Nonparametric Identification of Kronecker Networks

Mattia Zorzi

Dipartimento di Ingegneria dell’Informazione, Università degli studi di Padova, via Gradenigo 6/B, 35131 Padova, Italy

Abstract

We address the problem to estimate a dynamic network whose edges describe Granger causality relations and whose topology has a Kronecker structure. Such a structure arises in many real networks and allows to understand the organization of complex networks. We proposed a kernel-based PEM method to learn such networks. Numerical examples show the effectiveness of the proposed method.

Key words: Linear system identification; Sparsity inducing priors; Kernel-based methods; Gaussian processes.

1 Introduction

In many applications we collect high dimensional data which describe systems having a wide amount of variables. Thus, there is the need to understand how those variables are “connected each other”, i.e. we also need to learn from data the topology of the graphical model representing those interactions. It is worth noting that a graphical model is meaningful only if it is not complete, i.e. it has some degree of sparsity in terms of edges. It is clear that the network identification paradigm depends on the definition of “interactions”. The latter can describe conditional dependence relations between the stochastic processes characterizing the variables of the system and whose resulting network is undirected (Avventi et al., 2013; Zorzi & Sepulchre, 2016; Ciccone et al., 2018; Zorzi, 2019). In the case of directed graphical models there is an edge from node $h$ to node $j$ if we need the process at node $h$ in order to reconstruct the process at node $j$. It is worth noting that such reconstruction can be both acausal (Materassi & Innocenti, 2010; Materassi & Salapaka, 2020; Veedu et al., 2020; Sepehr & Materassi, 2019; Doddi et al., 2020) and causal (Chiuso & Pillonetto, 2012; Zorzi & Chiuso, 2015). In the latter case, we say that edges describes Granger causality relations (Granger, 1969). Finally, it is worth noting that a closely related topic is the problem to learn modules of a network only using data from neighbors nodes, see Ramaswamy et al., 2021; Ramaswamy & Vandenhof, 2020.

In this paper we focus our attention on Kronecker networks whose topology possesses some properties emerging in many real networks, e.g. heavy-tailed degree distribution, small diameter, see Leskovec et al., 2010 for more details. Such a structure is also useful to understand the organization of complex networks (Leskovec, 2009). Tsiligkaridis et al., (2013) consider a network identification problem whose Kronecker structure is not only imposed on the topology of the network but also on the parameters of the model. The latter constraint, however, could be restrictive in some applications, e.g. for spatio-temporal MEG/EEG modeling (Bijma et al., 2005). A possible way to overcome this restriction is to impose the structure “sum of Kronecker products” on the parameters of the model (Sinquin & Verhaegen, 2019; Tsiligkaridis & Hero, 2013) at the price that we loose a meaningful definition of interaction, i.e. the resulting network is fully connected. In Zorzi (2020a, 2018), instead, it has been considered the problem to learn undirected dynamic networks having the Kronecker structure on the topology, but not on the parameters of the model. Such a framework, however, has not been extended to the case of directed dynamic networks yet.

The present paper considers the problem to learn directed dynamic networks whose edges characterize Granger causality relations and whose topology has a Kronecker structure.

A well established system identification paradigm is the so called prediction error method (PEM), see Ljung (1999); Söderström & Stoica (1989). Within this framework, candidate models are described in fixed parametric model structures, e.g. ARMAX. Thus, the main
difficulty is the correct choice of the best model structure which is usually performed by AIC and BIC criteria \cite{Akaike1974}. Kernel-based PEM methods aim to overcome this issue, see Pillonetto \& De Nicolao \cite{Pillonetto2010}; \cite{Chen2012}; \cite{Chiuso2016}; \cite{Mu2018}; \cite{Ljung2020}; \cite{Zorzi2020b}. More precisely, the candidate model, described through the predictor impulse responses, is searched in an infinite dimensional nonparametric model class; this is clearly an ill posed problem because we have a finite set of measured data. However, it can be made into a well posed one using a penalty term which favors models with specific features. In the Bayesian viewpoint, this is equivalent to introduce an a priori Gaussian probability (prior) on the unknown model. Hence, the prior distribution is characterized by the covariance (i.e. kernel) function.

The contribution of this paper is the introduction of a kernel-based PEM method to estimate Kronecker networks. The a priori information is that the impulse responses must be Bounded Input Bounded Output (BIBO) stable and the topology of the network respects the Kronecker structure. We derive the corresponding kernel functions by using the maximum entropy principle.

The kernel functions are characterized by the decay rate of the predictor impulse responses and by the number of edges in the network. These features are not known and characterized by the so-called hyperparameters. We estimate them by minimizing the negative log-marginal likelihood of the measured data, see \cite{Rasmussen2006}. Moreover, we show that the negative log-marginal likelihood automatically sets some hyperparameters in such a way that the a priori information is that the network has a sparse Kronecker structure. The degree of sparsity depends on the variance of the noise process affecting each node.

Finally, we provide some numerical experiments on synthetic data in order to test the effectiveness of the proposed method. Moreover, we use the latter for learning Granger causality relations in a bike sharing system.

The paper is organized as follows. In Section 2 we introduce the Kronecker model corresponding to a network characterized in terms of Granger causality relations. In Section 3 we introduce the Kronecker network identification problem. In Section 4 we derive the maximum entropy kernels inducing BIBO stability and a Kronecker structure for the topology of the network, while Section 5 is devoted to the estimation of the hyperparameters. In Section 6 we present some numerical examples. Finally, we draw the conclusions in Section 7.

### Notation

\(\mathbb{N}\) is the set of natural numbers. Given a finite set \(\mathcal{I}\), \(|\mathcal{I}|\) denotes its cardinality. \(\mathbb{E}[\cdot]\) denotes the expectation, while \(\mathbb{E}[\cdot \mid \cdot]\) denotes the conditional mean. Given three (possibly infinite dimensional) random vectors \(a, b\) and \(c\) we say that \(a\) is conditionally independent of \(b\) given \(c\) if \(\mathbb{E}[a \mid b, c] = \mathbb{E}[a \mid c]\). Given \(G \in \mathbb{R}^{n \times p}\), \([G]_{i,j}\) denotes the entry of \(G\) in position \((i, j)\); \(G > 0\) \((G \geq 0)\) means that \(G\) is a positive (semi-)definite matrix. \(\mathcal{D}_p\) denotes the vector space of diagonal matrices of dimension \(p\). \(\ell_2^p(\mathbb{N})\) denotes the space of \(\mathbb{R}\)-valued infinite length sequences, which we think as infinite dimensional column vectors \(g := [g_1, g_2, \ldots, g_j, \ldots]^\top\), \(g_k \in \mathbb{R}, k \in \mathbb{N}\), such that \(\|g\|_2 := \sqrt{\sum_{k=1}^{\infty} |g_k|^2} < \infty\). \(\ell_2^{p \times n}(\mathbb{N})\) is the space of matrices of sequences in \(\ell_2^p(\mathbb{N})\)

\[
\Phi = \begin{pmatrix}
(\phi^{(11)})^\top & \ldots & (\phi^{(1n)})^\top \\
\vdots & \ddots & \vdots \\
(\phi^{(p1)})^\top & \ldots & (\phi^{(pn)})^\top
\end{pmatrix}
\]

where \(\phi^{(ij)} \in \ell_2^p(\mathbb{N}), i = 1 \ldots p\) and \(j = 1 \ldots n\). \(\ell_1(\mathbb{N})\) denotes the space of \(\mathbb{R}\)-valued infinite length sequences \(g\) such that \(\|g\|_1 := \sum_{k=1}^{\infty} |g_k| < \infty\). \(\ell_1^{p \times n}(\mathbb{N})\) is defined in similar way. \(\mathcal{S}_2^p(\mathbb{N})\) denotes the space of symmetric infinite dimensional matrices \(K\) such that \(\|K\|_2 := \sqrt{\sum_{i,j=1}^{p} |[K]_{i,j}|^2} < \infty\). \(\mathcal{S}_2^{p \times n}(\mathbb{N})\) is the space of symmetric infinite dimensional matrices

\[
K = \begin{bmatrix}
K^{[11]} & K^{[12]} & \ldots & K^{[1p]} \\
K^{[12]} & K^{[22]} & \ldots & K^{[2p]} \\
\vdots & \vdots & \ddots & \vdots \\
K^{[1p]} & K^{[2p]} & \ldots & K^{[pp]}
\end{bmatrix}
\]

where \(K^{[ij]} \in \mathcal{S}_2^p(\mathbb{N}), i, j = 1 \ldots p\). Given \(\Phi \in \ell_2^{p \times n}(\mathbb{N}), \Psi \in \ell_2^{m \times p}(\mathbb{N})\) and \(K \in \mathcal{S}_2^{p \times n}(\mathbb{N})\), the products \(\Phi \Psi^\top\) and \(\Phi K \Psi^\top\) are understood as \(p \times m\) matrices whose entries are limits of infinite sequences \(\{\text{jorgensen et al.}\ 2011\}\). Given \(g \in \ell_2^{1 \times n}(\mathbb{N})\) and \(K \in \mathcal{S}_2^{p \times n}(\mathbb{N})\), \(\|g\|_K^{-1} := g^\top K^{-1} g\). The definition is similar in the case that \(g\) and \(K\) have finite dimension. With some abuse of notation the symbol \(\mathcal{z}\) will denote both the complex variable as well as the shift operator \(z^{-1} y(t) := y(t - 1)\). Given a stochastic process \(y = \{y(t)\}_{t \in \mathbb{Z}}\), with some abuse of notation, \(y(t)\) will both denote a random vector and its sample value. From now on the time \(t\) will denote present and we shall talk about past and future with respect to time \(t\). With this convention in mind,

\[
y^{-} = \begin{bmatrix}
y(t-1)^\top \
y(t-2)^\top \\
\vdots
\end{bmatrix}^\top
\]

denotes the (infinite length) past data vector of \(y\) at time \(t\). We denote as \(\text{supp}(G(z))\) the support of the transfer matrix \(G(z)\), i.e. the entries of \(G(z)\) different from the null function correspond to entries equal to one in \(\text{supp}(G(z))\), otherwise the latter are equal to zero.
2 Kronencker Models

We consider the following nonparametric model

\[ y(t) = G(z)y(t) + F(z)u(t) + e(t) \]  

where \( y(t) \in \mathbb{R}^{p_1 \times p_2} \) is the output, \( u(t) \in \mathbb{R}^m \) is the input, \( e(t) \) is zero mean normalized white Gaussian noise (WGN) whose components have variance \( \sigma_k^2 \) with \( h = 1 \ldots p_1 \) and \( k = 1 \ldots p_2; G(z) = \sum_{i=1}^\infty G_i z^{-i} \) is a BIBO stable transfer matrix of dimension \( p_1 \times p_2 \times p_1 \times p_2 \), while \( F(z) = \sum_{i=1}^\infty F_i z^{-i} \) is a BIBO stable transfer matrix of dimension \( p_1 \times p_2 \times m \). The minimum variance one-step ahead predictor of \( y(t) \) based on the past data \( y^- \), denoted by \( \hat{y}(t|t-1) \), is given by

\[ \hat{y}(t|t-1) = G(z)y(t) + F(z)u(t). \]

