2017 IEEE 56th Annual Conference on Decision and Control (CDC)
December 12-15, 2017, Melbourne, Australia

Causality based graph structure of stochastic linear state-space representations

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Abstract— **This paper deals with different approaches to interpret the connectivity structure of complex systems. We connect the graph structure of linear state-space representations of a weakly stationary stochastic process and the non-causal relations between its components.**

I. Introduction

Complex systems, viewed as networks of simpler subsystems, occur in a wide variety of fields, ranging from cyber-physical systems to systems biology and neuroscience. For such systems, it is of interest to study the network topology or in other words, the connectivity structure. The connectivity structure of complex systems can be viewed in two ways: either as a relationship between the components of the outputs of the system, or as the internal structure of a representation of these outputs. In the latter case, the graph structure of a representation describes the interconnection of the components of a representation. Defining the connectivity structure on outputs has the advantage of being independent of the choice of the representation, which is not unique. However, it does not allow us to view the connectivity structure as interconnections of sub-systems. The second approach, which defines the internal connectivity structure of the system is more intuitive, but it may depend on the choice of the representation. In this paper we make a step towards reconciling these two approaches, by connecting the graph structure of state-space representations with their observed behavior.

Contribution: We consider stochastic linear time-invariant state-space representations (LTI-SS representation for short) whose observed behavior is a vector stochastic process. Regarding the network structure we restrict attention to the class of *transitive acyclic directed graphs (TADG)*, as an example see Fig. 1.

For a TADG graph G, we will say that a stochastic process is *consistent with* G, if conditional Granger causality relations among the components of the process are consistent with the edges of G. Granger causality [1] is a classical notion. We postpone the formal definition but informally, a

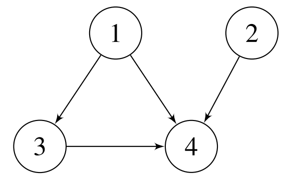

Fig. 1: Example of a TADG graph

stochastic process $\mathbf{z}_1$ *does not Granger cause* $\mathbf{z}_2$ (denoted by $\mathbf{z}_1 \not\to \mathbf{z}_2$), if the prediction of $\mathbf{z}_2$ based on the past of $\mathbf{z}_1$ and $\mathbf{z}_2$ is the same as that of only based on the past of $\mathbf{z}_2$. If an additional process $\mathbf{z}_3$ is present then we say that $\mathbf{z}_1$ *conditionally does not to Granger cause* $\mathbf{z}_2$ with respect to $\mathbf{z}_3$ (denoted by $\mathbf{z}_1 \not\to \mathbf{z}_2|\mathbf{z}_3$) if the prediction of $\mathbf{z}_2$ based on the past of $\mathbf{z}_1, \mathbf{z}_2$ and $\mathbf{z}_3$ is the same as that of only based on the past of $\mathbf{z}_2$ and $\mathbf{z}_3$.

A process $\mathbf{y} = \left[\mathbf{y}_1^T, \dots, \mathbf{y}_k^T\right]^T$ is consistent with a G graph having k nodes (each node of G corresponds to components of $\mathbf{y}$) if whenever there is no edge from node i to node j the process $\mathbf{y}_i$ does not conditionally Granger cause the process $\mathbf{y}_j$ with respect to the joint process formed by those components $\mathbf{y}_l$ which correspond to the parent nodes of i.

For instance, a process $\mathbf{y} = \left[\ \mathbf{y}_1^T, \mathbf{y}_2^T, \mathbf{y}_3^T, \mathbf{y}_4^T\ \right]^T$ is consistent with the TADG graph G depicted in Fig. 1, if $\mathbf{y}_1 \not\to \mathbf{y}_2$, $\mathbf{y}_2 \not\to \mathbf{y}_1$, $\mathbf{y}_2 \not\to \mathbf{y}_3|\mathbf{y}_1$, $\mathbf{y}_3 \not\to [\mathbf{y}_1^T, \mathbf{y}_2^T]^T$, $\mathbf{y}_4 \not\to [\mathbf{y}_1^T, \mathbf{y}_2^T]$ and $\mathbf{y}_4 \not\to \mathbf{y}_3|\mathbf{y}_1$.

For a TADG graph G an LTI-SS representation has a *G-zero structure*, if subsystems representing components of the output are connected in the same way as the nodes in G. More precisely, if there is an edge from one node to another then the state and noise process of the subsystem corresponding to the source node serves as an input of the subsystem corresponding to the target node. Example of an LTI-SS representation which has a G-zero structure for the TADG G in Fig. 1 is presented in Fig. 2.

We will show that if a process $\mathbf{y}$ is G-consistent with a TADG G, then there exists an LTI-SS representation of $\mathbf{y}$ which has a G-zero structure. We propose a construction of such an LTI-SS representation which built up of LTI-SS representations of the components of $\mathbf{y}$. In combination with stochastic realization algorithms, it leads to a procedure for computing an LTI-SS representation of $\mathbf{y}$ from the second order moments of $\mathbf{y}$. The latter can be estimated from data.

Motivation: The results of the paper could be useful for reverse engineering of the network structure of dynamical systems and structured model reduction [2], [3] and [4]. By reverse engineering of the network structure we mean finding out how various subsystems of a dynamical system interact with each other based on observed data. This problem arises

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This work was partially supported by the ESTIREZ project of Region Nord-Pas de Calais, France

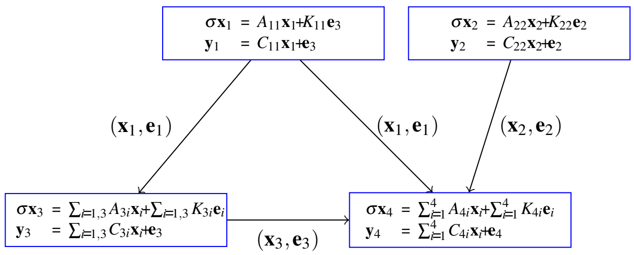

Fig. 2: LTI-SS representation with a TADG-zero structure

in several domains such as systems biology, neuroscience, smart grids, econometrics etc. [5], [6], [7], [8], [9], [10], [11], [12]. By structure preserving model reduction we mean replacing an interconnected model of the system by another interconnected model with smaller state dimension which has the same or similar network structure as the original model [2], [3]. In both cases, there is a need to understand when there exists a state-space representation admitting a specific graph structure for a certain behavior and how to compute such a realization.

