the quadratic form $|\Psi_L \boldsymbol{\beta}|^2$ in (40) is also indefinite, the optimization problem in (40) is not necessarily convex. In the particular case when the distortion $D_{\mathbf{P}}(\hat{\mathbf{p}}_{\text{pg}}, |\Psi_L \boldsymbol{\beta}|^2) = \|\hat{\mathbf{p}}_{\text{pg}} - |\Psi_L \boldsymbol{\beta}|^2\|_2^2$ is the Euclidean 2-norm, efficient (phase-retrieval) solvers with probabilistic guarantees are available [21], [22]. Alternative tractable formulations of (39) and (40) when the shifts are symmetric, or, when the shifts are positive semidefinite and the filter coefficients are nonnegative are discussed below.

Symmetric shifts. If the shift \mathbf{S} is symmetric, the expression for the covariance matrix in (37) can be simplified to a polynomial of degree $2(L - 1)$ in \mathbf{S} ,

$$\mathbf{C}_x(\boldsymbol{\beta}) = \sum_{l=0, l'=0}^{L-1} \beta_l \beta_{l'} \mathbf{S}^{l+l'} := \sum_{l=0}^{2(L-1)} \gamma_l \mathbf{S}^l := \mathbf{C}_x(\boldsymbol{\gamma}) \quad (41)$$

In the second equality in (41) we have defined the coefficients $\gamma_l := \sum_{l'+l''=l} \beta_{l'} \beta_{l''}$ summing all the coefficient crossproducts that multiply \mathbf{S}^l and introduced $\mathbf{C}_x(\boldsymbol{\gamma})$ to denote the covariance matrix written in terms of the $\boldsymbol{\gamma}$ coefficients. We propose now a relaxation of (39) in which $\mathbf{C}_x(\boldsymbol{\gamma})$ is used in lieu of $\mathbf{C}_x(\boldsymbol{\beta})$ to yield the optimization problem

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\gamma}}{\operatorname{argmin}} D_{\mathbf{C}}(\hat{\mathbf{C}}_x, \mathbf{C}_x(\boldsymbol{\gamma})). \quad (42)$$

If we add the constraints $\gamma_l = \sum_{l'+l''=l} \beta_{l'} \beta_{l''}$, the problem in (42) is equivalent to (39). By dropping these constraints we end up with a tractable relaxation because (42) is convex for all convex distortion metrics $D_{\mathbf{C}}(\hat{\mathbf{C}}_x, \mathbf{C}_x(\boldsymbol{\gamma}))$. A tractable relaxation of (40) can be derived analogously.

Nonnegative filter coefficients. When the shift \mathbf{S} is positive semidefinite, the elements of the matrix Ψ are all nonnegative. If we further restrict the coefficients $\boldsymbol{\beta}$ to be nonnegative, all the elements in the product $\Psi_L \boldsymbol{\beta}$ are also nonnegative. This means that in (40) we can replace the comparison $D_{\mathbf{P}}(\hat{\mathbf{p}}_{\text{pg}}, |\Psi_L \boldsymbol{\beta}|^2)$ by the comparison $D_{\mathbf{P}}(\sqrt{\hat{\mathbf{p}}_{\text{pg}}}, \Psi_L \boldsymbol{\beta})$. We can then replace (40) by

$$\hat{\boldsymbol{\beta}} := \underset{\boldsymbol{\beta} \geq 0}{\operatorname{argmin}} D_{\mathbf{P}}(\sqrt{\hat{\mathbf{p}}_{\text{pg}}}, \Psi_L \boldsymbol{\beta}). \quad (43)$$

The optimization problem in (43) is convex, therefore tractable, for all convex distortion metrics $D_{\mathbf{P}}(\sqrt{\hat{\mathbf{p}}_{\text{pg}}}, \Psi_L \boldsymbol{\beta})$. Do notice that the objective costs in (43) and (40) are *not* equivalent and that (43) requires positive semidefinite shifts –such as the Laplacian– and restricts coefficients to satisfy $\boldsymbol{\beta} \geq 0$. A tractable restriction of (39) can be derived analogously.

B. Autoregressive Graph Processes

For some processes it is more convenient to use a parametric model that generates an infinite impulse response through an autoregressive filter. As a simple example consider the heat diffusion process in Example 3 that is completely characterized

by the diffusion rate α and the scaling coefficient α_0 . This process can be represented with the filter $\mathbf{H} = \alpha_0 \sum_{l=0}^{\infty} \alpha^l \mathbf{S}^l$. If the series is summable, the filter can be rewritten as $\mathbf{H} = \alpha_0 (\mathbf{I} - \alpha \mathbf{S})^{-1}$ from where we can conclude that its frequency response is $\tilde{\mathbf{h}} = \text{diag}(\mathbf{V}^H \mathbf{H} \mathbf{V}) = \alpha_0 \text{diag}(\mathbf{I} - \alpha \mathbf{\Lambda}^{-1})$. This demonstrates that \mathbf{H} can be viewed as a single pole AR filter – see also [10].

Suppose now that \mathbf{x} is a random graph process whose realizations are generated by applying $\mathbf{H} = \alpha_0 (\mathbf{I} - \alpha \mathbf{S})^{-1}$ to a white input \mathbf{w} . Then, it readily holds that its covariance \mathbf{C}_x is [cf. (5)]

$$\mathbf{C}_x(\alpha_0, \alpha) = \mathbf{H} \mathbf{H}^H = \alpha_0^2 (\mathbf{I} - \alpha \mathbf{S})^{-1} (\mathbf{I} - \alpha \mathbf{S})^{-H}, \quad (44)$$

which implies that the PSD of \mathbf{x} is

$$\mathbf{p}(\alpha_0, \alpha) = \text{diag}[\alpha_0^2 |\mathbf{I} - \alpha \mathbf{\Lambda}|^{-2}], \quad (45)$$

confirming the fact that the expression for the PSD of \mathbf{x} is similar to that of a first-order AR time-varying process. We can now proceed to estimate the PSD utilizing the AR parametric models in (44) and (45) as we did in Section V-A for MA models. Substituting $\mathbf{C}_x(\alpha_0, \alpha)$ for $\mathbf{C}_x(\beta)$ in (39) yields a graph domain formulation and substituting $\mathbf{p}(\alpha_0, \alpha)$ for $|\Psi_L \beta|^2$ in (40) yields a graph frequency domain formulation. Since only two parameters must be estimated the corresponding optimization problems are tractable.