Thus, \( e(t) \) is the one-step-ahead prediction error

\[ e(t) = y(t) - \hat{y}(t|t-1). \]

We assume that

\[ \text{supp}(G(z)) = E_1 \otimes E_2 \]

\[ \text{supp}(F(z)) = A_1 \otimes A_2 \]

where \( E_1 \), \( E_2 \), \( A_1 \) and \( A_2 \) denote the adjacency matrices of dimension \( p_1 \times p_1 \), \( p_2 \times p_2 \), \( p_1 \times 1 \) and \( p_2 \times m \), respectively. Let \( y_{hk} \) denote the scalar process of \( y \) in position \( (h-1)p_2 + k \) with \( h \in I_1 := \{1 \ldots p_1 \} \) and \( k \in I_2 := \{1 \ldots p_2 \} \). In a similar way, \( y^{-}_{hk} \) denotes the past of \( y_{hk} \) at time \( t \). Finally, \( u_i \) denotes the scalar component of \( u \) in position \( i \in I_u := \{1 \ldots m \} \) and \( u^-_{i} \) the \( i \)-th component of \( u^- \). Throughout the paper we assume that \( E_1, E_2, A_1 \) and \( A_2 \) are different from the null matrix.

It is possible to describe the structure of model (1)-(2) using a Bayesian network [Lauritzen 1996]. The nodes correspond to the scalar processes \( y_{hk} \)'s, with \( h \in I_1 \) and \( k \in I_2 \), while \( u_i \)'s, with \( i \in I_u \), represent exogenous variables affecting some nodes of the network. Then, the connections among the nodes obey the following rules:

- there is a directed link from node \( y_{jl} \) to node \( y_{hk} \) if

\[ \mathbb{E}[y_{hk}(t)|y^-, u^-] \neq \mathbb{E}[y_{hk}(t)|y^-_{jl}, \tilde{j} \neq j, \tilde{l} \neq l, u^-], \]

i.e. if \( y^*_{jl} \) is needed to predict \( y_{hk}(t) \) given \( u^- \) and \( y^-_{jl} \), for any \( \tilde{j} \in I_1 \setminus \{j\} \) and \( \tilde{l} \in I_2 \setminus \{l\} \); in this case, we shall say \( y_{jl} \) conditionally Granger causes \( y_{hk} \).

- there is a directed link from \( u_i \) to node \( y_{hk} \) if

\[ \mathbb{E}[y_{hk}(t)|y^-, u^-] \neq \mathbb{E}[y_{hk}(t)|y^-, u^-_{i}, \tilde{i} \neq i] \]

i.e. if \( u^-_{i} \) is needed to predict \( y_{hk}(t) \) given \( y^- \) and \( u^-_{i} \), for any \( i \in I_u \setminus \{i\} \); in this case, we shall say \( u_i \) conditionally Granger causes \( y_{hk} \).

In such a network we can recognize \( p_1 \) modules containing \( p_2 \) nodes and sharing the same topology described by \( E_2 \), while the interaction among these \( p_1 \) modules is described by \( E_1 \). Finally, \( A_1 \) describes the topology among the input and the modules; \( A_2 \) describes the topology among the input components and the nodes in a module which is the same in each module. These facts are formalized by the next proposition.

**Proposition 1** Consider model (1)-(2). Let \( y^*_i \) be the process obtained by stacking \( y_{hk} \) with \( k \in I_2 \) and \( y^*_{ik} \) be the process obtained by stacking \( h \in I_1 \). Then:

- \( y^*_{kj} \) conditionally Granger causes \( y^*_{ih} \) if and only if \( |E_1|_{h,j} = 1 \);
- \( y^*_{ik} \) conditionally Granger causes \( y^*_{ij} \) if and only if \( |E_2|_{k,l} = 1 \);
- \( u_i \) conditionally Granger causes \( y^*_i \) if and only if \( |A_1|_{h} = 1 \);
- \( u_i \) conditionally Granger causes \( y^*_{ik} \) if and only if \( |A_2|_{k,i} = 1 \).

**Proof.** We only prove the first claim, the proof of the others is similar. Let \( g^{[kk,jl]} \) \( k \in \{1, \ldots, N\} \) denote the impulse response in \( G(z) \) having input \( y_{jl} \) and output \( y_{hk} \). By (2), we have

\[ g^{[kk,jl]} \neq 0 \quad \text{for some } k, l \in I_2 \iff |E_1|_{h,j} = 1. \]

From (1) we have that

\[ y_{hk}(t) = \sum_{j \in I_1, l \in I_2} [G(z)]_{(h-1)p_2+k,(j-1)p_2+l} y_{jl}(t) + \sum_{i \in I_u} [F(z)]_{(h-1)p_2+k,i} u_i(t) + e_{hk}(t). \]

Thus, condition (3) is equivalent to

\[ \mathbb{E}[y_{hk}(t)|y^-, u^-] \neq \mathbb{E}[y_{hk}(t)|y^-_{jl}, \tilde{j} \neq j, \tilde{l} \neq l, u^-], \]

for some \( k, l \in I_2 \iff |E_1|_{h,j} = 1. \]

By (4), we have

\[ \mathbb{E}[y_{hk}(t)|u^-, y^-] \neq \mathbb{E}[y_{hk}(t)|y^-_{jl}, \tilde{j} \neq j, u^-], \]

for some \( k \in I_2 \iff |E_1|_{h,j} = 1. \)

Staking condition (5) for any \( k \in I_2 \), we obtain

\[ \mathbb{E}[y_i(t)|y^-] \neq \mathbb{E}[y_i(t)|y^-_{jl}, \tilde{j} \neq j] \iff |E_1|_{h,j} = 1. \]
we have

\[ G_s(q) = G_{s+p_1}(q), \quad \hat{F}_s(q) = \hat{F}_{s+p_1}(q) \]  

(7)

where \( q^{-1} \) is the shift operator corresponding to time variable \( s \), e.g. \( q^{-1}x(s) = x(s-1) \). Then, if we define

\[
\begin{align*}
y(t) &= [x((t-1)p_1 + 1) \ldots x(tp_1)]^\top \in \mathbb{R}^{p_1p_2} \\
u(t) &= [w((t-1)p_1 + 1) \ldots w(tp_1)]^\top \in \mathbb{R}^{p_1\tilde{m}} \\
e(t) &= [v((t-1)p_1 + 1) \ldots v(tp_1)]^\top \in \mathbb{R}^{p_1p_2},
\end{align*}
\]

we can write (6) as (1) where \( G(z) \) and \( F(z) \) are BIBO stable transfer matrices of dimension \( p_1p_2 \times p_1p_2 \) and \( p_1p_2 \times p_1\tilde{m} \), respectively. Moreover,

\[
G(z) = \begin{bmatrix}
G_{1,1}(z) & G_{1,2}(z) & \cdots & G_{1,p_1}(z) \\
\vdots & \ddots & \vdots & \vdots \\
G_{p_1,1}(z) & \cdots & \cdots & G_{p_1,p_1}(z)
\end{bmatrix}
\]

where \( G_{hj}(z) = \sum_{t=1}^{\infty} G_{hj,t}z^{-t} \) is a transfer matrix of dimension \( p_2 \times p_2 \) and \( z^{-1} \) is the shift operator corresponding to time variable \( t \); \( F(z) \) is defined in a similar way: it is composed by the transfer matrices \( F_{hj}(z) = \sum_{t=1}^{\infty} F_{hj,t}z^{-t}, h, j = 1 \ldots p_1 \), of dimension \( p_2 \times \tilde{m} \) and the blocks in the strictly lower block triangular part are multiplied by \( z \). In plain words, we have written (6) as (1) where \( G(z) \) and \( F(z) \) satisfy condition (2), then by Proposition 1 we have that \( E_2 \) is the matrix describing the conditional Granger causality relations among the components of \( x(s) \), while \( A_2 \) is the matrix describing the conditional Granger causality relations among the components of \( w(s) \) and \( x(s) \). Moreover, \( E_1 \) describes the conditional Granger causality relations of \( x(s) \) over the period \( 1 \ldots p_1 \), while \( A_1 \) describes the conditional Granger causality relations among \( x(s) \) and \( w(s) \) over the period \( 1 \ldots p_1 \). We conclude that (1) can be understood as a dynamic spatio-temporal model. In particular, if we take

\[
G(z) = \tilde{G}, \quad F(z) = \tilde{F},
\]

i.e. constant matrices, then (1) describes a spatio-temporal model without dynamic. The latter has been used to model magnetoencephalography (MEG) measurements for mapping brain activity [Bijma et al., 2005]: \( z(k,t) = [x_k((t-1)p_1 + 1) \ldots x_k(tp_1)] \) models the measurements corresponding to the \( k \)-th brain region during the \( t \)-th trial of length \( p_1 \), while

2.1 Motivating examples

Dynamic spatio-temporal modeling. Consider a nonparametric time-varying model of the form

\[ x(s) = G_s(q)x(s) + \hat{F}_s(q)w(s) + v(s), \quad s \in \mathbb{Z} \]  

(6)

where \( x(s) \in \mathbb{R}^{p_2} \) is the output, \( w(s) \in \mathbb{R}^{\tilde{m}} \) is the input, \( v(t) \) is normalized WGN and \( \{G_s(q), s \in \mathbb{Z}\}, \{\hat{F}_s(q), s \in \mathbb{Z}\} \) are sequences of BIBO stable (strictly causal) transfer matrices of dimension \( p_2 \times p_2 \) and \( p_2 \times \tilde{m} \), respectively.
s(k, t) = [w_k((t - 1)p_1 + 1) \ldots w_k(tp_1)]^T is the stimulus applied to the k-th region during the t-th trial. These trials are assumed independent. Moreover, they are identically distributed because in each trial the task performed by the patient is the same and the way that the patient reacts to the stimulus is assumed to be the same. In our framework we do not impose the restrictive condition (8) and thus we let dependence among the trials. This means that the proposed model takes into account the fact that the trials are taken in a sequential way, and thus the fact that the behaviors of the patient in the next trial can be influenced by the previous one. Finally, such a dynamic spatio-temporal model could be also used for modeling the conditional Granger causality relations among the number rental bikes in a bikesharing system and the corresponding weather information, see Section 6.2.