Related work: The need to understand the relationship between the observed behavior and the graph structure of linear systems is an active research area, see for example [5], [6], [7]. In [5], [6], [13] the network structure of a deterministic system was defined on components of the observed output, by using the notion of the so-called dynamic structure function. However, the dynamic structure function itself is determined by the properties of a class of deterministic LTI state-space representations of that system. That is, in contrast with the current paper, the cited papers did not aim at relating network structures defined directly on the outputs with network structures defined based on state-space representations. Moreover, they dealt with deterministic systems. In [14] the relationship between dynamic structure function and Granger causality was investigated, however, in contrast to the current paper, [14] does not aim at establishing a relationship between the state-space defined network structure and the Granger causality based network structure.

Granger causality and graph structure of autoregressive-representations were related from the time Granger causality was introduced in [1]. The relationship between Granger causality of two processes and their innovation moving-average representation, the Wold decomposition, has been investigated in [15], [16], [17]. Granger causality for state-space representation was studied in [18], [19]. In contrast to [18] and [19], we consider multiple Granger causality relations by introducing the notion of conditional Granger causality and relate it to the graph structure of an innovation representation of the process. The notion of conditional Granger causality is a type of spurious causality [20]. The paper [20] related spurious causality with representations but did not discuss multiple causality conditions. In the paper [21] causality graph is defined for representing both spurious and direct causal relations, however the state-space representations of the processes are not discussed.

The closest papers to this paper are [22], [23] and [24] where also multiple causality conditions were studied in state-space representation driven by innovation noise. In comparison with the cited papers, we work on state-space representations without assuming the driving noise to have block diagonal covariance matrix and we focus on constructing the representation under consideration.

The paper [25] contains the result of the paper for TADGs of a special form, namely for the star graph, i.e., where there is one root node and all the other nodes are leaves. In contrast to [25], in this paper we consider arbitrary TADGs. In [26], stochastic processes which are realizable by stochastic LTI systems were investigated, but attention was restricted to so-called coercive stochastic processes and their transfer matrix representation. In contrast to [26], in this paper the output process needs not to be coercive, and we study the structure of state-space representations as opposed to transfer functions. Note that even for coercive processes, it is not clear how to derive the results of the present paper from those of [26].

Outline: In Section II we introduce the notation and the background material. In Section III we present our main result. The technical details of the main results, including the sketch of the proof, are written in Section IV. Finally in Section V we draw the conclusions of the paper.

II. Preliminaries

A. Hilbert spaces of random variables

The processes in this paper are discrete-time multivariate stochastic processes with the discrete-time axis being the set of integers $\mathbb{Z}$. The random variable of a process $\mathbf{z}$ at time t is denoted by $\mathbf{z}(t)$ and if $\mathbf{z}(t)$ takes its values from $\mathbb{R}^p$ then we write $\mathbf{z}(t) \in \mathbb{R}^p$ or for the process, $\mathbf{z} \in \mathbb{R}^p$.

We assume that the processes are zero mean, wide-sense stationary, square integrable, full-rank, purely non-deterministic and have strictly proper rational spectrum. These processes will be called *ZMSIR* processes.

The one-dimensional zero-mean, square integrable random variables form a Hilbert space $\mathscr{H}$ with the covariance matrix as the inner product (denoted by $E[z_1 z_2]$ for the variables z_1, z_2). By the Hilbert-space generated by a set $S \subset \mathscr{H}$ we mean the smallest (with respect to set inclusion) closed subspace of $\mathscr{H}$ which contains S. For a ZMSIR process $\mathbf{z} \in \mathbb{R}^p$ we denote by $\mathscr{H}_{t-}^{\mathbf{z}}$, $t \in \mathbb{Z}$ the Hilbert-space generated by the sets $\{\ell^T \mathbf{z}(s) \mid s \in \mathbb{Z}, s \leq t-1, \ell \in \mathbb{R}^p\}$. Informally, $\mathscr{H}_{t-}^{\mathbf{z}}$ is the Hilbert-space generated by the coordinates of the past values $\{\mathbf{z}(s)\}_{s=-\infty}^{t-1}$ of $\mathbf{z}$ up to time $t-1$.

If $\eta \in \mathscr{H}$ and B is a closed subspace of $\mathscr{H}$, then we denote by $E_l[\eta \mid B]$ the coordinate-wise orthogonal projection of η onto B. For Gaussian processes the orthogonal projection is equivalent to the conditional expectation. The identity matrix is denoted by I and its dimension will be clear from the context.

B. Stochastic linear state-space representation

Below we review some basic notions from the theory of stochastic linear systems, for more details see [27]. For a stochastic process $\mathbf{z}$ we denote by $\sigma\mathbf{z}$ the time-shifted stochastic process defined by $(\sigma\mathbf{z})(t) = \mathbf{z}(t+1)$, $t \in \mathbb{Z}$. An LTI-SS representation of a ZMSIR process $\mathbf{y} \in \mathbb{R}^p$ is a tuple $(A,B,C,D,\mathbf{x},\mathbf{e})$ such that

$$\begin{aligned} \sigma\mathbf{x} &= A\mathbf{x} + B\mathbf{e} \\ \mathbf{y} &= C\mathbf{x} + D\mathbf{e}, \end{aligned} \tag{1}$$

where the state process $\mathbf{x} \in \mathbb{R}^n$ and the noise process $\mathbf{e} \in \mathbb{R}^m$ are square integrable zero mean processes and $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{p\times n}$, $D \in \mathbb{R}^{p\times m}$. Moreover, A is stable (all its eigenvalues are inside the unit circle), $\mathbf{e}$ is white noise process (for all $t,s \in \mathbb{Z}$, $t \neq s$, $E[\mathbf{e}(t)\mathbf{e}^T(s)] = 0$) and $\mathbf{e}(t)$ is uncorrelated with $\mathbf{x}(t-k)$ $t,k \in \mathbb{Z}$, $k \geq 0$. We say that the representation (1) is a *Kalman representation* if the noise process $\mathbf{e}$ is the innovation process of $\mathbf{y}$, $\mathbf{e}(t) := \mathbf{y}(t) - E_l[\mathbf{y}(t)|\mathscr{H}_{t-}^{\mathbf{y}}]$ $\forall t \in \mathbb{Z}$. For a Kalman representation $D = I$ and B equals the Kalman gain denoted by K.