If the filter $\mathbf{H} = \alpha_0 (\mathbf{I} - \alpha \mathbf{S})^{-1}$ is the equivalent of an AR process of order one, an AR process of order M can be written as $\mathbf{H} = \alpha_0 \prod_{m=1}^M (\mathbf{I} - \alpha_m \mathbf{S})^{-1}$ for some set of diffusion rates $\alpha = [\alpha_0, \dots, \alpha_M]^T$. The frequency response $\tilde{\mathbf{h}} = \text{diag}(\mathbf{V}^H \mathbf{H} \mathbf{V})$ of this filter is

$$\tilde{\mathbf{h}} = \alpha_0 \text{diag} \left[\prod_{m=1}^M (\mathbf{I} - \alpha_m \mathbf{\Lambda})^{-1} \right]. \quad (46)$$

If we define the graph process $\mathbf{x} = \mathbf{H} \mathbf{w}$ with \mathbf{w} white and unitary energy, the covariance matrix \mathbf{C}_x can be written as

$$\mathbf{C}_x(\alpha) = \alpha_0^2 \prod_{m=1}^M (\mathbf{I} - \alpha_m \mathbf{S})^{-1} (\mathbf{I} - \alpha_m \mathbf{S})^{-H}. \quad (47)$$

The process \mathbf{x} is stationary with respect to \mathbf{S} , because of, e.g., Definition 2. The PSD of \mathbf{x} can be written as

$$\mathbf{p}(\alpha) = \alpha_0^2 \text{diag} \left[\prod_{m=1}^M |\mathbf{I} - \alpha_m \mathbf{\Lambda}|^{-2} \right]. \quad (48)$$

As before, we substitute $\mathbf{C}_x(\alpha)$ for $\mathbf{C}_x(\beta)$ in (39) to obtain a graph domain formulation and substitute $\mathbf{p}(\alpha)$ for $|\Psi_L \beta|^2$ in (40) to obtain a graph frequency domain formulation. For large degree M the problems can become intractable. Yule-Walker schemes [5, Sec. 3.4] tailored to graph signals may be of help. Their derivation and analysis are left as future work.

Remark 3 To further motivate AR processes, consider the example of $\mathbf{x} = \mathbf{H} \mathbf{w}$ with \mathbf{H} being a single-pole filter and \mathbf{w} a white and Gaussian input, so that \mathbf{x} is Gaussian too. The covariance of this first-order AR process is given by (44), with its inverse covariance (precision matrix) being simply $\Theta := \mathbf{C}_x^{-1} = (\rho)^{-2} (\mathbf{I} - \alpha \mathbf{S})^H (\mathbf{I} - \alpha \mathbf{S})$. Since \mathbf{S} is sparse, the precision matrix Θ is sparse too. Specifically, $\Theta_{i,j} \neq 0$ only if j is in the two-hop neighborhood of i . Then, it follows that a Gaussian AR process of order one on the shift \mathbf{S} is a Gaussian Markov Random Fields (GMRF) [23, Ch. 19], with the Markov blanket of a node i being given by $\mathcal{N}_2(i)$, i.e., the nodes that are within the two-hop neighborhood of i . As explained in Example 2, such a process is stationary both on \mathbf{S} and on Θ . The same holds true for an AR

process of order M , which in this case will give rise to a GMRF whose Markov blankets are given by the $2M$ -hop neighborhoods of the original graph.

C. Autoregressive Moving Average Graph Processes

The techniques in sections V-A and V-B can be combined to form ARMA models for PSD estimation. However, as is also done for time signals, we formulate ARMA filters directly in the frequency domain as a ratio of polynomials in the graph eigenvalues. We then define coefficients $\mathbf{a} := [a_1, \dots, a_M]^T$ and $\mathbf{b} := [b_0, \dots, b_{L-1}]^T$ and postulate filters with frequency response

$$\tilde{\mathbf{h}} = \text{diag} \left[\left(\sum_{l=0}^{L-1} b_l \mathbf{\Lambda}^l \right) \left(1 - \sum_{m=1}^M a_m \mathbf{\Lambda}^m \right)^{-1} \right]. \quad (49)$$

To find the counterpart of (49) in the graph domain define the matrices $\mathbf{B} := \sum_{l=0}^{L-1} b_l \mathbf{S}^l$ and $\mathbf{A} := \sum_{m=1}^M a_m \mathbf{S}^m$. It then follows readily that the filter whose frequency response is in (49) is $\mathbf{H} = (\mathbf{I} - \mathbf{A})^{-1} \mathbf{B} = \mathbf{B} (\mathbf{I} - \mathbf{A})^{-1}$. These expressions confirm that we can interpret the filter as the sequential application of finite and infinite response filters.

If we now define the graph process $\mathbf{x} = \mathbf{H} \mathbf{w}$, its covariance matrix follows readily as

$$\mathbf{C}_x(\mathbf{a}, \mathbf{b}) = (\mathbf{I} - \mathbf{A})^{-1} \mathbf{B} \mathbf{B}^H (\mathbf{I} - \mathbf{A})^{-H}. \quad (50)$$

Since $\mathbf{C}_x(\mathbf{a}, \mathbf{b})$ is diagonalized by the GFT \mathbf{V} , the process \mathbf{x} is stationary with PSD [cf. (49)]

$$\mathbf{p}(\mathbf{a}, \mathbf{b}) = \text{diag} \left[\left| \sum_{l=0}^{L-1} b_l \mathbf{\Lambda}^l \right|^2 \left| 1 - \sum_{m=1}^M a_m \mathbf{\Lambda}^m \right|^{-2} \right]. \quad (51)$$

As in the AR and MA models, we can identify the model coefficients by minimizing the covariance distortion $D_C(\hat{\mathbf{C}}_x, \mathbf{C}_x(\mathbf{a}, \mathbf{b}))$ or the PSD distortion $D_p(\hat{\mathbf{p}}_{\text{pg}}, \mathbf{p}(\mathbf{a}, \mathbf{b}))$ [cf. (38) and (39)]. These optimization problems are computationally difficult.

