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# IDENTIFIABILITY IN CONTINUOUS LYAPUNOV MODELS

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September 9, 2022

## ABSTRACT

The recently introduced graphical continuous Lyapunov models provide a new approach to statistical modeling of correlated multivariate data. The models view each observation as a one-time cross-sectional snapshot of a multivariate dynamic process in equilibrium. The covariance matrix for the data is obtained by solving a continuous Lyapunov equation that is parametrized by the drift matrix of the dynamic process. In this context, different statistical models postulate different sparsity patterns in the drift matrix, and it becomes a crucial problem to clarify whether a given sparsity assumption allows one to uniquely recover the drift matrix parameters from the covariance matrix of the data. We study this identifiability problem by representing sparsity patterns by directed graphs. Our main result proves that the drift matrix is globally identifiable if and only if the graph for the sparsity pattern is simple (i.e., does not contain directed two-cycles). Moreover, we present a necessary condition for generic identifiability and provide a computational classification of small graphs with up to 5 nodes.

**Keywords** Covariance matrix · Graphical Modelling · Lyapunov Equation · Parameter Identification

## 1 Introduction

In this paper, we study statistical models in which the covariance matrix  $\Sigma$  of random multivariate observations in  $\mathbb{R}^p$  is the solution of a continuous Lyapunov equation

$$M\Sigma + \Sigma M^\top + C = 0, \tag{1}$$

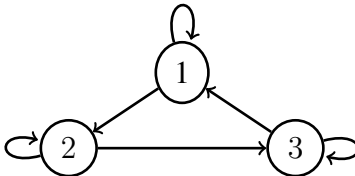
where the matrices  $M, C \in \mathbb{R}^{p \times p}$  play the role of parameters. This setting arises from work of Fitch (2019) and Varando and Hansen (2020) who propose a new approach to probabilistic graphical modeling (Maathuis et al., 2019). When capturing cause-effect relations among observations,

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**Figure 1:** The directed 3-cycle.

standard graphical models directly postulate noisy functional relations among the considered random variables (Pearl, 2009; Peters et al., 2017; Spirtes et al., 2000). In contrast, the new Lyapunov models view an available sample of  $n$  independent and identically distributed random vectors as cross-sectional observations of  $p$ -dimensional dynamic processes in equilibrium. A similar perspective was presented by Young et al. (2019) for discrete time autoregressive models, which leads to an equilibrium covariance matrix solving the *discrete* Lyapunov equation. Explicitly introducing a temporal perspective simplifies, in particular, modeling of feedback loops. When working in continuous time, the natural process to consider is the Ornstein-Uhlenbeck process which leads to precisely the setting in (1). In this context, the matrix  $M$  is a drift matrix that quantifies temporal cause-effect relations among the variables, and  $C$  is a positive definite volatility matrix. For the Lyapunov equation to yield a positive definite covariance matrix  $\Sigma$ , the matrix  $M$  has to be stable (all eigenvalues have a strictly negative real part).

A graphical continuous Lyapunov model as defined by Fitch (2019) and Varando and Hansen (2020) refines this setup by assuming that the drift matrix  $M = (m_{ij})$  exhibits a specific zero pattern that is given by a directed graph  $G$  on the set of nodes  $[p] = \{1, \dots, p\}$ , with  $m_{ji} = 0$  whenever  $i \rightarrow j$  is not an edge in  $G$ . In this setting our graphs will always include self-loops  $i \rightarrow i$ .