The minimality and uniqueness of LTI-SS representations are not as simple as in deterministic case in general. However, a Kalman representation $(A,K,C,I,\mathbf{x},\mathbf{e})$ is minimal (in the sense that the dimension n of its state space is minimal among all the LTI-SS representations of $\mathbf{y}$) if and only if (C,A) is an observable pair and (A,K) is a controllable pair. Moreover, minimal Kalman representations of $\mathbf{y}$ are unique up to a state-space transformation.

III. Main result

In this section we present the main result of the paper. To this end, the notion of (conditional) Granger causality is introduced, which enables us to define an interconnection structure for ZMSIR processes. Then, the concept of a ZMSIR process being consistent with a graph G is defined together with the notion of G-zero structure of LTI-SS representations.

We start by reviewing the definition of Granger acausality between two processes.

Definition 1 (Granger acausality $\cdot \not\to \cdot$) *Consider a ZMSIR process $\mathbf{y} = [\mathbf{y}_1^T, \mathbf{y}_2^T]^T$. We say that* $\mathbf{y}_2$ does not Granger cause $\mathbf{y}_1$*, denoted by $\mathbf{y}_2 \not\to \mathbf{y}_1$, if for all $t,k \in \mathbb{Z}$, $k \geq 0$*

$$E_l[\mathbf{y}_1(t+k) \mid \mathscr{H}_{t-}^{\mathbf{y}_1}] = E_l[\mathbf{y}_1(t+k) \mid \mathscr{H}_{t-}^{\mathbf{y}}].$$

In the presence of a third component $\mathbf{y}_3$, Granger acausality from $\mathbf{y}_2$ to $\mathbf{y}_1$ without the effect of $\mathbf{y}_3$ is formalized by the notion of conditional Granger acausality.[1]

Definition 2 (conditional Granger acausality $\cdot \not\to \cdot|\cdot$) *Consider a ZMSIR process $\mathbf{y} = [\mathbf{y}_1^T, \mathbf{y}_2^T, \mathbf{y}_3^T]^T$. We say that* $\mathbf{y}_2$ conditionally does not Granger cause $\mathbf{y}_1$ *with respect to* $\mathbf{y}_3$*, denoted by $\mathbf{y}_2 \not\to \mathbf{y}_1|\mathbf{y}_3$, if for all $t,k \in \mathbb{Z}$, $k \geq 0$*

$$E_l[\mathbf{y}_1(t+k) \mid \mathscr{H}_{t-}^{\mathbf{y}_1,\mathbf{y}_3}] = E_l[\mathbf{y}_1(t+k) \mid \mathscr{H}_{t-}^{\mathbf{y}}].$$

[1] These notions can also be found as feedback freeness and conditional orthogonality in the literature.

In order to state our main result, we need some concepts from graph theory.

Definition 3 (TADG) *A directed graph $G = (V,E)$, with set of nodes $V = \{1,\dots,k\}$ and set of directed edges $E \subseteq V \times V$ is called* acyclic *if there is no cycle i.e., closed directed path. Furthermore, it is* transitive *if for $i,j,l \in V$ the implication $(i,j),(j,l) \in E \Longrightarrow (i,l) \in E$ holds. We denote by* TADG *the class of transitive acyclic directed graphs.*

We use TADG graphs to model the interconnection structure of systems, both in terms of their outputs and their state-space representations. More precisely, for a TADG graph G, we define the class of output processes which are G-consistent and the class of LTI-SS representations which have G-zero structure.

Notation 1 (I_j) *For a TADG graph $G=(V,E)$ and node $j \in V$ denote the set of parent nodes of j by $I_j = \{i \in V | (i,j) \in E\}$.*

Notation 2 *Consider a TADG graph $G = (V,E)$ with $V = \{1,\dots,k\}$. For a ZMSIR process $\mathbf{y} = \left[\mathbf{y}_1^T,\dots,\mathbf{y}_k^T\right]^T$ and a set of nodes $J = \{j_1,\dots,j_l\} \subseteq V$ define the sub-process $\mathbf{y}_J := [\mathbf{y}_{j_1}^T,\dots,\mathbf{y}_{j_l}^T]^T$.*

Definition 4 (G-consistent process) *Consider a ZMSIR process $\mathbf{y} = \left[\mathbf{y}_1^T,\dots,\mathbf{y}_k^T\right]^T$ and a TADG graph $G = (V,E)$ with $V = \{1,\dots,k\}$. We say that $\mathbf{y}$ is* G-consistent *if $\mathbf{y}_i$ conditionally does not Granger cause $\mathbf{y}_j$ with respect to $\mathbf{y}_{I_j}$ for any $i,j \in V, i \neq j$ such that $(i,j) \notin E$.*

Next, we define the counterpart of G-consistency for LTI-SS representations. For this, we need the following notation.