Alternative estimation schemes can be obtained by reordering (50) into $(\mathbf{I} - \mathbf{A}) \mathbf{C}_x (\mathbf{I} - \mathbf{A})^H = \mathbf{B} \mathbf{B}^H$ and solving for either the graph domain distortion

$$(\hat{\mathbf{a}}, \hat{\mathbf{b}}) := \underset{\mathbf{a}, \mathbf{b}}{\text{argmin}} D_C((\mathbf{I} - \mathbf{A}) \hat{\mathbf{C}}_x (\mathbf{I} - \mathbf{A})^H, \mathbf{B} \mathbf{B}^H). \quad (52)$$

or the graph frequency domain distortion

$$(\hat{\mathbf{a}}, \hat{\mathbf{b}}) := \underset{\mathbf{a}, \mathbf{b}}{\text{argmin}} \quad (53)$$

$$D_p \left[\left| 1 - \sum_{m=1}^M a_m \mathbf{\Lambda}^m \right|^2 \hat{\mathbf{p}}_{\text{pg}}, \text{diag} \left[\left| \sum_{l=0}^{L-1} b_l \mathbf{\Lambda}^l \right|^2 \right] \right].$$

The formulations in (52) and (53) can still be intractable but we observe that the problems have the same structure as the ones considered in Section V-A. The tractable relaxation that we discussed for symmetric shifts and the tractable restriction to nonnegative filter coefficients for positive semidefinite shifts can be then used here as well.

Remark 4 The parametric methods in this section are well tailored to PSD estimation of diffusion processes – see Section III-B. When $L \ll N$ the dynamics in (15) are accurately represented by a low-order FIR model. Parametric estimation with a MA model as in Section V-A is recommendable. Single pole AR models arise when $\gamma^{(l)} = \gamma$ for all l and $L = \infty$ as we already explained in Section V-B. An AR model of order M arises when M single pole models are applied sequentially. The latter implies that AR models are applicable when the diffusion constants $\gamma^{(l)}$ are constant during stretches of time or vary slowly with time. If we consider now M diffusion dynamics with constant coefficients $\gamma^{(l)} = \gamma_m$ for all l running in *parallel* and we produce an output

as the sum of the M outcomes we obtain an ARMA system with M poles and $M - 1$ zeros [10].

Remark 5 The methods for PSD estimation that we presented in Sections IV and V can be used for covariance estimation as well. This follows directly for some of the parametric formulations in which we estimate filter coefficients that minimize a graph domain distortion – these include (39), its relaxation in (42), and the analogous formulations in Sections V-B and V-C. When this is not done, an estimate for \mathbf{C}_x can be computed from a PSD estimate as $\hat{\mathbf{C}}_x = \mathbf{V} \text{diag}(\hat{\mathbf{p}}_{\text{pg}}) \mathbf{V}^H$.

VI. NUMERICAL EXPERIMENTS

The implementation and associated benefits of the proposed schemes are illustrated through three test cases (TC). TC1 and TC2 rely on synthetic graphs to evaluate the performance of nonparametric and parametric PSD estimation methods. TC3 illustrates how the concepts and tools of stationary graph processes can be leveraged in practical applications involving real-world signals and graphs. Unless otherwise stated, the results shown are averages across 100 realizations of the particular experiment.

TC1. Nonparametric methods: We first evaluate the estimation performance of the average periodogram [cf. (16) and (21)] as a function of R , the number of realizations observed. Consider a baseline Erdős-Rényi (ER) graph with $N = 100$ nodes and edge probability $p = 0.05$ [24]. We define its adjacency matrix as the shift and generate signals by filtering white Gaussian noise with a filter of degree 3. In this case, the normalized MSE equals $2/R$ [cf. (21)] as can be corroborated in Fig. 1a (top). To further confirm this result, we consider three variations of the baseline setting: i) a smaller ER graph with $N = 10$ nodes and $p = 0.3$, ii) a small-world graph [25] obtained by rewiring with probability $q = 0.1$ the edges in a regular graph of the same size as the baseline ER, and iii) filtering the noise with a longer filter of degree 6. As expected, Fig. 1a (top) indicates that the normalized MSE is independent of these variations. We then repeat the above setting but for signals generated as filtered versions of *non-Gaussian* white noise drawn from a uniform distribution of unit variance. Even though the MSE expression in (21) was shown for Gaussian signals, we observe that in the tested non-Gaussian setup the evolution of the MSE with R is the same; see Fig. 1a (bottom).

The second experiment evaluates the performance of window-based estimators. To assess the role of locality in the window design, we consider graphs generated via a stochastic block model [26] with $N = 100$ nodes and 10 communities with 10 nodes each. The edge probability within each community is $p = 0.9$, while the probability for edges across communities is $q = 0.1$. We design rectangular non-overlapping windows where the nodes are chosen following two strategies: i) $M = 10$ local windows corresponding to the 10 communities, and ii) $M = 10$ windows of equal size with randomly chosen nodes. We use the Laplacian as shift and generate the graph process using a filter with $L = 2$ coefficients. Fig. 1b shows the theoretical and empirical normalized MSE for the two designs as well as that of the periodogram for a single window. We first observe that the periodogram has no bias and that the theoretical and empirical errors coincide for the three cases, validating the results in Propositions 3 and 5, respectively. Moreover, we corroborate that windowing contributes to reduce the variance of the estimator. Fig. 1b also illustrates that windows that leverage the community structure of the graph yield a better estimation performance. To gain insights on the latter observation, we now consider a small-world graph of size $N = 100$ obtained by rewiring with probability

$q = 0.05$ a regular graph where each node has 10 neighbors. Both local and random windows are considered, where the local windows are obtained by applying complete linkage clustering [27] to a metric space given by the shortest path distances between nodes. In order to obtain increasing number of windows M , we cut the output dendrogram at smaller resolutions [28]. The random windows are designed to have the same sizes as the local ones. The windows are tested for graph processes generated by two filters of different degrees: i) $L = 2$, so that nodes that are more than 2 hops away are not correlated (cf. Property 2); and ii) $L = 10$, which is greater than the graph diameter, inducing correlations between every pair of nodes. In Fig. 1c we illustrate the performance of local and random windows in these two settings as a function of M . We first observe that as M increases, the error first decreases until it reaches an optimal point and then starts to increase. Intuitively, this indicates that at first the reduction in variance outweighs the increase in bias but, after some point, the marginal variance reduction when adding one extra window does not compensate the detrimental effect on the bias. Moreover, it can be seen that local windows outperform the random ones, especially for localized graph processes ($L = 2$). These findings are consistent for other types of graphs, although for graphs with a weaker clustered structure the benefits of local windows are less conspicuous.