**Multi-task learning.** Consider a network composed by \( p_2 \in N \) agents (i.e. each node correspond to an agent). One agent is described by a model having an input and output. Our aim is to model such a network under \( p_1 \in N \) heterogeneous conditions (i.e. tasks). The k-th agent under the h-th task has input \( u_k(t) \) and output \( y_{h,k}(t) \). Then, we could model the network through the \( p_1 \) models:

\[
y_h^*(t) = G_h(z)y_h^* + F_h(z)u(t) + e_h(t), \quad h \in I_1
\]  

where \( y_h^*(t) \) has been defined in Proposition 1. A more flexible approach is to model all the models in (9) together in order to exploit commonalities and differences across the tasks, see [Yu et al.] (2009). More precisely, we consider the model

\[
y(t) = G(z)y(t) + F(z)u(t)
\]

where \( y(t) \) is obtained by stacking \( y_h^*(t) \) with \( h \in I_1 \). Under the assumption that (2) holds, and in view of Proposition 1, we have that \( E_1 \) describes the conditional Granger causality relations among the tasks; \( E_2 \) describes the conditional Granger causality relations among the agents in each task; \( A_1 \) describes the conditional Granger causality relations from the input to the tasks; \( A_2 \) describes the conditional Granger causality relations from the input components to the agents in each task.

### 3 Problem Formulation

Assume to measure the data \( \{y(t), u(t)\}_{t=0,\ldots,N} \) generated by (1). In this section, we address the problem of estimating \( G(z) \) and \( F(z) \) which admit the Kronecker product decomposition in (2).

The transfer matrices \( G(z), F(z) \) are parametrized in terms of their impulse response coefficients \( G_i \) and \( F_i \). In particular, defining \( g^{[hk, jl]} \in \ell_1(N) \) to be the impulse response from input \((j-1)p_2 + l \) to output \((h-1)p_2 + k \), we have:

\[
g^{[hk, jl]} = \left[ \begin{array}{c} G_1((h-1)p_2+k,(j-1)p_2+l) \\ \vdots \\ G_s((h-1)p_2+k,(j-1)p_2+l) \end{array} \right]^T,
\]

defining \( f^{[hk, i]} \in \ell_1(N) \) to be the impulse response from input \( u_i \) to output \((h-1)p_2 + k,i \), we have

\[
f^{[hk, i]} = \left[ \begin{array}{c} F_1((h-1)p_2+k,i) \\ \vdots \\ F_s((h-1)p_2+k,i) \end{array} \right]^T.
\]

The coefficient vectors \( \theta_g^\top \in \ell_1^{(1)1x(1)p_2^2}(N) \) and \( \theta_f^\top \in \ell_1^{(1)1xp_1p_2m}(N) \) are defined as follows:

\[
\theta_g^\top = \left[ (\theta_g^{[11]})^\top \ldots (\theta_g^{[p_2]})^\top \right] \ldots
\]

\[
\theta_f^\top = \left[ (\theta_f^{[11]})^\top \ldots (\theta_f^{[p_2]})^\top \right] \ldots
\]

where

\[
\theta_g^{[hk]} = \left[ (g^{[hk,11]})^\top \ldots (g^{[hk,1p_2]})^\top \right] \ldots
\]

\[
\theta_f^{[hk]} = \left[ (f^{[hk,1]})^\top \ldots (f^{[hk,m]})^\top \right].
\]

The measured data \( y(1) \ldots y(N) \) are stacked in the vector \( y^+ \) as follows

\[
y^+ = \left[ \begin{array}{c} y_{11}^+ \ldots y_{1p_2}^+ \\ \vdots \\ y_{p_11}^+ \ldots y_{p_1p_2}^+ \end{array} \right]^T
\]

where

\[
y_{hk}^+ = \left[ y_{hk}(N) \ldots y_{hk}(1) \right]^T.
\]

The vector \( e^+ \) is defined analogously. Let us also introduce the Toeplitz matrices \( \phi_{hk} \in \ell_2^{N\times1}(N), \psi_i \in \ell_2^{N\times1}(N) \):

\[
[\phi_{hk}]^\top_{sn} := y_{hk}(N-s-n+1)
\]

\[
[\psi_i]^\top_{sn} := u_i(N-s-n+1)
\]

with \( s = 1 \ldots N \) and \( n \in N \). Then, we define the regression matrices \( \Phi \in \ell_2^{p_1p_2N\times p_1^2p_2^2}(N) \) and
\(\Psi \in \ell_2^{p_2 N \times p_1 P_2 m}(N)\) as:
\[
\Phi = I_{p_1 P_2} \otimes \begin{bmatrix} \phi_{11} & \ldots & \phi_{1 p_2} & \ldots & \phi_{p_1 1} & \ldots & \phi_{p_1 p_2} \end{bmatrix} \\
\Psi = I_{p_1 P_2} \otimes \begin{bmatrix} \psi_1 & \ldots & \psi_m \end{bmatrix}
\]
so that, from (1) the vector \(y^+\) containing the measured output data satisfies the linear regression model
\[
y^+ = \Phi \theta_g + \Psi \theta_f + e^+ \tag{10}\]
and \(\hat{y}^+ := \Phi \hat{\theta}_g + \Psi \hat{\theta}_f\) is the one-step ahead predictor of \(y^+\). It is worth noting that to construct \(\Phi\) and \(\Psi\) we need the remote past of the output and the input which is not available. Thus, model (10) has to be approximated truncating \(\Phi\) and \(\Psi\) (and thus \(\theta_g\) and \(\theta_f\)). This is equivalent to impose zero initial conditions, which is a reasonable approximation given the decay, as a function of \(t\), of the coefficients \(G_t, F_t\) by the BIBO stability conditions.

**Remark 2** In the case that we consider the dynamic spatio-temporal model of Section 2.1, the regression matrices in (10) are different because the strictly lower block triangular parts of \(G(z)\) and \(F(z)\) do not contain a delay. More precisely, \(\Phi\) and \(\Psi\) are \(p_1 \times p_1\) block diagonal matrices where the block in position \((h, h)\), with \(h \in I_1\), is, respectively,
\[
I_{p_2} \otimes \begin{bmatrix} \phi_{h-1,1} & \ldots & \phi_{h-1, p_2} \end{bmatrix} \\
I_{p_2} \otimes \begin{bmatrix} \psi_{h-1,1} & \ldots & \psi_{h-1, m} \end{bmatrix}
\]
and the Toeplitz matrices \(\tilde{\phi}_{hk}, \tilde{\psi}_{hk} \in \ell_2^{N \times 1}(N)\) are:
\[
[\tilde{\phi}_{hk}]_{sn} := y_{hk}(N - s - n + 2) \\
[\tilde{\psi}_{hk}]_{sn} := u_{hk}(N - s - n + 2)
\]
Therefore, our Kronecker identification problem can be formulated in terms of PEM as follows.

**Problem 3** Assume to collect the measurements \(\{y(t), u(t)\}_{t=0}^{N}\) and that the dimensions \(p_1\) and \(p_2\) are known. Find \(\theta^T_g \in \ell_2^{1 \times p_2 \beta^2}(N)\) and \(\theta^T_f \in \ell_2^{1 \times p_1 P_2 m}(N)\) corresponding to a Kronecker model minimizing the prediction error squared norm \(\|y^+ - \Phi \theta\|_{\Sigma^{-1} \otimes I_N}^2\) with \(\Sigma = \operatorname{diag}(\sigma^2_1, \ldots, \sigma^2_{p_2 m}, \ldots, \sigma^2_1, \ldots, \sigma^2_{p_1 1}, \ldots, \sigma^2_{p_1 p_2})\).

Following the nonparametric Gaussian regression approach in Pillonetto et al [2011], we model \(\theta_g\) and \(\theta_f\) as zero-mean processes with kernels \(K_g \in S_2^{p_2 \beta^2}(N)\) and \(K_f \in S_2^{p_1 P_2 m}(N)\), respectively. These kernels may depend upon some tuning parameters, usually called hyperparameters and denoted with \(\zeta\) hereafter. As illustrated in Section 4, according to the maximum entropy principle \(\theta_g\) and \(\theta_f\) will be modeled as Gaussian and independent. In the following \(H_K\) denotes the reproducing Hilbert space of deterministic functions on \(N\), associated with \(K\) and with norm denoted by \(\|\cdot\|_{K-1}\).

We assume that the past data \(y^-\) neither affects the a priori probability on \(\theta_g\) and \(\theta_f\) nor carries information on \(\zeta\) and \(\Sigma\) (Pillonetto & De Nicolao [2010]), that is
\[
p(y^+, \theta_g, \theta_f, y^-|\zeta, \Sigma) \\
= p(y^+|\theta_g, \theta_f, y^-, \zeta, \Sigma)p(\theta_g, \theta_f|y^-, \zeta, \Sigma)p(y^-|\zeta, \Sigma) \\
\approx p(y^+|\theta_g, \theta_f, y^-, \zeta, \Sigma)p(\theta_g, \theta_f|\zeta, \Sigma)p(y^-) \tag{11}
\]
Let \(\hat{\theta}_g = \mathbb{E}[\theta_g|y^+, \zeta, \Sigma]\) and \(\hat{\theta}_f = \mathbb{E}[\theta_f|y^+, \zeta, \Sigma]\) be the minimum variance estimator, respectively, of \(\theta_g\) and \(\theta_f\) given \(y^+, \zeta\) and \(\Sigma\). It is well known that \(\hat{\theta}_g\) and \(\hat{\theta}_f\) are almost surely solution to the following Tikhonov-type variational problem
\[
\arg\min_{\theta_g \in H_{K_g}, \theta_f \in H_{K_f}}\|y^+ - \Phi \theta_g - \Psi \theta_f\|_{\Sigma^{-1} \otimes I_N}^2 + \|\theta_g\|_{K_g^{-1}}^2 + \|\theta_f\|_{K_f^{-1}}^2.
\]
Moreover, almost surely:
\[
\hat{\theta}_g = K_g \Phi^T(\Phi K_g \Phi^T + \Psi K_f \Psi^T + \Sigma \otimes I)^{-1}y^+ \\
\hat{\theta}_f = K_f \Psi^T(\Phi K_g \Phi^T + \Psi K_f \Psi^T + \Sigma \otimes I)^{-1}y^+.
\]
In what follows, \(\hat{G}(z)\) and \(\hat{F}(z)\) denote the transfer matrices corresponding to \(\hat{\theta}_g\) and \(\hat{\theta}_f\), respectively. The main task now is to design the kernels \(K_g\) and \(K_f\) in such a way that \(\hat{G}(z)\) and \(\hat{F}(z)\) are almost surely BIBO stable while favoring a sparse Kronecker decomposition of \(\mathbb{P}(G(z))\) and \(\mathbb{P}(F(z))\).