Notation 3 *We call the set $\{n_i,m_i\}_{i=1}^k$ a* partition *of (n,m), if $\sum_{i=1}^k n_i = n$, $\sum_{i=1}^k m_i = m$, $n_i,m_i > 0, i \in \{1,\dots,k\}$. For a matrix $M \in \mathbb{R}^{n\times m}$ and a partition $\{n_i,m_i\}_{i=1}^k$ of (n,m) the partitioning of M is of the form*

$$M = \begin{bmatrix} M_{11} & \dots & M_{1k} \\ \vdots & \ddots & \vdots \\ M_{k1} & \dots & M_{kk} \end{bmatrix}$$

where the ij block is $M_{ij} \in \mathbb{R}^{n_i \times m_j}$. Note that in this paper the indexing of matrices refers to blocks of block matrices and does not refer directly to the elements of them. It is parallel to the component-wise indexing of processes where the components can be multidimensional.

Definition 5 *Consider a ZMSIR process $\mathbf{y} = \left[\mathbf{y}_1^T,\dots,\mathbf{y}_k^T\right]^T$ and a TADG graph $G = (V,E)$ with $V = \{1,\dots,k\}$. We say that a Kalman representation $(A,K,C,I,\mathbf{x} \in \mathbb{R}^n,\mathbf{e} \in \mathbb{R}^m)$ of $\mathbf{y} \in \mathbb{R}^m$ has a* G-zero structure *if there exists a partition $\{n_i,m_i\}_{i=1}^k$ of (n,m) for which $A_{j,i} = 0$, $K_{j,i} = 0$, $C_{j,i} = 0$ whenever $(i,j) \notin E$.*

Consider the TADG graphs $G_1 := (\{1,2\},\{(1,2)\})$, $G_2 := (\{1,2\},\emptyset)$ and $G_3 := (\{1,2,3\},\{(1,3),(2,3)\})$. For these cases instead of saying that a Kalman representation has a G_1-, G_2- or G_3-zero structure we say that *it is in block* *triangular, block diagonal or coordinated form*, respectively [25].

Now we are ready to state our main result.

Theorem 1 *Consider a ZMSIR process $\mathbf{y} = [\mathbf{y}_1^T, \ldots, \mathbf{y}_k^T]^T$ and a TADG graph $G = (V,E)$ with $V = \{1,\ldots,k\}$. If the process $\mathbf{y}$ is G-consistent, then there exists an observable Kalman representation of $\mathbf{y}$ with a G-zero structure.*

The proof of Theorem 1 is based on constructing an observable Kalman representation with a G-zero structure. This, along with the sketch of the proof of Theorem 1 is presented in Section IV.

IV. Construction of Kalman representations with a G-zero structure

In this section we present the construction of a Kalman representation of $\mathbf{y}$ with a G-zero structure. For this, we will need the following auxiliary results.

A. Auxiliary results

To construct the representation in Theorem 1 we first take an ordering of the components of the process being consistent with a topological ordering of the nodes of the TADG graph. We take a minimal Kalman representation of the first component and then extend this representation one by one to the other components obtaining observable Kalman representation in each step. The extension step can happen in three different ways; if all or none of the preceding nodes are parent nodes of the new node then the corresponding extended representation is in block triangular or block diagonal form, respectively. If some of the preceding nodes are parent nodes, some are non-parent nodes then the corresponding extended representation has a so-called coordinated form, see [25]. The extension of the LTI-SS representations uses the following Lemmas.

Lemma 1 *Corollary of [25, Theorem 1]. Consider a ZMSIR process $\mathbf{y} = [\mathbf{y}_1^T, \mathbf{y}_2^T]^T$ and an observable Kalman representation $(A_{11}, K_{11}, C_{11}, I, \mathbf{x}_1, \mathbf{e}_1)$ of $\mathbf{y}_1$. If $\mathbf{y}_2$ does not Granger cause $\mathbf{y}_1$ then there exists an observable Kalman representation of $\mathbf{y}$ in the form of*

$$\begin{aligned}\sigma\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix} &= \begin{bmatrix}A_{11} & 0\\ A_{21} & A_{22}\end{bmatrix}\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix} + \begin{bmatrix}K_{11} & 0\\ K_{21} & K_{22}\end{bmatrix}\begin{bmatrix}\mathbf{e}_1\\ \mathbf{e}_2\end{bmatrix}\\ \begin{bmatrix}\mathbf{y}_1\\ \mathbf{y}_2\end{bmatrix} &= \begin{bmatrix}C_{11} & 0\\ C_{21} & C_{22}\end{bmatrix}\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix} + \begin{bmatrix}\mathbf{e}_1\\ \mathbf{e}_2\end{bmatrix}.\end{aligned} \tag{2}$$

We call (2) the extension of $(A_{11}, K_{11}, C_{11}, I, \mathbf{x}_1, \mathbf{e}_1)$ for $\mathbf{y}$ in block triangular form.

To the best of our knowledge, the results of Lemma 2-3-4 have not been published before; the proofs are not presented here because of the lack of space.

Lemma 2 *Consider a ZMSIR process $\mathbf{y} = [\mathbf{y}_1^T, \mathbf{y}_2^T]^T$ and an observable Kalman representation $(A_{11}, K_{11}, C_{11}, I, \mathbf{x}_1, \mathbf{e}_1)$ of $\mathbf{y}_1$. If $\mathbf{y}_1$ and $\mathbf{y}_2$ mutually do not Granger cause each other then there exists an observable Kalman representation of $\mathbf{y}$ in the form of*

$$\begin{aligned}\sigma\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix} &= \begin{bmatrix}A_{11} & 0\\ 0 & A_{22}\end{bmatrix}\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix} + \begin{bmatrix}K_{11} & 0\\ 0 & K_{22}\end{bmatrix}\begin{bmatrix}\mathbf{e}_1\\ \mathbf{e}_2\end{bmatrix}\\ \begin{bmatrix}\mathbf{y}_1\\ \mathbf{y}_2\end{bmatrix} &= \begin{bmatrix}C_{11} & 0\\ 0 & C_{22}\end{bmatrix}\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix} + \begin{bmatrix}\mathbf{e}_1\\ \mathbf{e}_2\end{bmatrix}\end{aligned} \tag{3}$$

We call (3) the extension of $(A_{11}, K_{11}, C_{11}, I, \mathbf{x}_1, \mathbf{e}_1)$ for $\mathbf{y}$ in block diagonal form.