The last experiment evaluates the performance of filter-bank estimators, where two types of bandpass filters are considered. The first type designs the k -th filter as an ideal bandpass filter with unit response for the k -th frequency and the B frequencies closest to it, and zero otherwise [cf. (32)]. More precisely, being λ_k the eigenvalue associated to the k -th frequency, we consider the closest frequencies as those with eigenvalues $\lambda_{k'}$ minimizing $|\lambda_k - \lambda_{k'}|$. The second filter bank type designs the filters using the FIR approach in (36). To run the experiments we consider the adjacency matrix of an ER graph with $N = 100$ and $p = 0.05$, and generate signals by filtering white noise. Fig. 1d shows the MSE performance of both approaches as a function of the degree of the filter that generates the process as well as the nonparametric periodogram estimation. We consider two ideal bandpass filters with $B = 3$ and $B = 7$ and two FIR bandpass filters with $L = 5$ and $L = 10$. Fig. 1d indicates that filter banks contribute to reduce the MSE compared to the periodogram. Moreover, the ideal bandpass filter outperforms the FIR design and, within each type, filters with larger bandwidth ($B = 7$ and $L = 5$) tend to perform better. The reason being that the periodogram-based estimation for a single observation is very noisy, thus, it benefits from the averaging effect of larger bandwidths.

TC2. Parametric methods: We first illustrate the parametric estimation of a MA process. Consider the Laplacian of an ER graph with $N = 100$ and $p = 0.2$ and processes generated by an FIR filter of length L whose coefficients β are selected randomly. The performance of a periodogram is contrasted with that of two parametric approaches: i) an algorithm that estimates the L values in β by minimizing (40) via phase-retrieval [22]; and ii) a least squares algorithm that estimates the $2L - 1$ values in γ by minimizing (41). The results are shown in Fig. 1e (solid lines). It can be observed that both parametric methods outperform the periodogram since they leverage the FIR structure of the generating filter. Moreover, this difference is largest for smaller values of the degree, since in these cases a few parameters are sufficient to completely characterize the filter of interest. Furthermore, we also test our schemes for a model mismatch (MM) scenario where the MA schemes assume that the order of the process is $L + 2$ instead of L (dashed lines in Fig. 1e).

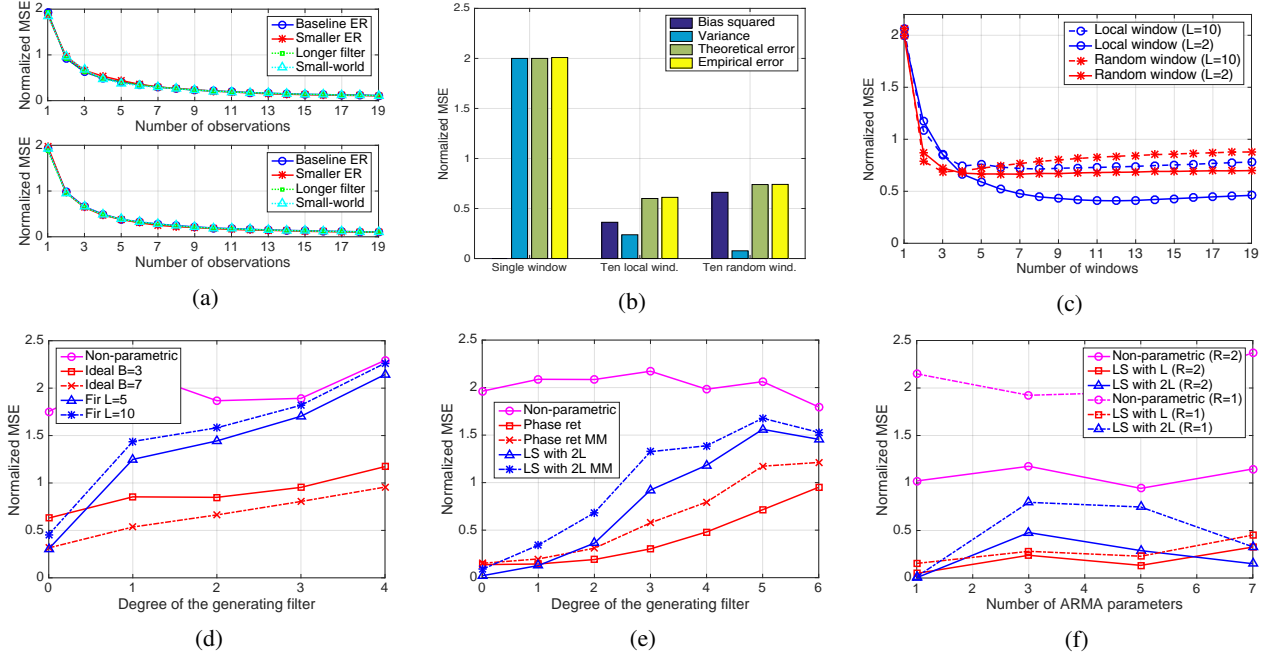


Fig. 1: Normalized MSE (NMSE) for different PSD estimation schemes. (a) Top: NMSE for the periodogram using Gaussian inputs. Bottom: NMSE for non-Gaussian inputs. (b) Theoretical and empirical NMSE for different window strategies. (c) NMSE as a function of the number of windows for local and random windows. (d) NMSE for filter banks as a function of the degree of the generating filter. (e) NMSE for MA parametric estimation as a function of the degree of the generating filter. (f) NMSE for different ARMA parametric estimators based on $R = 1$ and $R = 2$ signal realizations.