**4 Maximum entropy priors**

The probability law for the joint process \(\theta = [\theta^T_g \theta^T_f]^T\) under desired constraints can be obtained by the maximum entropy principle. Indeed, maximum entropy solutions rely on “information” arguments which essentially state that the maximum entropy distribution is the one satisfying the given constraints and containing the largest amount of “uncertainty” (Jaynes [1982]). In plain words, this principle guarantees that this solution does not satisfy additional constraints that are undesired and unnecessary. We shall make the rather mild assumption that the process \(\theta\) is zero-mean and absolutely continuous with respect to the Lebesgue measure. We will see that the optimal solution (i.e. maximizing the differential entropy) is a Gaussian process where \(\theta_g\) and \(\theta_f\) are independent. Then, we will also characterize the corresponding kernel functions.

We start with the constraints on \(\theta_g\) inducing BIBO stability on \(G(z)\). Let \(P \in S_2(N)\) be a strictly positive def-
finite kernel (in the sense of Moore) such that \(|P|_{t,t} \leq \kappa e^{-\beta t}, t \in \mathbb{N}\), with \(\kappa, \beta > 0\) and \(\alpha \in \mathbb{R}\). Let also \(\vartheta\) be a zero-mean process which satisfies the moment constraint

\[
E[\|\vartheta\|^2_{p-1}] \leq c
\]

where \(c > 0\). Then, for any \(\varepsilon > 1\) there exists \(\tilde{c}_e > 0\) such that the covariance function (kernel) \(K\) of \(\vartheta\) satisfies (Zorzi & Chiuso [2017] Proposition 4):

\[
[K]_{t,t} \leq \tilde{c}_e t^{\alpha + \varepsilon} e^{-\beta t}, \quad t \in \mathbb{N}.
\]

It is not difficult to see that the condition above on \(P\) is satisfied by the kernels usually employed in the identification of dynamical models (e.g. stable spline, tuned/correlated and so on, see Pillonetto et al. [2014]). Thus, we consider the constraints

\[
E[\|g[h,k,j;l]\|^2_{p-1}] \leq \tilde{c}_{h,k,j,l}, \quad \forall h, k, j \in I_1, \forall k, l \in I_2 \quad (12)
\]

where \(\tilde{c}_{h,k,j,l} \geq 0\) and \(P \in \mathcal{S}_2(\mathbb{N})\) as above. Then, by (12), the covariance of the \(k\)-th element of \(g[h,k,j;l]\) decays exponentially. Accordingly, its posterior mean is a BIBO stable transfer function.

**Remark 4** The kernel \(P\) induces a prior about the decay rate of the impulse responses \(g[h,k,j;l]\). On the other hand, the hyperparameters of \(P\) are estimated from the measured data, see Section 5. Therefore, although \(P\) could assign high probability to a small subset of BIBO stable systems, the latter is a “wise” set because it has been extrapolated from the data.

It remains to derive the constraints inducing a sparse Kronecker decomposition as in (2), i.e.:

\[
\begin{align*}
[E_1]_{h,j} = 0 & \iff g[h,k,j;l] = 0, \forall k, l \in I_2 \quad (13) \\
[E_2]_{k,l} = 0 & \iff g[h,k,j;l] = 0, \forall h, j \in I_1. \quad (14)
\end{align*}
\]

We consider the constraints:

\[
\begin{align*}
\sum_{k,l \in I_2} E[\|g[h,k,j;l]\|^2_{p-1}] & \leq c_{h,j}, \quad \forall h, j \in I_1; \quad (15) \\
\sum_{h,j \in I_1} E[\|g[h,k,j;l]\|^2_{p-1}] & \leq c_{k,l}^{(s)}, \quad \forall k, l \in I_2 \quad (16)
\end{align*}
\]

where \(c_{h,j}^{(s)} \geq 0\). First, notice that (15) and (16) imply (12) provided that \(\max(c_{h,j}^{(s)}, c_{k,l}^{(s)}) \leq \tilde{c}_{h,k,j,l}\) for any \(h, k, j, l\). Accordingly, the posterior mean of \(G(z)\), under the constraints (15)-(16), is BIBO stable. Let \(c_{h,j}^{(s)} = 0\), by (15) we have that \(g[h,k,j;l] \forall k, l \in I_2\) are the null sequence in mean square and so are their posterior mean, i.e. the latter satisfy (13). Let \(c_{k,l}^{(s)} = 0\), by (16) we have that \(g[h,k,j;l] \forall h, j \in I_1\) are the null sequence in mean square and so are their posterior mean, i.e. the latter satisfy (14). In a similar way, condition (2) on \(F(z)\) can be written as:

\[
\begin{align*}
[A_1]_{h} = 0 & \iff f[h,k,j;l] = 0, \forall k \in I_2, \forall i \in I_u \quad (17) \\
[A_2]_{k,i} = 0 & \iff f[h,k,j;l] = 0, \forall h \in I_1. \quad (18)
\end{align*}
\]

Thus, the constraints inducing BIBO stability and a sparse Kronecker decomposition are:

\[
\begin{align*}
\sum_{k \in I_2} \sum_{l \in I_2} E[\|f[h,k,j;l]\|^2_{R-1}] & \leq d_{h}^{(s)}, \forall h \in I_1; \quad (17) \\
\sum_{h \in I_1} \sum_{i \in I_u} E[\|f[h,k,j;l]\|^2_{R-1}] & \leq d_{k,i}^{(s)}, \forall k \in I_2, \forall i \in I_u \quad (18)
\end{align*}
\]

where \(d_{h}^{(s)}, d_{k,i}^{(s)} \geq 0\) and \(R \in \mathcal{S}_2(\mathbb{N})\) is a strictly positive kernel such that \([-R]_{t,t} \leq \kappa e^{-\beta t}, t \in \mathbb{N}, \kappa, \beta > 0\) and \(\alpha \in \mathbb{R}\).

In order to build the desired prior distribution we make use of the Kolmogorov extension Theorem, see Øksendal [1998], and work with finite vectors extracted from process \(\theta = [\theta_g^T \theta_f^T]^T\). More precisely, consider a finite index set \(\mathcal{I} = I_g \times I_f\) and \(I_g, I_f \subset \mathbb{N}\). Let \(\theta\) be the random vector whose components are extracted, from processes \(\theta_g\) and \(\theta_f\) according to the index sets \(I_g\) and \(I_f\), respectively. We denote by \(p_\mathcal{I}(\theta)|\mathcal{I}\) the probability density of \(\theta\). In view of the Kolmogorov extension Theorem, process \(\theta\) can be characterized by specifying the joint probability density \(p_\mathcal{I}\) for all finite sets \(\mathcal{I} \subset \mathbb{N} \times \mathbb{N}\). Thus, the maximum entropy process \(\theta\) can be constructed building all the marginals \(p_\mathcal{I}\) using the maximum entropy principle, which can thus be extended by the Kolmogorov extension theorem. Such principle states that among all the probability densities \(p_\mathcal{I}\) satisfying the desired constraints, the optimal one should maximize the differential entropy [Cover & Thomas [1991]]. Let \(P_{\mathcal{I}}\) and \(R_{\mathcal{I}}\) be the kernel matrices whose entries are extracted from \(P\) and \(R\) according to \(I_g\) and \(I_f\), respectively. Therefore, the corresponding maximum entropy problem is

\[
\begin{align*}
\max_{p_\mathcal{I} \in \mathcal{P}} H(p_\mathcal{I}) \\
\text{s.t.} \quad (15) \ (16) \ (17) \ (18) \text{ hold for } \mathcal{I}
\end{align*}
\]

where \(\mathcal{P}\) is the class of probability densities in \(\mathbb{R}^{[2]}\) which are bounded and taking positive values and \(H(p_\mathcal{I})\) denotes the differential entropy of \(\theta\). Moreover, the constraints in (19) must be understood as follows: (15), (16), (17) and (18) hold with \(\theta, P\) and \(R\) replaced by \(\tilde{\theta}_g, P_{\mathcal{I}}\) and \(R_{\mathcal{I}}\), respectively.

**Theorem 5** Under the assumption that \(c_{h,j}^{(s)} , c_{k,l}^{(s)}, d_{h}^{(s)}, d_{k,i}^{(s)} \geq 0\), \(h,j \in I_1, k,l \in I_2\) and \(i \in I_u\), the unique optimal solution to the maximum entropy problem (19) is such that \(\theta = [\theta_g^T \theta_f^T]^T\) is Gaussian with zero mean. Moreover, \(\tilde{\theta}_g\) and \(\tilde{\theta}_f\) are independent and with kernel matrix,
respectively,
\[
\begin{align*}
\hat{K}_g &= X_g \otimes P_x, \\
\hat{K}_f &= X_f \otimes R_x, \\
X_g &= (\Lambda \otimes \Gamma) (\Lambda \otimes I_p^2 + I_p^2 \otimes \Gamma)^{-1}, \\
X_f &= (\Pi \otimes \Omega) (\Pi \otimes I_p^2 + P_{I_p} \otimes \Omega)^{-1}, \\
\Lambda &= \text{diag}(\lambda_{11} \ldots \lambda_{1p_1} \ldots \lambda_{p_1p_1}), \\
\Gamma &= \text{diag}(\gamma_{11} \ldots \gamma_{1p_1} \ldots \gamma_{p_1p_1}), \\
\Pi &= \text{diag}(\pi_1 \ldots \pi_{p_1}), \\
\Omega &= \text{diag}(\omega_{11} \ldots \omega_{1m} \ldots \omega_{p_2m}).
\end{align*}
\]

where \(\lambda_{hj}, \gamma_{kl}, \pi_h, \omega_{ki} > 0\).