Lemma 3 *Consider a ZMSIR process $\mathbf{y} = [\mathbf{y}_1^T, \mathbf{y}_2^T, \mathbf{y}_3^T]^T$ and let*

$$S = \left(\begin{bmatrix}A_{11} & 0\\ A_{21} & A_{22}\end{bmatrix}, \begin{bmatrix}K_{11} & 0\\ K_{21} & K_{22}\end{bmatrix}, \begin{bmatrix}C_{11} & 0\\ C_{21} & C_{22}\end{bmatrix}, I, \begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix}, \begin{bmatrix}\mathbf{e}_1\\ \mathbf{e}_2\end{bmatrix}\right)$$

be an observable Kalman representation of $[\mathbf{y}_1^T, \mathbf{y}_2^T]^T$ in block triangular form. If

(I) $\mathbf{y}_2 \not\to \mathbf{y}_1$
(II) $\mathbf{y}_2 \not\to \mathbf{y}_3 | \mathbf{y}_1$
(III) $\mathbf{y}_3 \not\to \mathbf{y}_1$
(IV) $\mathbf{y}_3 \not\to [\mathbf{y}_1^T, \mathbf{y}_2^T]^T$

then there exists an observable Kalman representation of $\mathbf{y}$ in the form of

$$\begin{aligned}\sigma\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\\ \mathbf{x}_3\end{bmatrix} &= \begin{bmatrix}A_{11} & 0 & 0\\ A_{21} & A_{22} & 0\\ A_{31} & 0 & A_{33}\end{bmatrix}\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\\ \mathbf{x}_3\end{bmatrix} + \begin{bmatrix}K_{11} & 0 & 0\\ K_{21} & K_{22} & 0\\ K_{31} & 0 & K_{33}\end{bmatrix}\begin{bmatrix}\mathbf{e}_1\\ \mathbf{e}_2\\ \mathbf{e}_3\end{bmatrix}\\ \begin{bmatrix}\mathbf{y}_1\\ \mathbf{y}_2\\ \mathbf{y}_3\end{bmatrix} &= \begin{bmatrix}C_{11} & 0 & 0\\ C_{21} & C_{22} & 0\\ C_{31} & 0 & C_{33}\end{bmatrix}\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\\ \mathbf{x}_3\end{bmatrix} + \begin{bmatrix}\mathbf{e}_1\\ \mathbf{e}_2\\ \mathbf{e}_3\end{bmatrix}.\end{aligned} \tag{4}$$

We call (4) the extension of S for $\mathbf{y}$ in coordinated form.

In the next lemma we relate Theorem 1 to Lemma 1-2 and Lemma 3. For this, note that for any TADG graph $G = (V,E)$, the set of nodes V has a so-called *topological ordering*. By topological ordering we mean an ordering of V such that for every directed edge $(i,j) \in E$ the node i comes before j in the ordering. From now on, we assume topological ordering for the nodes of TADG graphs. That is, we can assume that if $(i,j) \in E$ then $i < j$. Recall that for a node $j \in V$ we denote the set of parent nodes by $I_j = \{i \in V | (i,j) \in E\}$. Define also the set of preceding non-parent nodes of j by $\bar{I}_j = \{i \in V | i < j, (i,j) \notin E\}$. Note that because of the topological ordering $I_j \cup \bar{I}_j = \{1,\ldots,j-1\}$.

Lemma 4 *Consider a ZMSIR process $\mathbf{y} = [\mathbf{y}_1^T, \ldots, \mathbf{y}_k^T]^T$ and a TADG graph $G = (V,E)$ with $V = \{1,\ldots,k\}$ having topological ordering, and assume that $\mathbf{y}$ is G-consistent. Then for any $j \in V$ the following holds:*

(i) $\mathbf{y}_{\bar{I}_j} \not\to \mathbf{y}_{I_j}$
(ii) $\mathbf{y}_{\bar{I}_j} \not\to \mathbf{y}_j | \mathbf{y}_{I_j}$
(iii) $\mathbf{y}_j \not\to \mathbf{y}_{I_j}$
(iv) $\mathbf{y}_j \not\to [\mathbf{y}_1^T, \ldots, \mathbf{y}_{j-1}^T]^T$.

In case $I_j = \emptyset$, it follows that $\{1,\ldots,j-1\} = \bar{I}_j$ and the Granger causality conditions above simplify to

- $\mathbf{y}_{\bar{I}_j} \not\to \mathbf{y}_j$
- $\mathbf{y}_j \not\to \mathbf{y}_{\bar{I}_j}$.

In case $\bar{I}_j = \emptyset$ it follows that $\{1,\ldots,j-1\} = I_j$ and the Granger causality conditions simplify to $\mathbf{y}_j \not\to \mathbf{y}_{I_j}$.

Before the sketch of the proof of Theorem 1 for an index set, we define sub-matrices on block matrices with partition and the notion of restriction of a graph.

Notation 4 *Consider the block matrix $M \in \mathbb{R}^{n\times m}$ with the partition $\{n_i,m_i\}_{i=1}^{k}$ of (n,m). Then, for $\mathrm{I} := \{i_1,\dots,i_p\}$, $\mathrm{J} := \{j_1,\dots,j_q\}, \subseteq \{1,\dots,k\}$ the sub-matrix M_{IJ} is defined by*

$$M_{\mathrm{IJ}} := \begin{bmatrix} M_{i_1 j_1} & \dots & M_{i_1 j_q} \\ \vdots & \ddots & \vdots \\ M_{i_p j_1} & \dots & M_{i_p j_q} \end{bmatrix}.$$

Notation 5 *The restriction of a TADG graph $G = (V,E)$ with $V = \{1,\dots,k\}$ to $\mathrm{I} := \{i_1,\dots,i_p\} \subseteq V$ is the graph defined by $G|_{\mathrm{I}} := (\{i_1,\dots,i_p\},\{(i,j) \in E | i,j \in \mathrm{I}\})$.*