The results show that, although the model mismatch degrades the performance, the parametric estimates are still superior to the periodogram.

The second experiment considers ARMA processes with L poles and L zeros. The coefficients are drawn randomly from a uniform distribution with support $[0, 1]$ and the shift is selected as in the previous experiment. We compare the periodogram estimation with two schemes: i) a least squares (LS) algorithm that estimates $2L$ coefficients, i.e., the counterpart of (41) for the problem in (53); and ii) a LS algorithm that estimates L nonnegative coefficients, i.e., the counterpart of (43) for (53). Note that the latter is computationally tractable because both the eigenvalues of the shift and the coefficients of the filters are nonnegative. The algorithms are tested in two scenarios, with one and two signal realizations available, respectively. Fig. 1f shows that the parametric methods attain smaller MSEs compared to the periodogram. Moreover, note that while increasing the number of observations reduces the MSE for all tested schemes, the reduction is more pronounced for nonparametric schemes. This is a manifestation of the fact that parametric approaches tend to be more robust to noisy or imperfect observations.

TC3. Real-world graphs and signals: We now demonstrate how the tools developed in this paper can be useful in practice through two real-world experiments. The first one deals with source identification in opinion formation dynamics. We consider the social network of Zachary’s karate club [29] represented by a graph \mathcal{G} consisting of 34 nodes or members of the club and 78 undirected edges symbolizing friendships among members. Denoting by \mathbf{L} the 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. We assume that an opinion profile \mathbf{x} is generated by the diffusion through the network of an initially sparse (rumor) signal \mathbf{w} . More precisely, we model \mathbf{w} as a white process such that $w_i = 1$ with probability 0.05, $w_i = -1$ with

probability 0.05, and $w_i = 0$ otherwise. We are given a set $\{\mathbf{x}_r\}_{r=1}^R$ of opinion profiles generated from different sources $\{\mathbf{w}_r\}_{r=1}^R$ diffused through a filter of unknown nonnegative coefficients β . Our goal is to identify the sources of the different opinions, i.e., the nonzero entries of \mathbf{w}_r for every r . Our approach proceeds in two phases. First, we use $\{\mathbf{x}_r\}_{r=1}^R$ to identify the parameters β of the generating filter. We do this by solving (43) via least squares. Second, given the set of coefficients β , we have that $\mathbf{x}_r = \sum_{l=0}^{L-1} \beta_l \mathbf{S}^l \mathbf{w}_r$. Thus, we estimate the sources \mathbf{w}_r by solving a ℓ_1 -regularized least squares problem to promote sparsity in the input. In Fig. 2a (blue) we show the proportion of sources misidentified as a function of the number of observations R . As R increases, the estimates of the parameters β become more reliable, thus leading to a higher success rate. Finally, we consider cases where the observations are noisy. Formally, we define noisy observations $\hat{\mathbf{x}}_r$ by perturbing the original ones $\hat{\mathbf{x}}_r = \mathbf{x}_r + \sigma \mathbf{z} \circ \mathbf{x}_r$ where σ denotes the magnitude of the perturbation and \mathbf{z} is a vector with elements drawn from a standard normal distribution. As expected, higher levels of noise have detrimental effects on the recovery of sources. Nevertheless, for moderate noise levels ($\sigma = 0.1$) a performance comparable to the noiseless case can be achieved when observing 20 signals or more.

For our last experiment, we consider a set of 100 grayscale images $\{\mathbf{x}_i\}_{i=1}^{100}$ corresponding to 10 face pictures of 10 different people². Since spectral representations of images can be used for successful face recognition [30], our goal is to use PSD estimation to generate consistent spectral signatures for different faces of the same person. Formally, every image is represented by a vector $\mathbf{x}_i \in \mathbb{R}^{10304}$ where the entries correspond to grayscale values of pixels, normalized to have zero mean. We consider the images \mathbf{x}_i to be realizations of a graph process which, by definition, is stationary on the shift given by its covariance, here approximated by the sample covariance $\mathbf{S} = \hat{\mathbf{C}}_x = \mathbf{V} \mathbf{\Lambda}_c \mathbf{V}^H$. Moreover, denote by \mathcal{I}_j the set of images corresponding to faces of person j and consider the sample covariance $\hat{\mathbf{C}}_x^{(j)} = \mathbf{V}_x^{(j)} \mathbf{\Lambda}_c^{(j)} \mathbf{V}_x^{(j)}$ of the

²<http://www.cl.cam.ac.uk/research/dtg/attarchive/facedatabase.html>

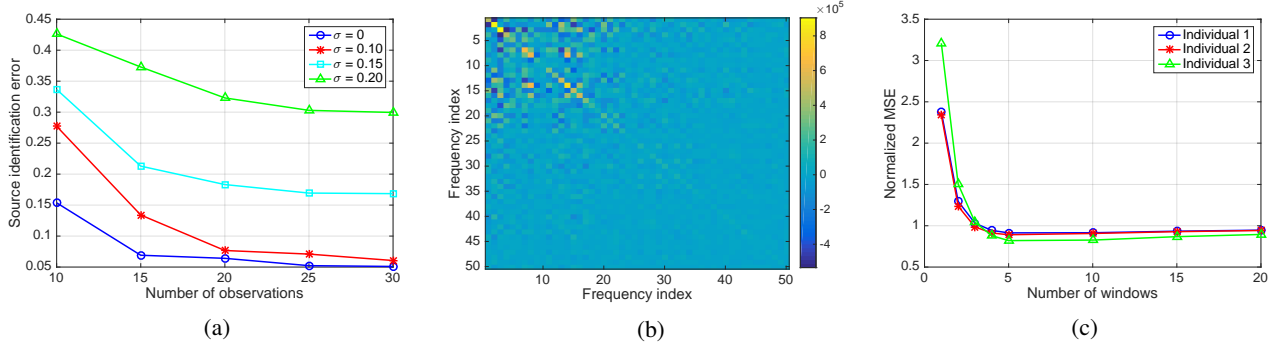


Fig. 2: (a) Error in the identification of sources in opinion formation dynamics as a function of the number of observed opinions and parametrized by the noise level σ . (b) Diagonalization of the sample covariance of the images of an individual with the basis of the ensemble sample covariance. (c) Normalized MSE for the windowed average periodogram as a function of the number of windows for individual face processes.