**Proof.** We prove the claim by using the duality theory. The Lagrangian is

\[
L(p_x, \tilde{\Lambda}, \tilde{\Gamma}, \tilde{\Pi}, \tilde{\Omega}) = H(p_x)
\]

\[
+ \frac{1}{2} \sum_{h,j \in I_1} \tilde{\lambda}_{hj} \left( c'_{hj} - \sum_{k,l \in I_2} E[\|g(h,k,j,l)\|_2] \right)
\]

\[
+ \frac{1}{2} \sum_{k,l \in I_2} \tilde{\gamma}_{kl} \left( c'_{kl} - \sum_{h,j \in I_1} E[\|g(h,k,j,l)\|_2] \right)
\]

\[
+ \frac{1}{2} \sum_{h \in I_1} d'_h \left( d''_h - \sum_{k \in I_2} E[\|f(h,k,i)\|_2^2] \right)
\]

\[
+ \frac{1}{2} \sum_{k \in I_2} \tilde{\omega}_{ki} \left( d''_{ki} - \sum_{h \in I_1} E[\|f(h,k,i)\|_2^2] \right)
\]

\[
- \frac{1}{2} \sum_{h,k \in I_1, j \in I_2} \tilde{\lambda}_{hj} \tilde{\gamma}_{kl}
\]

\[
- \frac{1}{2} \sum_{h \in I_1, k \in I_2} \tilde{\pi}_h d'_h + \frac{1}{2} \sum_{k \in I_2} \tilde{\omega}_{ki} d''_{ki}
\]

\[
= - E[\log(p_x)] + \frac{1}{2} \sum_{h,j \in I_1} \tilde{\lambda}_{hj} c'_{hj} + \frac{1}{2} \sum_{k,l \in I_2} \tilde{\gamma}_{kl} c'_{kl}
\]

\[
- \frac{1}{2} \sum_{h \in I_1, k \in I_2} \tilde{\pi}_h d'_h + \frac{1}{2} \sum_{k \in I_2} \tilde{\omega}_{ki} d''_{ki}
\]

\[
- \frac{1}{2} \sum_{h \in I_1, k \in I_2} \tilde{\pi}_h d'_h - \frac{1}{2} E[\|\tilde{\theta}_g\|^2_{(\tilde{\Lambda} \otimes I + I \otimes \tilde{\Gamma}) \otimes P_x}]
\]

\[
+ \frac{1}{2} \sum_{k \in I_2} \tilde{\omega}_{ki} d''_{ki} - \frac{1}{2} E[\|\tilde{\theta}_f\|^2_{(\tilde{\Pi} \otimes I + I \otimes \tilde{\Omega}) \otimes R_x}]
\]

where \(\tilde{\lambda} = \text{diag}(\tilde{\lambda}_{11} \ldots \tilde{\lambda}_{1p_1} \ldots \tilde{\lambda}_{p_1p_1}), \tilde{\Gamma} = \text{diag}(\tilde{\gamma}_{11} \ldots \tilde{\gamma}_{1p_1} \ldots \tilde{\gamma}_{p_1p_1}), \tilde{\Pi} = \text{diag}(\tilde{\pi}_1 \ldots \tilde{\pi}_{p_1}), \tilde{\Omega} = \text{diag}(\tilde{\omega}_{11} \ldots \tilde{\omega}_{1m} \ldots \tilde{\omega}_{p_2m})\); moreover, \(\tilde{\lambda}_{hj} + \tilde{\gamma}_{kl} \geq 0\) are the Lagrange multipliers corresponding to (15), (16), (17) and (18), respectively. It is not difficult to see that (21) is strictly concave in \(P\). Moreover, its point of maximum exists under the assumptions that \(\tilde{\lambda}_{hj} + \tilde{\gamma}_{kl} > 0\) and \(\tilde{\pi}_h + \tilde{\omega}_{ki} > 0\), and it is Gaussian distributed:

\[
p_x(\tilde{\theta}_g) = \frac{1}{\sqrt{2\pi}^p |I_x|} \exp(-\frac{1}{2} \tilde{\theta}_g^T \hat{K}_g^{-1} \tilde{\theta}_g)
\]

\[
p_x(\tilde{\theta}_f) = \frac{1}{\sqrt{2\pi}^p |I_x|} \exp(-\frac{1}{2} \tilde{\theta}_f^T \hat{K}_f^{-1} \tilde{\theta}_f)
\]

and

\[
\hat{K}_g = (\hat{\Lambda} \otimes I + I \otimes \hat{\Gamma})^{-1} \otimes P_x, \\
\hat{K}_f = (\hat{\Pi} \otimes I + I \otimes \hat{\Omega})^{-1} \otimes R_x.
\]

In the case that \(\tilde{\lambda}_{hj} + \tilde{\gamma}_{kl} = 0\) or \(\tilde{\pi}_h + \tilde{\omega}_{ki} = 0\) for some \(h, k, j, l, i\), then the maximum cannot be attained in \(P\). Substituting the optimal form of \(p_x\) in the Lagrangian we obtain the dual function (up to terms not depending on \(\tilde{\Lambda}, \tilde{\Gamma}, \tilde{\Pi}\) and \(\tilde{\Omega}\):

\[
J(\tilde{\Lambda}, \tilde{\Gamma}, \tilde{\Pi}, \tilde{\Omega}) = J_f(\tilde{\Lambda}, \tilde{\Gamma}) + J_g(\tilde{\Pi}, \tilde{\Omega})
\]

where

\[
J_f(\tilde{\Lambda}, \tilde{\Gamma}) = - \frac{|I_g|}{2} \sum_{h,j \in I_1, k,l \in I_2} \log(\tilde{\lambda}_{hj} + \tilde{\gamma}_{kl})
\]

\[
+ \frac{1}{2} \sum_{k \in I_2} \tilde{\lambda}_{hj} c'_{hj} + \frac{1}{2} \sum_{k \in I_2} \tilde{\gamma}_{kl} c'_{kl}
\]

\[
J_g(\tilde{\Pi}, \tilde{\Omega}) = - \frac{|I_f|}{2} \sum_{h \in I_1, k \in I_2} \log(\tilde{\pi}_h + \tilde{\omega}_{ki})
\]

\[
+ \frac{1}{2} \sum_{k \in I_2} \tilde{\pi}_h d'_h + \frac{1}{2} \sum_{k \in I_2} \tilde{\omega}_{ki} d''_{ki}
\]

Hence, we can minimize \((\tilde{\Lambda}, \tilde{\Gamma})\) and \((\tilde{\Pi}, \tilde{\Omega})\) in an independent way. We start to minimize \(J_f(\tilde{\Lambda}, \tilde{\Gamma})\) over the open and unbounded set

\[
C = \{ (\tilde{\Lambda}, \tilde{\Gamma}) \in D \text{ s.t. } \hat{\Lambda} \geq 0, \hat{\Gamma} \geq 0, \hat{\Lambda} \otimes I + I \otimes \hat{\Gamma} > 0 \}
\]

where \(D = D_{p_1^2} \times D_{p_2^2} \).
Next, we show that we can restrict the search of the minimum of $J_f$ over a compact set and thus by the Weierstrass’ theorem, the dual problem admits solution. Take a sequence $(\tilde{\Lambda}^{(n)}, \tilde{\Gamma}^{(n)}) \in C, n \in \mathbb{N},$ such that $\|\tilde{\Lambda}^{(n)}\| \to \infty$ and/or $\|\tilde{\Gamma}^{(n)}\| \to \infty$ as $n \to \infty.$ Then, $J_f(\tilde{\Lambda}^{(n)}, \tilde{\Gamma}^{(n)}) \to \infty$ because the linear terms dominate the logarithmic ones. Therefore, such a sequence cannot be an infinizing sequence. Accordingly, we can restrict the set $C$ as
\[
C_1 = \{(\tilde{\Lambda}, \tilde{\Gamma}) \in D \text{ s.t. } 0 \leq \tilde{\Lambda} \leq \lambda_{MAX} I, \\
0 \leq \tilde{\Gamma} \leq \gamma_{MAX} I, \tilde{\Lambda} \otimes I + I \otimes \tilde{\Gamma} > \epsilon I \}
\]
where $\lambda_{MAX}, \gamma_{MAX} > 0$ are constants taken sufficiently large. Take a sequence $(\tilde{\Lambda}^{(n)}, \tilde{\Gamma}^{(n)}) \in C_1, n \in \mathbb{N},$ such that $\lambda_{hj}^{(n)} + \gamma_{kl}^{(n)} \to 0$ as $n \to \infty$ for some $h,j \in I_1$ and $k,l \in I_2.$ Then, we have
\[
J_f(\tilde{\Lambda}^{(n)}, \tilde{\Gamma}^{(n)}) \geq \frac{-|I_g|}{2} \sum_{h,j \in I_1, k,l \in I_2} \log(\lambda_{hj} + \gamma_{kl}) \to \infty.
\]
Accordingly, it cannot be an infinizing sequence, and thus we can restrict the search to the set
\[
C_2 = \{(\tilde{\Lambda}, \tilde{\Gamma}) \in D \text{ s.t. } 0 \leq \tilde{\Lambda} \leq \lambda_{MAX} I, \\
0 \leq \tilde{\Gamma} \leq \gamma_{MAX} I, \tilde{\Lambda} \otimes I + I \otimes \tilde{\Gamma} \geq \epsilon I \}
\]
where $\epsilon$ is a constant taken sufficiently small. Thus, $C_2$ is closed and bounded and thus compact. We conclude that $J_f$ admits minimum over $C.$ In a similar way, it is possible to prove that $J_g$ admits minimum over the set
\[
C = \{ (\tilde{\Pi}, \tilde{\Omega}) \in D \text{ s.t. } \tilde{\Pi} \geq 0, \tilde{\Omega} \geq 0, \tilde{\Pi} \otimes I + I \otimes \tilde{\Omega} > 0 \}
\]
with $\tilde{D} = D_{p_h} \times D_{p_{ym}}.$ We conclude that the dual problem admits solution. Accordingly, (22) is the solution to the maximum entropy problem (19). Finally, by defining $\Lambda = \Lambda^{-1}, \Gamma = \Gamma^{-1}, \Pi = \Pi^{-1}$ and $\Omega = \Omega^{-1}$ we obtain (20).

We assumed that constraints (15), (16), (17) and (18) are totally binding in problem (19). However, we are interested in the limiting cases where $c_{hj}^{(n)}, c_{kl}^{(n)}$ and $d_{hj}^{(n)}, d_{kl}^{(n)}$ might be equal to zero in order to obtain a posterior corresponding to a Kronecker model. To include these scenarios, we consider the limits as $c_{hj}^{(n)} \to 0, c_{kl}^{(n)} \to 0, d_{hj}^{(n)} \to 0, d_{kl}^{(n)} \to 0$ and extend the maximum entropy solution by continuity.