B. Sketch of the proof of Theorem 1

Consider a ZMSIR process $\mathbf{y} = \left[\mathbf{y}_1^T,\dots,\mathbf{y}_k^T\right]^T$ and a TADG graph $G = (V,E)$ with $V = \{1,\dots,k\}$ such that $\mathbf{y}$ is G-consistent. Using induction on the number of nodes, we will show that with the help of Lemma 1-2 and Lemma 3 a Kalman representation with a G-zero structure can be constructed. Moreover, it also turns out that for $\mathbf{y} = [\mathbf{y}_1^T,\dots,\mathbf{y}_j^T]^T$, $j = 2,\dots,k$ there exists an observable Kalman representation S_j with a $G|_{\{1,\dots,j\}}$-zero structure such that S_j is an extension of S_{j-1}. Recall that the graph $G|_{\{1,\dots,j\}}$ is the restriction of G to the set of vertices $\{1,\dots,j\} \subseteq V$ and note that if G is TADG, then so is $G_{\{1,\dots,j\}}$.

For $k = 2$ there are two cases: either there is edge from the first node to the second $G = (\{1,2\},\{(1,2)\})$ or there is no edge in the graph at all $G = (\{1,2\},\emptyset)$. In the first case, by assumption $\mathbf{y}_2 \not\to \mathbf{y}_1$ and thus from Lemma 1 there exists an observable Kalman representation $(A,K,C,I,\mathbf{x} \in \mathbb{R}^n,\mathbf{e} \in \mathbb{R}^m)$ of $[\mathbf{y}_1^T,\mathbf{y}_2^T]^T$ in block triangular form

$$\begin{aligned} \sigma \begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix} &= \begin{bmatrix}A_{11} & 0\\ A_{21} & A_{22}\end{bmatrix}\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix} + \begin{bmatrix}K_{11} & 0\\ K_{21} & K_{22}\end{bmatrix}\begin{bmatrix}\mathbf{e}_1\\ \mathbf{e}_2\end{bmatrix}\\ \begin{bmatrix}\mathbf{y}_1\\ \mathbf{y}_2\end{bmatrix} &= \begin{bmatrix}C_{11} & 0\\ C_{21} & C_{22}\end{bmatrix}\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix} + \begin{bmatrix}\mathbf{e}_1\\ \mathbf{e}_2\end{bmatrix}. \end{aligned} \tag{5}$$

Defining a partition $n_i = \dim(\mathbf{x}_i)$ and $m_i = \dim(\mathbf{y}_i)$, $i \in \{1,2\}$ it follows that since $A_{n_1,n_2} = 0, K_{n_1,m_2} = 0$ and $C_{m_1,n_2} = 0$ the representation (5) has a G-zero structure. In the second case, by assumption $\mathbf{y}_1 \not\to \mathbf{y}_2$ and $\mathbf{y}_2 \not\to \mathbf{y}_1$ thus from Lemma 2 there exists an observable Kalman representation $(A,K,C,I,\mathbf{x} \in \mathbb{R}^n,\mathbf{e} \in \mathbb{R}^m)$ of $[\mathbf{y}_1^T,\mathbf{y}_2^T]^T$ in block diagonal form

$$\begin{aligned} \sigma \begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix} &= \begin{bmatrix}A_{11} & 0\\ 0 & A_{22}\end{bmatrix}\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix} + \begin{bmatrix}K_{11} & 0\\ 0 & K_{22}\end{bmatrix}\begin{bmatrix}\mathbf{e}_1\\ \mathbf{e}_2\end{bmatrix}\\ \begin{bmatrix}\mathbf{y}_1\\ \mathbf{y}_2\end{bmatrix} &= \begin{bmatrix}C_{11} & 0\\ 0 & C_{22}\end{bmatrix}\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix} + \begin{bmatrix}\mathbf{e}_1\\ \mathbf{e}_2\end{bmatrix}. \end{aligned} \tag{6}$$

Defining the same partition $n_i = \dim(\mathbf{x}_i)$ and $m_i = \dim(\mathbf{y}_i)$, we can see that the representation (6) has a G-zero structure.

Suppose now that we have an observable Kalman representation $(A,K,C,I,\mathbf{x} \in \mathbb{R}^n,\mathbf{e} \in \mathbb{R}^m)$ of $[\mathbf{y}_1^T,\dots,\mathbf{y}_{j-1}^T]^T$ with a $G|_{\{1,\dots,j-1\}}$-zero structure with the partition $\{n_i,m_i\}_{i=1}^{j-1}$ for (n,m). Note that $\mathbf{x}$ is partitioned as $\mathbf{x} = [\mathbf{x}_1^T,\dots,\mathbf{x}_n^T]^T$ where $\mathbf{x}_i \in \mathbb{R}^{n_i}$ and the notation for sub-processes was introduced in Notation 2. Notice that because of $I_j \cup \bar{I}_j = \{1,\dots,j-1\}$ we can define permutation matrices $P_{\mathbf{y}}$ and $P_{\mathbf{x}}$ such that

$$\begin{bmatrix}\mathbf{y}_{I_j}\\ \mathbf{y}_{\bar{I}_j}\end{bmatrix} = P_{\mathbf{y}}\begin{bmatrix}\mathbf{y}_1\\ \vdots\\ \mathbf{y}_{j-1}\end{bmatrix}; \quad \begin{bmatrix}\mathbf{e}_{I_j}\\ \mathbf{e}_{\bar{I}_j}\end{bmatrix} = P_{\mathbf{y}}\begin{bmatrix}\mathbf{e}_1\\ \vdots\\ \mathbf{e}_{j-1}\end{bmatrix}; \quad \begin{bmatrix}\mathbf{x}_{I_j}\\ \mathbf{x}_{\bar{I}_j}\end{bmatrix} = P_{\mathbf{x}}\begin{bmatrix}\mathbf{x}_1\\ \vdots\\ \mathbf{x}_{j-1}\end{bmatrix}.$$