subset $\{\mathbf{x}_i\}_{i \in \mathcal{I}_j}$. Matrix $\hat{\mathbf{C}}_x^{(j)}$ is perfectly diagonalized by $\mathbf{V}_x^{(j)}$ but only approximately diagonalized by the principal component basis \mathbf{V} . To confirm this in Fig. 2b we show a block of the matrix $\hat{\mathbf{\Lambda}}_1 = \mathbf{V}^H \hat{\mathbf{C}}_x^{(1)} \mathbf{V}$ for the first individual. The diagonally dominant structure indicates that the process generating face images of subject j is approximately stationary in \mathbf{S} , motivating looking at the (squared) frequency coefficients $\hat{\mathbf{p}}_j = \text{diag}(\hat{\mathbf{\Lambda}}_j)$. Given a new unobserved image \mathbf{x}_i of individual j , our goal is to implement the windowed average periodogram with random windows of equal size to improve the estimate of $\hat{\mathbf{p}}_j$ from the single new realization \mathbf{x}_i . In Fig. 2c we plot the estimation error as a function of the number of windows for three different individuals $j \in \{1, 2, 3\}$ and observe that using multiple windows enhances the PSD estimation. Interestingly, even though the process associated with the images of a given individual is only approximately stationary, the MSE gains with random windows are similar to those in bonafide stationary processes (cf. Fig. 1c).

VII. CONCLUSION

Three equivalent ways of generalizing the notion of stationarity to graph processes were proposed. Given that stationary processes were shown to be diagonalized by the Graph Fourier basis, the concept of power spectral density for graph processes was introduced and several estimation methods were studied in detail. We first generalized nonparametric methods including periodograms, window-based average periodograms, and filter banks. Their performance was analyzed, comparisons with the traditional time domain schemes were established and open issues, such as how to group nodes and frequencies in a graph, were identified. We then focused on parametric estimation, where we examined MA, AR, and ARMA processes. We not only showed that those processes are useful to model linear diffusion dynamics, but also identified particular scenarios where the optimal parameter estimation problem is tractable.

APPENDICES

A. Proof of Proposition 3

To prove that the estimate is unbiased, we use the equivalence result in Proposition 2 combined with (17) to conclude that $\mathbb{E}[\hat{\mathbf{p}}_{\text{pg}}] = \text{diag}[\mathbf{V}^H R^{-1} (\sum_{r=1}^R \mathbb{E}[\mathbf{x}_r \mathbf{x}_r^H]) \mathbf{V}] = \text{diag}[\mathbf{V}^H R^{-1} R \mathbf{C}_x \mathbf{V}] = \mathbf{p}$. Hence, $\mathbf{b}_{\text{pg}} = \mathbb{E}[\hat{\mathbf{p}}_{\text{pg}}] - \mathbf{p} = \mathbf{0}$.

To compute the covariance, start by writing $\Sigma_{\text{pg}} = \mathbb{E}[\hat{\mathbf{p}}_{\text{pg}} \hat{\mathbf{p}}_{\text{pg}}^H] - \mathbf{p} \mathbf{p}^H$. We may expand the leftmost term as

$$\mathbb{E}[\hat{\mathbf{p}}_{\text{pg}} \hat{\mathbf{p}}_{\text{pg}}^H] = \mathbb{E}[\text{diag}(\mathbf{V}^H \hat{\mathbf{C}}_x \mathbf{V}) \text{diag}(\mathbf{V}^H \hat{\mathbf{C}}_x \mathbf{V})^H] \quad (54)$$

$$= \frac{1}{R^2} \sum_{r=1}^R \sum_{r'=1}^R \mathbb{E}[\text{diag}(\mathbf{V}^H \mathbf{x}_r \mathbf{x}_r^H \mathbf{V}) \text{diag}(\mathbf{V}^H \mathbf{x}_{r'} \mathbf{x}_{r'}^H \mathbf{V})^H]. \quad (55)$$

We may split the above summation into the terms where $r \neq r'$ and those where $r = r'$. For the former case, since \mathbf{x}_r is assumed to be independent from $\mathbf{x}_{r'}$, we have that

$$\mathbb{E}[\text{diag}(\mathbf{V}^H \mathbf{x}_r \mathbf{x}_r^H \mathbf{V})] \mathbb{E}[\text{diag}(\mathbf{V}^H \mathbf{x}_{r'} \mathbf{x}_{r'}^H \mathbf{V})^H] = \mathbf{p} \mathbf{p}^H. \quad (56)$$

By contrast, for the case where $r = r'$ we undertake an elementwise analysis of the elements in the expected value in (55). Notice that if we denote by \mathbf{v}_i the i th column of \mathbf{V} we have that $[\text{diag}(\mathbf{V}^H \mathbf{x}_r \mathbf{x}_r^H \mathbf{V})]_i = \mathbf{v}_i^H \mathbf{x}_r \mathbf{x}_r^H \mathbf{v}_i$. Replacing this expression in (55), setting $r = r'$, and using the formula for the quartic form of a Gaussian, see e.g. [31, pp. 43], we obtain that

$$\begin{aligned} & \mathbb{E}[\text{diag}(\mathbf{V}^H \mathbf{x}_r \mathbf{x}_r^H \mathbf{V}) \text{diag}(\mathbf{V}^H \mathbf{x}_r \mathbf{x}_r^H \mathbf{V})^H]_{ij} \quad (57) \\ &= \mathbb{E}[\mathbf{v}_i^H \mathbf{x}_r \mathbf{x}_r^H \mathbf{v}_i \mathbf{v}_j^H \mathbf{x}_r \mathbf{x}_r^H \mathbf{v}_j] = \mathbf{v}_i^H \mathbb{E}[\mathbf{x}_r \mathbf{x}_r^H \mathbf{v}_i \mathbf{v}_j^H \mathbf{x}_r \mathbf{x}_r^H] \mathbf{v}_j \\ &= p_i p_j + \mathbf{v}_i^H \mathbf{C}_x \mathbf{v}_j^* \mathbf{v}_i^T \mathbf{C}_x \mathbf{v}_j + \mathbf{v}_j^H \mathbf{C}_x \mathbf{v}_i \mathbf{v}_i^H \mathbf{C}_x \mathbf{v}_j. \end{aligned}$$