**Proposition 6** Let $\cal E_1 := \{(h,j) \text{ s.t. } c_{hj}^{(n)} > 0\}, \cal E_2 := \{(k,l) \text{ s.t. } d_{kl}^{(n)} > 0\}.$ If the sets $\cal E_1, \cal E_2$ are nonempty, then the maximum entropy solution extended by continuity is the probability density such that $\theta_g$ is Gaussian, zero-mean and with kernel matrix as in (20) where:

- $(i,j) \notin \cal E_1 \implies \lambda_{hj} = 0,$
- $(k,l) \notin \cal E_2 \implies \gamma_{kl} = 0.$

**Proof.** First, recall that $\lambda_{hj} = \tilde{\lambda}_{hj}^{-1}, \gamma_{kl} = \tilde{\gamma}_{kl}^{-1}$ and $\tilde{\lambda}_{hj}, \tilde{\gamma}_{kl}$ are the original Lagrange multipliers. The maximum entropy solution $\tilde{\theta}_{ME}$ is such that, by Theorem 5, $\tilde{g}_{ME}^{[h,k,l]}$ is a zero-mean process with kernel matrix
\[
\frac{1}{\tilde{\lambda}_{hj} + \tilde{\gamma}_{kl}} P_{\delta_q}.
\]
Moreover, if $\tilde{\gamma}_{kl} > 0$ then the maximum entropy solution $\tilde{\theta}_{ME}$ satisfies the corresponding constraint with equality. We consider two sequences $\{c_{hj}^{(n)}\}_{n \in \mathbb{N}}, c_{hj}^{(n)} > 0,$ and $\{c_{kl}^{(n)}\}_{n \in \mathbb{N}}, c_{kl}^{(n)} > 0,$ such that $c_{hj}^{(n)} \to c_{hj}$ and $c_{kl}^{(n)} \to c_{kl}'$ as $n \to \infty.$ For any $c_{hj}^{(n)},$ we have
\[
c_{hj}^{(n)} \geq \sum_{k,l \in I_2} \E[\|g_{ME}^{[h,k,l]}[2]^T_{\delta_q}] \\
= \sum_{k,l \in I_2} \tr \left( \E[g_{ME}^{[h,k,l]}]^T P_{\delta_q}^{-1} \right) \\
= |I_g| \sum_{k,l \in I_2} \frac{1}{\tilde{\lambda}_{hj}^{(n)} + \tilde{\gamma}_{kl}^{(n)}} > 0.
\]
In a similar way, we have
\[
c_{kl}^{(n)} \geq |I_g| \sum_{h,j \in I_1} \frac{1}{\tilde{\lambda}_{hj}^{(n)} + \tilde{\gamma}_{kl}^{(n)}} > 0.
\]
Let $(h,j) \notin \cal E_1,$ then $c_{hj}^{(n)} \to 0.$ Then, we consider the arbitrary subsequences $\lambda_{hj}^{(n_r)}$ and $\gamma_{kl}^{(n_r)},$ with $r \in \mathbb{N},$ which admit limit. Taking into account (23), we may have two possible cases. First case. $\tilde{\gamma}_{kl}^{(n_r)}$ converges for some $k,l \in I_2.$ By (23), this implies that $\tilde{\lambda}_{hj}^{(n_r)} \to \infty$ and thus $\lambda_{hj}^{(n_r)} \to 0.$ Second case, $\tilde{\gamma}_{kl}^{(n_r)} \to \infty$ for any $k,l \in I_2.$ This means that there exists $\tilde{r} \in \mathbb{N}$ sufficiently large for which $\tilde{\gamma}_{kl}^{(n_r)} > 0$ for any $k,l \in I_2$ and $r \geq \tilde{r},$ Accordingly, the corresponding constraints in (24) are satisfied with equality for $r \geq \tilde{r}$ and $n = n_r.$ Hence $c_{hj}^{(n)} \to 0$ for any $k,l \in I_2$ and thus $\cal E_2 = \emptyset.$ This is not possible because $\cal E_2 \neq \emptyset$ by assumption. We conclude that $c_{hj}^{(n)} \to 0$ implies $\lambda_{hj}^{(n)} \to 0$ for any arbitrary subsequence which admits limit and thus $\lambda_{hj}^{(n)} \to 0.$ Accordingly, in a similar way, it is possible to prove that $c_{kl}^{(n)} \to 0$ implies $\gamma_{kl}^{(n)} \to 0.$

**Proposition 7** Let $\cal A_1 := \{(h) \text{ s.t. } d_{hj}^{(n)} > 0\}, \cal A_2 := \{(k,l) \text{ s.t. } d_{kl}^{(n)} > 0\}.$ If the sets $\cal A_1, \cal A_2$ are nonempty,
then the maximum entropy solution extended by continuity is the probability density such that \( \theta_f \) is Gaussian, zero-mean and with kernel matrix as in (20) where

- \( h \notin A_1 \implies \pi_h = 0 \),
- \( (k, l) \notin A_2 \implies \omega_{kli} = 0 \).

**Proof.** The proof is similar to one of Proposition 6. \( \square \)

Finally, in view of the Kolmogorov extension Theorem, the probability density of \( \theta \) we can characterize the probability law of \( \theta \) maximizing the differential entropy.

**Corollary 8** Consider the zero-mean Gaussian process \( \theta = [\theta_g^T \theta_f^T]^T \) with kernel, respectively,

\[
K_g = X_g \otimes P, \quad K_f = X_f \otimes R \tag{25}
\]

where \( X_g \) and \( X_f \) are defined as in (20). For all finite sets \( \mathcal{I} \subset \mathbb{N} \times \mathbb{N} \), its joint probability density is the extended solution to the maximum entropy problem (19).

It is worth noting that the maximum entropy solution is such that \( g^{[hk,jl]} \) and \( f^{[hk,i]} \) are zero-mean Gaussian processes with kernel function, respectively,

\[
K_g^{[hk,jl]} := \frac{\lambda_{hj} \gamma_{kl}}{\lambda_{hj} + \gamma_{kl}} P, \quad K_f^{[hk,i]} := \frac{\pi_h \omega_{kli}}{\pi_h + \omega_{kli}} R. \tag{26}
\]

In the case that both \( \lambda_{hj} \) and \( \gamma_{kl} \) are equal to zero, we define by continuity \( \lambda_{hj} \gamma_{kl}/(\lambda_{hj} + \gamma_{kl}) = 0 \). Accordingly, \( K_g^{[hk,jl]} = 0 \) if \( \lambda_{hj} = 0 \) or \( \gamma_{kl} = 0 \). Similarly, in the case that \( \pi_h \) or \( \omega_{kli} \) is equal to zero, we define \( \pi_h \omega_{kli}/(\pi_h + \omega_{kli}) = 0 \).

In Chiuso & Pillonetto (2012) the transfer matrices in model (1) are modeled as zero mean Gaussian processes with kernels

\[
K_g^{[hk,jl]} := \lambda_{hj} \gamma_{kl} P, \quad K_f^{[hk,i]} := \pi_h \omega_{kli} R \tag{27}
\]

where \( \lambda_{hj}, \pi_{h,k} \geq 0 \), with \( h, j \in I_1, k, l \in I_2 \) and \( i \in I_u \), are the hyperparameters representing the so called scale factors. The prior in (27) has been used to learn sparse networks. Finally, it is worth noting that there are many more hyperparameters in (27) compared with (26).

**Remark 9** It is worth noting that the constants \( c_{hj}'s \), \( c_{kl}'s \), \( d_{hj}'s \) and \( d_{kl}'s \) were needed only to derive the kernel structure in (25). Indeed, we are not interested in their particular values because, as we will show in the next section, the hyperparameters of the kernel will be found through another paradigm which exploits the measured data.

**Hierarchical dynamic networks.** An interesting scenario included in this framework is the case of a system without input (i.e. \( y(t) \) is a stationary stochastic process which is characterized by the transfer matrix \( G(z) \) with \( p_1 = p_2 \) and \( E_1 = E_2 \). It is then natural to take

\[
K_g = (\Lambda \otimes \Lambda)(\Lambda \otimes I_{p_1} + I_{p_2} \otimes \Lambda)^{-1} \otimes P
\]

and thus \( g^{[hk,jl]} \) is modeled is a Gaussian process with kernel function

\[
K_g^{[hk,jl]} := \frac{\lambda_{hj} \lambda_{kl}}{\lambda_{hj} + \lambda_{kl}} P. \tag{28}
\]

This model corresponds to a network which is hierarchically organized into communities (clusters), the communities then grow, creating miniature copies of themselves. This idea can be applied recursively at the price that the dimension of \( G(z) \) increases exponentially. Thus, \( \Lambda \) is the Kronecker initiator for the prior on \( G(z) \). These models have been proposed in Leskovec et al. (2010); the main difference with respect to our approach is the fact that we do not impose the Kronecker decomposition on \( G(z) \), but on \( \text{supp}(G(z)) \); moreover \( y(t) \) is not white noise (i.e. we consider a process with dynamics).

**5 Hyperparameters Estimation**

In order to compute \( \hat{\theta}_g \) and \( \hat{\theta}_f \), we have to estimate \( \Sigma \) and \( \zeta \). The latter contains the hyperparameters of \( P, R \) and \( \xi := \{\Lambda, \Gamma, \Pi, \Omega\} \). The noise covariance matrix \( \Sigma \) can be estimated using a low-bias ARX-model as suggested in Goodwin et al. (1992). To estimate the hyperparameters of \( P \) and \( R \) we consider a nonparametric unstructured model, i.e. we consider model (1) but we do not require that \( G(z) \) and \( F(z) \) satisfy condition (2). Then, the hyperparameters of \( P \) can be estimated by minimizing the negative log-marginal likelihood of \( y^+ \) computed using the unstructured model, see Pillonetto et al. (2011). Throughout the paper, kernel \( P \) is chosen as Stable Spline (SS) with a modulation factor Zorzi & Chiuso 2018:

\[
[P]_{t,s} = \left[ e^{-\beta(t-s)} e^{-\beta \max(t,s)} \frac{e^{-3\beta \max(t,s)}}{6} \right] \cos(\omega_0(t-s))
\]

where \( \beta \in (0, 1) \) and \( \omega_0 \in (0, \pi) \) tune, respectively, the a priori information about the decay rate and the frequency content of the impulse responses. Kernel \( R \) is chosen likewise. As explained in Pillonetto et al. (2011), kernels of this type represent a good prior in the case that the impulse responses of the predictor have “fast dynamics”.

Then, an estimate of \( \xi \) is given by minimizing the negative log-marginal likelihood \( \ell \) of \( y^+ \) under model (1),
We have attained for $\ell$ a gradient based method and the gradient

\[ \ell(y^+, \xi) = \log \det V + \frac{1}{2}(y^+)^T V^{-1} y^+ \]

\[ V = \Phi K_\gamma \Phi^T + \Psi K_f \Psi^T + \Sigma \otimes I \]  

(29)

where $K_\gamma$ and $K_f$ have been defined in (25) and $\xi$ belongs to the compact set

\[ \Xi = \{(\Lambda, \Gamma, \Pi, \Omega) \in \mathcal{D} \text{ s.t. } 0 \leq \Lambda, \Gamma, \Pi, \Omega \leq \kappa I \} \]  

(30)

where $\mathcal{D} = \mathcal{D}_{p_1} \times \mathcal{D}_{p_2} \times \mathcal{D}_{p_1} \times \mathcal{D}_{p_2}$ and $\kappa > 0$ is a constant taken sufficiently large. Notice that the choice of $\Xi$ is not restrictive. Indeed, if we take $\Gamma \geq 0$ such that $\gamma_{kl} > 0$ for some $k, l \in I_2$, $\Lambda \geq 0$ such that $\lambda_{hj} \to \infty$ for some $h, j \in I_1$, then $\lambda_{hj} \gamma_{kl} / (\lambda_{hj} + \gamma_{kl}) \to \infty$ and thus $\ell(y^+, \xi) \to \infty$. This means that the minimum cannot be attained for $\lambda_{hj} > \kappa$. In the case that $\Gamma = 0$, then we have $\ell(y^+, \{\lambda, \gamma, \Pi, \Omega\}) = \ell(y^+, \{\lambda + \hat{\Lambda}, \gamma, \Pi, \Omega\})$ for any $\hat{\Lambda} \in \mathcal{D}_{p_2}$ such that $\lambda + \hat{\Lambda} \geq 0$; accordingly, we can restrict the values of $\Lambda$ as in (30). A similar reasoning holds for $\Gamma, \Pi$ and $\Omega$. Since $\ell$ is a continuous function over the compact set $\Xi$, it follows that $\ell$ admits a point of minimum over $\Xi$.