The transitive property of $G|_{\{1,\dots,j-1\}}$ implies that there is no edge from any node in $\bar{I}_j$ to any node in I_j. Hence, since $(A,K,C,I,\mathbf{x},\mathbf{e})$ has a $G|_{\{1,\dots,j-1\}}$-zero structure we know that $A_{li} = 0$, $K_{li} = 0$ and $C_{li} = 0$ for $i \in \bar{I}_j, l \in I_j$ or equivalently, $A_{I_j\bar{I}_j} = 0$, $K_{I_j\bar{I}_j} = 0$ and $C_{I_j\bar{I}_j} = 0$. We discuss three cases now: when I_j is the empty set, when $\bar{I}_j$ is the empty set and when neither I_j nor $\bar{I}_j$ is the empty set. If neither I_j nor $\bar{I}_j$ is the empty set then the representation $(P_{\mathbf{x}}AP_{\mathbf{x}}^{-1},P_{\mathbf{x}}KP_{\mathbf{y}}^{-1},P_{\mathbf{y}}CP_{\mathbf{x}}^{-1},I,P_{\mathbf{x}}\mathbf{x},P_{\mathbf{y}}\mathbf{e})$ is an observable Kalman representation of $[\mathbf{y}_{I_j}^T,\mathbf{y}_{\bar{I}_j}^T]^T$ in the form of

$$\begin{aligned} \sigma \begin{bmatrix}\mathbf{x}_{I_j}\\ \mathbf{x}_{\bar{I}_j}\end{bmatrix} &= \underbrace{\begin{bmatrix}A_{I_jI_j} & 0\\ A_{\bar{I}_jI_j} & A_{\bar{I}_j\bar{I}_j}\end{bmatrix}}_{\tilde{A}}\begin{bmatrix}\mathbf{x}_{I_j}\\ \mathbf{x}_{\bar{I}_j}\end{bmatrix} + \underbrace{\begin{bmatrix}K_{I_jI_j} & 0\\ K_{\bar{I}_jI_j} & K_{\bar{I}_j\bar{I}_j}\end{bmatrix}}_{\tilde{K}}\begin{bmatrix}\mathbf{e}_{I_j}\\ \mathbf{e}_{\bar{I}_j}\end{bmatrix}\\ \begin{bmatrix}\mathbf{y}_{I_j}\\ \mathbf{y}_{\bar{I}_j}\end{bmatrix} &= \underbrace{\begin{bmatrix}C_{I_jI_j} & 0\\ C_{\bar{I}_jI_j} & C_{\bar{I}_j\bar{I}_j}\end{bmatrix}}_{\tilde{C}}\begin{bmatrix}\mathbf{x}_{I_j}\\ \mathbf{x}_{\bar{I}_j}\end{bmatrix} + \begin{bmatrix}\mathbf{e}_{I_j}\\ \mathbf{e}_{\bar{I}_j}\end{bmatrix}. \end{aligned} \tag{7}$$

From Lemma 4 the conditions of Lemma 3 are satisfied for the process $[\mathbf{y}_{I_j}^T,\mathbf{y}_{\bar{I}_j}^T,\mathbf{y}_j^T]^T$. Applying Lemma 3 for $[\mathbf{y}_{I_j}^T,\mathbf{y}_{\bar{I}_j}^T,\mathbf{y}_j^T]^T$ and (7) we obtain an observable Kalman representation, that is the extension of (7) for $[\mathbf{y}_{I_j}^T,\mathbf{y}_{\bar{I}_j}^T,\mathbf{y}_j^T]^T$ in coordinated form

$$\begin{aligned} \sigma \begin{bmatrix}\mathbf{x}_{I_j}\\ \mathbf{x}_{\bar{I}_j}\\ \mathbf{x}_j\end{bmatrix} &= \begin{bmatrix}A_{I_jI_j} & 0 & 0\\ A_{\bar{I}_jI_j} & A_{\bar{I}_j\bar{I}_j} & 0\\ A_{jI_j} & 0 & A_{jj}\end{bmatrix}\begin{bmatrix}\mathbf{x}_{I_j}\\ \mathbf{x}_{\bar{I}_j}\\ \mathbf{x}_j\end{bmatrix} + \begin{bmatrix}K_{I_jI_j} & 0 & 0\\ K_{\bar{I}_jI_j} & K_{\bar{I}_j\bar{I}_j} & 0\\ K_{jI_j} & 0 & K_{jj}\end{bmatrix}\begin{bmatrix}\mathbf{e}_{I_j}\\ \mathbf{e}_{\bar{I}_j}\\ \mathbf{e}_j\end{bmatrix}\\ \begin{bmatrix}\mathbf{y}_{I_j}\\ \mathbf{y}_{\bar{I}_j}\\ \mathbf{y}_j\end{bmatrix} &= \begin{bmatrix}C_{I_jI_j} & 0 & 0\\ C_{\bar{I}_jI_j} & C_{\bar{I}_j\bar{I}_j} & 0\\ C_{jI_j} & 0 & C_{jj}\end{bmatrix}\begin{bmatrix}\mathbf{x}_{I_j}\\ \mathbf{x}_{\bar{I}_j}\\ \mathbf{x}_j\end{bmatrix} + \begin{bmatrix}\mathbf{e}_{I_j}\\ \mathbf{e}_{\bar{I}_j}\\ \mathbf{e}_j\end{bmatrix}. \end{aligned} \tag{8}$$

To transform (8) into a representation of $\mathbf{y}_{\{1,\dots,j\}}$, apply the inverse permutation transformations $P_{\mathbf{x}}^{-1}$ and $P_{\mathbf{y}}^{-1}$ for the sub-processes and sub-matrices indexed by $I_j \cup \bar{I}_j$ such as

$$\left(P_{\mathbf{x}}^{-1}\tilde{A}P_{\mathbf{x}},P_{\mathbf{x}}^{-1}\tilde{K}P_{\mathbf{y}},P_{\mathbf{y}}^{-1}\tilde{C}P_{\mathbf{x}},I,P_{\mathbf{x}}^{-1}\begin{bmatrix}\mathbf{x}_{I_j}\\ \mathbf{x}_{\bar{I}_j}\end{bmatrix},P_{\mathbf{y}}^{-1}\begin{bmatrix}\mathbf{e}_{I_j}\\ \mathbf{e}_{\bar{I}_j}\end{bmatrix}\right).$$