When \mathbf{S} is symmetric, hence \mathbf{V} is real, the above expression can be further simplified to obtain

$$\mathbb{E}[\text{diag}(\mathbf{V}^H \mathbf{x}_r \mathbf{x}_r^H \mathbf{V}) \text{diag}(\mathbf{V}^H \mathbf{x}_r \mathbf{x}_r^H \mathbf{V})^H] = 2 \text{diag}^2(\mathbf{p}) + \mathbf{p} \mathbf{p}^H. \quad (58)$$

Upon substituting (56) and (58) into (55), the result follows.

B. Proof of Proposition 5

From the definition of $\hat{\mathbf{p}}_{\mathcal{W}}$ in (25), it follows that

$$\hat{\mathbf{p}}_{\mathcal{W}} = \frac{1}{M} \sum_{m=1}^M \text{diag}(\mathbf{V}^H \text{diag}(\mathbf{w}_m) \mathbf{V} \tilde{\mathbf{x}} \tilde{\mathbf{x}}^H \mathbf{V}^H \text{diag}(\mathbf{w}_m^*) \mathbf{V}). \quad (59)$$

Thus, using the definition of $\tilde{\mathbf{W}}_m$, we may write

$$\mathbb{E}[\hat{\mathbf{p}}_{\mathcal{W}}] = \frac{1}{M} \sum_{m=1}^M \text{diag}(\tilde{\mathbf{W}}_m \mathbb{E}[\tilde{\mathbf{x}} \tilde{\mathbf{x}}^H] \tilde{\mathbf{W}}_m^H). \quad (60)$$

Leveraging the fact that $\mathbb{E}[\tilde{\mathbf{x}} \tilde{\mathbf{x}}^H] = \text{diag}(\mathbf{p})$ is diagonal and recalling that $\tilde{\mathbf{W}}_{mm} = \tilde{\mathbf{W}}_m \circ \tilde{\mathbf{W}}_m^*$, the result in (27) follows.

In order to show (28), notice that only the diagonal elements of $\Sigma_{\mathcal{W}}$ are needed. Each of them can be found as

$$[\Sigma_{\mathcal{W}}]_{k,k} = \mathbb{E}[[\hat{\mathbf{p}}_{\mathcal{W}}]_k [\hat{\mathbf{p}}_{\mathcal{W}}]_k] - \mathbb{E}[[\hat{\mathbf{p}}_{\mathcal{W}}]_k]^2. \quad (61)$$

Rewriting $\hat{\mathbf{p}}_{\mathcal{W}}$ as a sum across the M windows, it holds that

$$\begin{aligned} \mathbb{E}[[\hat{\mathbf{p}}_{\mathcal{W}}]_k [\hat{\mathbf{p}}_{\mathcal{W}}]_k] &= \mathbb{E}\left[\frac{1}{M} \sum_{m=1}^M [|\tilde{\mathbf{W}}_m \tilde{\mathbf{x}}|^2]_k \frac{1}{M} \sum_{m'=1}^M [|\tilde{\mathbf{W}}_{m'} \tilde{\mathbf{x}}|^2]_k\right] \\ &= \frac{1}{M^2} \sum_{m=1, m'=1}^M \mathbb{E}[[|\tilde{\mathbf{W}}_m \tilde{\mathbf{x}}|^2]_k [|\tilde{\mathbf{W}}_{m'} \tilde{\mathbf{x}}|^2]_k]. \quad (62) \end{aligned}$$

Denoting the k th row of $\tilde{\mathbf{W}}_m$ by $\tilde{\mathbf{w}}_{k|m}^T$, each of the $[|\hat{\mathbf{W}}_m \tilde{\mathbf{x}}|^2]_k$ above can be written as $\tilde{\mathbf{w}}_{k|m}^T \tilde{\mathbf{x}} \tilde{\mathbf{x}}^H \tilde{\mathbf{w}}_{k|m}^*$. Consequently, we may write

$$\begin{aligned} \mathbb{E} \left[[|\hat{\mathbf{W}}_m \tilde{\mathbf{x}}|^2]_k [|\hat{\mathbf{W}}_{m'} \tilde{\mathbf{x}}|^2]_k \right] &= \mathbb{E} \left[\tilde{\mathbf{w}}_{k|m}^T \tilde{\mathbf{x}} \tilde{\mathbf{x}}^H \tilde{\mathbf{w}}_{k|m}^* \tilde{\mathbf{w}}_{k|m'}^T \tilde{\mathbf{x}} \tilde{\mathbf{x}}^H \tilde{\mathbf{w}}_{k|m'}^* \right] \\ &= \tilde{\mathbf{w}}_{k|m}^T \mathbb{E} \left[\tilde{\mathbf{x}} \tilde{\mathbf{x}}^H \tilde{\mathbf{w}}_{k|m}^* \tilde{\mathbf{w}}_{k|m'}^T \tilde{\mathbf{x}} \tilde{\mathbf{x}}^H \right] \tilde{\mathbf{w}}_{k|m'}^*, \end{aligned} \quad (63)$$

where the middle factor is a quartic form of a Gaussian with covariance $\text{diag}(\mathbf{p})$ (cf. Property 3). Solving this fourth moment, see e.g. [31, pp. 43], it follows that

$$\begin{aligned} \mathbb{E} \left[[|\hat{\mathbf{W}}_m \tilde{\mathbf{x}}|^2]_k [|\hat{\mathbf{W}}_{m'} \tilde{\mathbf{x}}|^2]_k \right] &= \\ &|\tilde{\mathbf{w}}_{k|m}^T \mathbf{p} \tilde{\mathbf{w}}_{k|m'}^T \mathbf{p}|^2 + |\tilde{\mathbf{w}}_{k|m}^T \text{diag}(\mathbf{p}) \tilde{\mathbf{w}}_{k|m'}^*|^2 \\ &+ \tilde{\mathbf{w}}_{k|m}^T \text{diag}(\mathbf{p}) \mathbf{V}^H \mathbf{V}^* \tilde{\mathbf{w}}_{k|m'}^* \tilde{\mathbf{w}}_{k|m}^H \mathbf{V}^T \mathbf{V} \text{diag}(\mathbf{p}) \tilde{\mathbf{w}}_{k|m'}^* \end{aligned} \quad (64)$$