The minimization of (29) with respect to $\xi$ in the numerical examples presented in the next section is performed through the nonlinear optimization Matlab solver *fmincon.m* which uses a gradient based method and the gradient, i.e. $\partial \ell(y^+, \xi) / \partial \xi$, is supplied. The computation of the gradient can be done in a similar way to that explained in [Chen & Ljung, 2013, Section 5]. In the case one is interested to make more efficient the algorithm, it is possible to perform the minimization by means of the scaled gradient projection method proposed in [Bonet-tini et al., 2015]. Finally, it is worth noting that only a local minimum can be found because $\ell(y^+, \xi)$ is not convex with respect to $\xi$.

Next, we prove that the posterior mean of $\theta_g$ and $\theta_f$ under the prior defined through kernels in (25) leads to a sparse Kronecker network. The analysis is performed by drawing inspiration from [Aravkin et al., 2014] which deals with the case of a sparse Bayesian network (Chiuso & Pillonetto, 2012), i.e. the prior is defined through kernels in (27), and indeed our prior is closely related to Auto Relevance Determination (ARD) method [MacKay, 1994]. First, notice that the estimates $\hat{\theta}_g$ and $\hat{\theta}_f$ describe a sparse Kronecker network only if $\xi = \{\hat{\Lambda}, \hat{\Gamma}, \hat{\Pi}, \hat{\Omega}\}$ is such that $\hat{\Lambda}, \hat{\Gamma}, \hat{\Pi}, \hat{\Omega}$ are spare matrices. We assume that the variance noise at each node is the same, i.e. $\sigma_{kk}^2 = \sigma^2$ with $h \in I_1$ and $k \in I_2$, and that

\[ (I \otimes P^{1/2}) \Phi^T \Phi (I \otimes P^{1/2}) = N I, \]

\[ (I \otimes P^{1/2}) \Psi^T \Psi (I \otimes R^{1/2}) = 0, \]

\[ (I \otimes R^{1/2}) \Psi^T \Psi (I \otimes R^{1/2}) = N I. \]

(31)

Moreover $\sigma^2, P$ and $R$ are fixed. First, we consider the case that $\tilde{g}_{h, k, l, j}^g$ and $\tilde{f}_{h, k, l, j}^f$ are finite dimensional vectors, say $T$ their dimension. Accordingly, the corresponding transfer matrices $G(z)$ and $F(z)$ are finite impulse responses (FIR) and $T$ represents their practical length. Moreover, we assume that $N \geq T$. We define

\[ \hat{\theta}_{g, LS} = (\Phi^T \Phi)^{-1} \Phi^T y^+, \]

\[ \hat{\theta}_{f, LS} = (\Psi^T \Psi)^{-1} \Psi^T y^+, \]

\[ \hat{g}_{LS}^g = \frac{1}{N} P \hat{\phi}_{g}^T y^+, \]

\[ \hat{f}_{LS}^f = \frac{1}{N} P \hat{\psi}_{f}^T y^+, \]

which are the least squares estimators of $\theta_g$ and $\theta_f$. Thus, we have

\[ \hat{g}_{LS}^g = \frac{1}{N} P \hat{\phi}_{g}^T y^+, \]

\[ \hat{f}_{LS}^f = \frac{1}{N} P \hat{\psi}_{f}^T y^+, \]

(32)

**Proposition 10** Let $\lambda_{hj}$, $\gamma_{kl}$, $\pi_h$ and $\omega_k$ be the entries in the main diagonal of $\Lambda, \Gamma, \Pi, \Omega$, respectively. The following facts hold:

- if

\[ \frac{T}{N} \sigma^2 - \|\hat{g}_{LS}^g\|_{2^{-1}}^2 \geq 0, \quad \forall k, l \in I_2, \]  

then the subset

\[ \Xi_1 = \{\Lambda, \Gamma, \Pi, \Omega \text{ s.t. } \Lambda, \Gamma, \Pi, \Omega \geq 0, \lambda_{hj} = 0\} \]

contains a local minimum for $\ell$;

- if

\[ \frac{T}{N} \sigma^2 - \|\hat{f}_{LS}^f\|_{2^{-1}}^2 \geq 0, \quad \forall h, j \in I_1, \]  

then the subset

\[ \Xi_2 = \{\Lambda, \Gamma, \Pi, \Omega \text{ s.t. } \Lambda, \Gamma, \Pi, \Omega \geq 0, \gamma_{kl} = 0\} \]

contains a local minimum for $\ell$;

- if

\[ \frac{T}{N} \sigma^2 - \|\hat{g}_{LS}^g\|_{2^{-1}}^2 \geq 0, \quad \forall k \in I_2, \quad i \in I_a, \]  

then the subset

\[ \Xi_3 = \{\Lambda, \Gamma, \Pi, \Omega \text{ s.t. } \Lambda, \Gamma, \Pi, \Omega \geq 0, \pi_h = 0\} \]

contains a local minimum for $\ell$;
if
\[ T \sigma^2 - \| \hat{f}_{LS} \|^2_{R^{-1}} \geq 0, \quad \forall h \in I_1, \]
then the subset
\[ \Xi_3 = \{ (\Lambda, \Gamma, \Pi, \Omega) \text{ s.t. } \Lambda, \Gamma, \Pi, \Omega \geq 0, \omega_{kl} = 0 \} \]
contains a local minimum for \( \ell \).

**Proof.** Let
\[
X := \begin{bmatrix} X_g \otimes I & 0 \\ 0 & X_f \otimes I \end{bmatrix}, \quad \hat{K} := \begin{bmatrix} I \otimes P & 0 \\ 0 & I \otimes R \end{bmatrix},
\]
thus
\[
K := \begin{bmatrix} K_g & 0 \\ 0 & K_f \end{bmatrix} = X\hat{K} = \hat{K}X = \hat{K}^{1/2}X\hat{K}^{1/2}
\]
and condition (31) can be written as
\[
\hat{K}^{1/2} \begin{bmatrix} \Phi^T \\ \Psi^T \end{bmatrix} \begin{bmatrix} \Phi \\ \Psi \end{bmatrix} \hat{K}^{1/2} = NI. \tag{35}
\]
In what follows, the symbol \( \equiv \) means “equal to up to terms not depending on \( \xi \).” Next, we rewrite \( \ell(\gamma^+, \xi) \) using (32) and (35). First,

\[
\log \det(\Phi K_g \Phi^T + \Psi K_f \Psi^T + \sigma^2 I) \\
\equiv \log \det \left( \frac{1}{\sigma^2} \begin{bmatrix} \Phi & \Psi \end{bmatrix} K \begin{bmatrix} \Phi^T \\ \Psi^T \end{bmatrix} + I \right) \\
\equiv \log \det \left( \frac{1}{\sigma^2} \begin{bmatrix} \Phi & \Psi \end{bmatrix} \hat{K}^{1/2} X^{1/2} X^{1/2} \hat{K}^{1/2} \begin{bmatrix} \Phi^T \\ \Psi^T \end{bmatrix} + I \right) \\
\equiv \log \det \left( \frac{1}{\sigma^2} X^{1/2} \hat{K}^{1/2} \begin{bmatrix} \Phi^T \\ \Psi^T \end{bmatrix} \hat{K}^{1/2} X^{1/2} + I \right) \\
= \log \det \left( \frac{N}{\sigma^2} \begin{bmatrix} X_g \otimes I & 0 \\ 0 & X_f \otimes I \end{bmatrix} + I \right) \\
= \log \det \left( \frac{N}{\sigma^2} X_g \otimes I_T + I \right) + \log \det \left( \frac{N}{\sigma^2} X_f \otimes I_T + I \right) \\
= T \sum_{h \in I_1} \sum_{l \in I_2} \log \det \left( \frac{N}{\sigma^2} \lambda_{hl} + \gamma_{hl} + 1 \right) \\
+ \sum_{i \in I_u} \log \det \left( \frac{N}{\sigma^2} \pi_h \omega_{ki} + 1 \right).
\]

Next, we prove the first statement regarding \( \lambda_{hl} \). The expression of the partial derivative of \( \ell \) with respect to \( \lambda_{hl} \) depends on the value of \( \gamma_{kl} \)'s. Given \( \gamma_{kl} \geq 0 \) for \( k, l \in I_2 \), let \( \hat{J} \) denotes the subset of \( I_2 \times I_2 \) containing the indexes \((k, l)\) such that \( \gamma_{kl} > 0 \). Then, we have:

\[
\frac{\partial \ell(\gamma^+, \xi)}{\partial \lambda_{hl}} = \sum_{(k, l) \in \hat{J}} \left( \frac{\gamma_{kl}}{\lambda_{hl} + \gamma_{hl}} \right) T\frac{\gamma_{kl} \omega_{ki}}{\lambda_{hl} + \gamma_{hl} + 1} \frac{\lambda_{hl} \gamma_{kl} + \sigma^2}{\sigma^2} - \frac{\| \hat{f}_{LS} \|^2_{R^{-1}}}{\sigma^2}.
\]

Thus
\[
\frac{\partial \ell(\gamma^+, \xi)}{\partial \lambda_{hl}} \bigg|_{\lambda_{hl}=0} = \sum_{(k, l) \in \hat{J}} \frac{T}{N} \frac{\sigma^2 - \| \hat{f}_{LS} \|^2_{P^{-1}}}{\sigma^4/N^2}. \tag{36}
\]
If condition (33) holds, and in view of (36), then
\[
\frac{\partial \ell(y^*, \xi)}{\partial \lambda_{hj}} \bigg|_{\lambda_{hj}=0} \geq 0. \tag{37}
\]
Notice that \( \ell \) is continuous in the compact set \( \Xi_1 \) and thus \( \ell \) admits a point of minimum in \( \Xi_1 \). Therefore, if (37) holds, then \( \Xi_1 \) contains a local minimum for \( \ell \). The remaining statements can be proved in a similar way. \( \square \)

**Remark 11** In the nonparametric case, i.e. the limit case \( T \to \infty \), the above result holds provided that the length of the data diverges in the same way. More precisely, assume that \( T \to \infty \), \( N \to \infty \) and \( T/N \to 1 \), then Proposition 10 holds where conditions (33)-(34) are replaced by

\[
\sigma^2 - \|g_{[h,k,j]}^{[l]}\|^2_{P^{-1}} \geq 0, \quad \forall k, l \in I_2
\]
\[
\sigma^2 - \|g_{[h,k,j]}^{[l]}\|^2_{P^{-1}} \geq 0, \quad \forall h, j \in I_1
\]
\[
\sigma^2 - \|f_{[h,k,j]}^{[l]}\|^2_{R^{-1}} \geq 0, \quad \forall k \in I_2, \quad i \in I_u
\]
\[
\sigma^2 - \|f_{[h,k,j]}^{[l]}\|^2_{R^{-1}} \geq 0, \quad \forall h \in I_1.
\]

Let \( \hat{G}_{LS}(z) \) and \( \hat{F}_{LS}(z) \) be the transfer matrices corresponding to the least squares estimates in (32). Then, the corresponding model is

\[
y(t) = \hat{G}_{LS}(z)y(t) + \hat{F}_{LS}(z) + e(t)
\]

The first statement of Remark 11 means that if the \( \ell_2 \) norms of \( g_{[h,k,j]}^{[l]} \)'s describing the conditional Granger causality relations from \( y_j^* \) to \( y_h^* \) do not dominate the variance of the noise process, then \( \hat{\lambda}_{hj} = \{1 \} \) and thus the posterior mean of \( g_{[h,k,j]}^{[l]} \)'s belonging to the block \((h,j)\) are null functions. Similar reasoning hold for the other statements.