Then, for the ordered index set $J := \{1,\dots,j-1\}$ we obtain that after the transformation above (8) becomes

$$\begin{aligned} \sigma \begin{bmatrix}\mathbf{x}_J\\ \mathbf{x}_j\end{bmatrix} &= \begin{bmatrix}P_{\mathbf{x}}^{-1}\tilde{A}P_{\mathbf{x}} & 0\\ \begin{bmatrix}A_{jI_j} & 0\end{bmatrix}P_{\mathbf{x}} & A_{jj}\end{bmatrix}\begin{bmatrix}\mathbf{x}_J\\ \mathbf{x}_j\end{bmatrix} + \begin{bmatrix}P_{\mathbf{x}}^{-1}\tilde{K}P_{\mathbf{y}} & 0\\ \begin{bmatrix}K_{jI_j} & 0\end{bmatrix}P_{\mathbf{y}} & K_{jj}\end{bmatrix}\begin{bmatrix}\mathbf{e}_J\\ \mathbf{e}_j\end{bmatrix}\\ \begin{bmatrix}\mathbf{y}_{I_j}\\ \mathbf{y}_j\end{bmatrix} &= \begin{bmatrix}P_{\mathbf{y}}^{-1}\tilde{C}P_{\mathbf{x}} & 0\\ \begin{bmatrix}C_{jI_j} & 0\end{bmatrix}P_{\mathbf{x}} & C_{jj}\end{bmatrix}\begin{bmatrix}\mathbf{x}_J\\ \mathbf{x}_j\end{bmatrix} + \begin{bmatrix}\mathbf{e}_J\\ \mathbf{e}_j\end{bmatrix}. \end{aligned} \tag{9}$$

The representation (9) is an observable Kalman representation of $\mathbf{y}_{\{1,\dots,j\}}$; it is because $[\mathbf{e}_J^T,\mathbf{e}_j^T]^T$ is the innovation process of $\mathbf{y}_{\{1,\dots,j\}}$ and $(\tilde{A},\tilde{C})$ together with (A_{jj},C_{jj}) are observable pairs. Furthermore, $A_{ji} = 0$, $K_{ji} = 0$ and $C_{ji} = 0$

for any $i \in \bar{I}_j$ and $A = P_{\mathbf{x}}^{-1}\tilde{A}P_{\mathbf{x}}$, $K = P_{\mathbf{x}}^{-1}\tilde{K}P_{\mathbf{y}}$ and $C = P_{\mathbf{y}}^{-1}\tilde{C}P_{\mathbf{x}}$. Therefore, (9) is an observable Kalman representation of $\mathbf{y}_{1,\dots,j}$ with a $G|_{\{1,\dots,j\}}$-zero structure for the partitioning $\{n_i, m_i\}_{i=1}^{j}$ where $n_j = \dim(\mathbf{x}_j)$, $m_j = \dim(\mathbf{y}_j)$.

When $\bar{I}_j = \emptyset$ then the representation of $[\mathbf{y}_{\{1,\dots,j-1\}}^T, \mathbf{y}_j^T]^T$ with a G-zero structure is in block triangular form. Similarly, when $I_j = \emptyset$ then the representation of $[\mathbf{y}_{\{1,\dots,j-1\}}^T, \mathbf{y}_j^T]^T$ with a G-zero structure is in block diagonal form. In these cases we can leave aside to use permutation transformations and can directly apply Lemma 1 or Lemma 2. If $\bar{I}_j = \emptyset$ then $I_j = \{1,\dots,j-1\}$ and thus from condition (iv) in Lemma 4 we can apply Lemma 1 to obtain an observable Kalman representation of $[\mathbf{y}_{\{1,\dots,j-1\}}^T, \mathbf{y}_j^T]^T$ in block triangular form, i.e., with a $G|_{\{1,\dots,j\}}$-zero structure. If $I_j = \emptyset$ then $\bar{I}_j = \{1,\dots,j-1\}$ and thus from condition (iv) in Lemma 4 we can apply Lemma 2 to obtain an observable Kalman representation of $[\mathbf{y}_{\{1,\dots,j-1\}}^T, \mathbf{y}_j^T]^T$ in block diagonal form i.e., with a $G|_{\{1,\dots,j\}}$-zero structure. With this, the induction for the nodes is completed.

In summary, for a G-consistent ZMSIR process $\mathbf{y} = [\mathbf{y}_1^T, \dots, \mathbf{y}_k^T]^T$ we can construct a Kalman representation with a G-zero structure in the following way: we start with a Kalman representation of $\mathbf{y}_1$ and extend it for $[\mathbf{y}_1^T, \mathbf{y}_2^T]^T$ applying Lemma 1, Lemma 2 (or Lemma 3) depending on the causal relation between $\mathbf{y}_1$ and $\mathbf{y}_2$. Then, we continue this step for $j = 2,\dots,k$ extending the representation of $[\mathbf{y}_1^T, \dots, \mathbf{y}_{j-1}^T]^T$ for $[\mathbf{y}_1^T, \dots \mathbf{y}_j^T]^T$ depending on the causal relation between $\mathbf{y}_{1,\dots,j-1}$ and $\mathbf{y}_j$. Kalman representations of ZMSIR processes can be calculated from the second order statistics of the process. Therefore, all the representations presented here can be calculated form output data of an LTI-SS representation.

V. Conclusion

In this paper we have studied the relationship between the causality structure of the observed behavior of a stochastic LTI system and the graph structure of its state-space representation. The former is determined by statistical properties (conditional Granger causality) of the output process, the latter by the subsystems which form the state-space representation. That is, we have shown that the internal interconnection structure of an LTI system can be read of from the statistical properties of its observed output.

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