When \mathbf{S} is symmetric, hence \mathbf{V} is real, the third summand in (64) is equal to the second one. Thus, substituting first (64) into (62) and then, (62) into (61) yields

$$[\Sigma_{\mathcal{W}}]_{k,k} = \frac{2}{M^2} \sum_{m=1, m'=1}^M |\tilde{\mathbf{w}}_{k|m}^T \text{diag}(\mathbf{p}) \tilde{\mathbf{w}}_{k|m'}^*|^2. \quad (65)$$

Since $\tilde{\mathbf{W}}_{mm'} = \tilde{\mathbf{W}}_m \circ \tilde{\mathbf{W}}_{m'}^*$, it follows that $|\tilde{\mathbf{w}}_{k|m}^T \text{diag}(\mathbf{p}) \tilde{\mathbf{w}}_{k|m'}^*| = [|\tilde{\mathbf{W}}_{mm'} \mathbf{p}|]_k$, thus

$$[\Sigma_{\mathcal{W}}]_{k,k} = \frac{2}{M^2} \sum_{m=1, m'=1}^M [|\tilde{\mathbf{W}}_{mm'} \mathbf{p}|]_k^2. \quad (66)$$

Finally, using (66) to write $\text{tr}[\Sigma_{\mathcal{W}}] = \sum_{k=1}^N [\Sigma_{\mathcal{W}}]_{k,k}$, we obtain (28) and the proof concludes.

C. Proof of Proposition 7

Rewriting the norm in (32) as the trace of the corresponding outer product we get that

$$\mathbb{E} [\hat{p}_{\tilde{\mathbf{q}}_k}] = \text{tr}[\text{diag}(\tilde{\mathbf{q}}_k) \mathbb{E} [\tilde{\mathbf{x}} \tilde{\mathbf{x}}^H] \text{diag}(\tilde{\mathbf{q}}_k^*)]. \quad (67)$$

Expression (33) follows from replacing $\mathbb{E} [\tilde{\mathbf{x}} \tilde{\mathbf{x}}^H]$ by $\text{diag}(\mathbf{p})$ and noting that the trace of the product of diagonal matrices equals the sum of the entrywise products of the diagonals.

To prove (34), we first find $\mathbb{E} [\hat{p}_{\tilde{\mathbf{q}}_k} \hat{p}_{\tilde{\mathbf{q}}_k}]$. Since $\hat{p}_{\tilde{\mathbf{q}}_k} = \text{tr}[\text{diag}(\tilde{\mathbf{q}}_k) \tilde{\mathbf{x}} \tilde{\mathbf{x}}^H \text{diag}(\tilde{\mathbf{q}}_k)^H] = \text{tr}[\tilde{\mathbf{x}}^H \text{diag}(|\tilde{\mathbf{q}}_k|^2) \tilde{\mathbf{x}}]$ then, since the argument of the trace is a scalar, we can write

$$\begin{aligned} \mathbb{E} [\hat{p}_{\tilde{\mathbf{q}}_k} \hat{p}_{\tilde{\mathbf{q}}_k}] &= \mathbb{E} [\text{tr}[\tilde{\mathbf{x}}^H \text{diag}(|\tilde{\mathbf{q}}_k|^2) \tilde{\mathbf{x}} \tilde{\mathbf{x}}^H \text{diag}(|\tilde{\mathbf{q}}_k|^2) \tilde{\mathbf{x}}]] \\ &= \text{tr}[\mathbb{E} [\tilde{\mathbf{x}} \tilde{\mathbf{x}}^H \text{diag}(|\tilde{\mathbf{q}}_k|^2) \tilde{\mathbf{x}} \tilde{\mathbf{x}}^H] \text{diag}(|\tilde{\mathbf{q}}_k|^2)], \end{aligned} \quad (68)$$

where we have a quartic form of a Gaussian. From the expression of this quartic form, see e.g. [31, pp. 43], we obtain

$$\begin{aligned} \mathbb{E} [\hat{p}_{\tilde{\mathbf{q}}_k} \hat{p}_{\tilde{\mathbf{q}}_k}] &= \|\text{diag}(|\tilde{\mathbf{q}}_k|^2) \mathbf{p}\|_2^2 + ((|\tilde{\mathbf{q}}_k|^2)^T \mathbf{p})^2 \\ &+ \text{tr}[\text{diag}(\mathbf{p}) \mathbf{V}^H \mathbf{V}^* \text{diag}(|\tilde{\mathbf{q}}_k|^2) \mathbf{V}^T \mathbf{V} \text{diag}(\mathbf{p}) \text{diag}(|\tilde{\mathbf{q}}_k|^2)]. \end{aligned} \quad (69)$$

When \mathbf{S} is symmetric, hence \mathbf{V} is real, the trace in (69) is equal $\|\text{diag}(|\tilde{\mathbf{q}}_k|^2) \mathbf{p}\|_2^2$ and, since $\text{var}[\hat{p}_{\tilde{\mathbf{q}}_k}] = \mathbb{E} [\hat{p}_{\tilde{\mathbf{q}}_k} \hat{p}_{\tilde{\mathbf{q}}_k}] - \mathbb{E} [\hat{p}_{\tilde{\mathbf{q}}_k}]^2$, using (69) and (33), the expression (34) follows.

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