6 Numerical experiments

In this section we test the performance of the proposed estimator.

6.1 Synthetic examples

We consider five Monte Carlo studies of 100 runs. For each run we generate an ARMAX model of the form

\[
y(t) = G_{TR}(z)y(t) + F_{TR}(z)u(t) + e(t) \tag{38}
\]
as follows:

- the rational transfer matrices \( G_{TR}(z) \) and \( F_{TR}(z) \) are strictly casual and generated through the MATLAB function `drmodel.m` where the order of the system is equal to 20; moreover, their poles are restricted to have absolute value less than 0.95.
- some entries of \( G_{TR}(z) \) and \( F_{TR}(z) \) are set equal to the null function in such a way that they satisfy condition (2); matrices \( E_1, E_2, A_1 \) and \( A_2 \) are randomly generated in such a way such that the fraction of non-null entries is equal to 0.6.

For each run we generate a dataset of length \( N = 500 \) if not otherwise specified; the input \( u \) has uncorrelated components which are generated through the MATLAB function `idinput.m` as a realization from a random Gaussian noise with band \([0, 0.4]\).

We compare the following estimators:

- **K**: this is the estimator based on model (1) where the transfer matrices are modeled as zero mean Gaussian processes with kernels (25);
- **S**: this is the estimator based on model (1) where the transfer matrices are modeled as zero mean Gaussian processes with kernels (27);
- **SS**: this is the estimator based on model (1) where the transfer matrices are modeled as zero mean Gaussian processes with kernels (27);

The impulse responses are truncated with length \( T = 50 \), i.e. we make the approximation \( G(z) = \sum_{t=1}^{\infty} G_{t} z^{-t} \approx \sum_{t=1}^{T} G_{t} z^{-t} \). Such a truncation does not affect the estimates because both \( P \) and \( R \) force the estimated impulse responses to decay exponentially, i.e. it does not involve any kind of trade-off between bias and variance [Pillonetto & De Nicolao, 2010]. In practice, it is only important to take the practical length very large.

The performance of these estimators is assessed through the following indexes:

- Average impulse response fit

\[
\text{AIRF} = \frac{fit(G_{TR}, \hat{G})}{2} + \frac{fit(F_{TR}, \hat{F})}{2}
\]

where

\[
fit(G_{TR}, \hat{G}) = 100 \left( 1 - \frac{1}{T} \sum_{t=1}^{T} \| G_{TR,t} - \hat{G}_{t} \|^2 \right)
\]

\[
\hat{G}_{TR} = \frac{1}{T} \sum_{t=1}^{T} G_{TR,t}
\]

and \( \hat{G}(z) \), \( \hat{F}(z) \) are the estimated transfer matrices;
PEM+OR, and

tors.

K is 3848. Figure 2 shows the performance of the estimation of parameters whose amount with polynomial orders equal to 15 has enough PEM, the latter has been chosen so large in such a way that PEM+OR AIRF while both PEM+OR, even though it owns the correct network topology, and PEM are the worst. Finally, K is better than S in terms of ERR. Notice that we did not plot ERR for PEM and SS because they always provide a full network. In particular, in regard to SS, the entries of G(z) share the same prior (and thus the same scale factor λ whose estimated value is always strictly positive). We also considered Monte Carlo studies where p1 and p2 are different: the results, in terms of performance, do not change.

First Monte Carlo study. We consider the case in which model (38) is without input u, i.e. we have a dynamic network corresponding to an ARMA stochastic process. In this case we only have to estimate G(z), accordingly AIRF = fit(GTR, ˜G) and ERR = ∥E1 ⊗ E2 − ˜E1 ⊗ ˜E2∥0/∥ρ1∥2). Besides the previous estimators, we also consider:

• PEM: this is the classical PEM approach that uses BIC for model order selection. The orders of the polynomials in the ARMA model ranges from 1 to 15 and are not allowed to be different from each other since this would lead to a combinatorial explosion of the number of competitive models.

• PEM+OR: this is the same as PEM with an additional oracle knowing which impulse responses are null functions.

The length of the dataset is N = 3900. It is worth noting the latter has been chosen so large in such a way that PEM with polynomial orders equal to 15 has enough data to estimate all the model parameters whose amount is 3848. Figure 2 shows the performance of the estimators. K outperforms all the other estimators in terms of AIRF while both PEM+OR, even though it owns the correct network topology, and PEM are the worst. Finally, K is better than S in terms of ERR. Notice that
Fig. 4. Third Monte Carlo study with $p_1 = 3$, $p_2 = 4$ and $m = 2$. Left panel. Average impulse response fit. Right panel. Fraction of misspecified edges.

Fig. 5. Fourth Monte Carlo study with $p_1 = 4$, $p_2 = 3$ and $m = 2$. Left panel. Average impulse response fit. Right panel. Fraction of misspecified edges.

Fig. 6. Fifth Monte Carlo study “ARMA case - hierarchical network” with $p_1 = 4$, $p_2 = 4$. Left panel. Average impulse response fit. Right panel. Fraction of misspecified edges.

study. In Figure 6 the performance of the estimators is depicted. $S$ and $SS$ are worse than $H$ and $K$. The latter perform in a similar way in terms of AIRF. $H$, however, outperforms $K$ in terms of ERR.

**Remark 12** The negative log-marginal likelihood function is not convex with respect to the hyperparameters even in the simplest case where the hyperparameters are only the scale factors, see [Chen et al. (2014)](https://example.com). Accordingly, the kernel-based PEM methods could suffer about local minima in the estimation of the hyperparameters. In particular, both $S$ and $K-H$ have the same issue. The main difference is the number of hyperparameters to estimate: $K-H$ have to estimate very less hyperparameters than $S$. More precisely, in $K$ we have to estimate $p_1^2 + p_2^2 + p_1 + p_2m$ ($p_1^2 + p_2^2$ in the case of systems without input) hyperparameters, in $H$ we have to estimate only applicable in the case of systems without input and $p_1 = p_2$), while in $S$ we have to estimate $p_1^2 + p_1 + p_2m$ ($p_1^2 + p_2^2$ in the case of systems without input) hyperparameters. Table 1 summarizes the number of hyperparameters needed in the previous Monte Carlo studies. Therefore, $K$ and $H$ alleviate the aforementioned issue since the search space for optimizing the marginal likelihood is small in respect to the one of $S$.

### Table 1

| M.C. study | $S$ | $K$ | $H$ |
|------------|-----|-----|-----|
| First      | 99  | 27  | -   |
| Second     | 168 | 36  | -   |
| Third      | 168 | 35  | -   |
| Fourth     | 256 | 32  | -   |
| Fifth      | 256 | 32  | 16  |

6.2 Learning a bike sharing system

Bike sharing systems aim to make automatic bike rentals, in particular the rental and the return back. We consider the number of users and some variables describing the weather, that is wind speed, humidity and apparent temperature. These quantities have been collected in the period 1 January 2011 - 14 May 2012 (500 days in total) from the Capital Bike Sharing (CBS) system at Washington, D.C., USA. The sampling time is equal to 1 hour. For more details see [Fanaee-T & Gama (2014)](https://example.com). These data describe a four dimensional stochastic process $x(s) = [x_1(s) x_2(s) x_3(s) x_4(s)]^T$, where $x_1(s)$ is the number of users, $x_2(s)$ is the wind
speed, $x_3(s)$ is the humidity and $x_4(s)$ is the apparent temperature. Process $x(s)$ is non-stationary during a day: for instance, we expect that the number of users during the night is smaller than the ones during the day. Accordingly, we consider the process

$$y(t) = [x(24(t-1)+1)^T \ldots x(24t)^T]^T$$

taking values in $\mathbb{R}^{96}$ and the corresponding sampling time is 1 day. Thus, the corresponding dataset has length $N = 500$. After detrending it, we model $y$ as the dynamic spatio-temporal model of Section 2.1 where $p_1 = 24$, $p_2 = 4$. Then, we estimate $G(z)$ by $K$ and the regression matrices are the ones in Remark 2. The estimated network describing the conditional Granger causality relations among the number of users, wind speed, humidity and apparent temperature is depicted in Figure 7.

As expected, the number of users does not conditionally Granger causes the weather variables. Moreover, the number of users is conditionally Granger caused by the apparent temperature. Figure 8 shows the weighted matrix describing the conditional Granger causality relations among hours. More precisely, the entry in position $(h, j)$ is the $\ell_1$ norm of the $4 \times 4$ impulse response, formed by $\hat{g}_k = \frac{\lambda_k}{\lambda_1}$ with $k, l \in \{1, 2, 3, 4\}$, which describes the strength of the conditional Granger causality relation from hour $j$ to hour $h$. We can notice that all the hours are mainly conditionally Granger caused by the previous hour.

7 Conclusions

We have considered the problem to estimate a dynamic network describing conditional Granger causality relations and having a Kronecker structure. We have proposed a kernel-based PEM method for estimating such a model from data. The kernel functions have been derived from the maximum entropy principle. Numerical simulation showed that the proposed estimator outperforms the one estimating dynamic networks without structure. Finally, we have used the proposed method to learn the conditional Granger causality relations in a bike sharing system.

Fig. 7. Estimated network describing conditional Granger causality relations among: the number of users (U), wind speed (W), humidity (H) and apparent temperature (T).

Fig. 8. Weighted matrix describing the estimated Granger causality relations among hours.

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