**Example 1.** *The directed 3-cycle  $G$  with vertex set  $V = \{1, 2, 3\}$  and edge set  $E = \{1 \rightarrow 1, 2 \rightarrow 2, 3 \rightarrow 3, 1 \rightarrow 2, 2 \rightarrow 3, 3 \rightarrow 1\}$ , which is displayed in Figure 1, encodes drift matrices of the form*

$$M = \begin{pmatrix} m_{11} & 0 & m_{13} \\ m_{21} & m_{22} & 0 \\ 0 & m_{32} & m_{33} \end{pmatrix}.$$

The Lyapunov equation from (1) is a symmetric matrix equation providing  $p(p+1)/2$  constraints. In contrast, the drift matrix  $M$  is a  $p \times p$  matrix that need not be symmetric. Hence, without any assumptions on its structure,  $M$  is never uniquely determined by the covariance matrix  $\Sigma$  of the observations. For graphical Lyapunov models, this leads to a key identifiability question: For which sparsity patterns can the drift matrix  $M$  be recovered from the positive definite covariance matrix  $\Sigma$ ? Our treatment of this question will assume that the volatility matrix  $C$  is a known positive definite matrix. Our main focus will be on the case where  $C$  is diagonal (i.e., the  $p$  noise processes driving the considered multivariate dynamic process are independent).

**Remark 2.** *Evidently, if a matrix  $\Sigma$  solves the Lyapunov equation (1) for a pair  $(M, C)$  then  $\Sigma$  also solves the equation given by  $(\gamma M, \gamma C)$  for any  $\gamma \in \mathbb{R}$ . An implication of this fact is that our results on recovery of  $M$  for fixed  $C$  also address the setting of models in which  $C = \gamma C'$ , with  $C'$  known and positive definite but  $\gamma > 0$  an unknown parameter. In this latter setting, one can only hope to recover  $M$  up to a scalar multiple and this is possible if and only if  $M$  can be recovered uniquely in the setting where we fix  $C = C'$ .*

Before proceeding to illustrate the identifiability problem for Example 1, we give a formal definition of graphical continuous Lyapunov models as sets of covariance matrices. We write  $\text{PD}_p$  for the cone of  $p \times p$  positive definite matrices.

**Definition 3.** Let  $G = (V, E)$  be a directed graph with vertex set  $V = [p]$  and an edge set  $E$  that includes all self-loops  $i \rightarrow i$ ,  $i \in [p]$ . Given a choice of  $C \in \text{PD}_p$ , the graphical continuous Lyapunov model of  $G$  is the set of covariance matrices

$$\mathcal{M}_{G,C} = \{\Sigma \in \text{PD}_p : M\Sigma + \Sigma M^\top = -C \text{ with } M \in \mathbb{R}^E\},$$

where we write  $\mathbb{R}^E$  for the space of matrices  $M = (m_{ij}) \in \mathbb{R}^{p \times p}$  with  $m_{ji} = 0$  whenever  $i \rightarrow j \notin E$ .

**Remark 4.** Let  $\text{Stab}(E) \subseteq \mathbb{R}^E$  be the subset of stable matrices, which is always non-empty and open. When  $C$  is positive definite, the Lyapunov equation from (1) has a positive definite solution  $\Sigma$  if and only if  $M$  is stable (Bhaya et al., 2003, Theorem 1.1). Hence, the definition of the model  $\mathcal{M}_{G,C}$  remains unchanged if we replace the requirement  $M \in \mathbb{R}^E$  by  $M \in \text{Stab}(E)$ .

The identifiability question we pose asks if a covariance matrix  $\Sigma$  in the model  $\mathcal{M}_{G,C}$  may simultaneously solve the Lyapunov equation for more than one choice of a matrix  $M \in \mathbb{R}^E$ . In other words, we study the injectivity of the (rational) parametrization map

$$\begin{aligned} \phi_{G,C} : \text{Stab}(E) &\rightarrow \text{PD}_p \\ M &\mapsto \Sigma(M, C), \end{aligned} \tag{2}$$

where  $\Sigma(M, C)$  is the unique matrix  $\Sigma$  that solves the Lyapunov equation given by the stable matrix  $M$  and positive definite  $C$ . See (6) for details on this uniqueness.

**Example 5.** By vectorization, the Lyapunov equation (1) is transformed into the linear equation system

$$A(\Sigma)\text{vec}(M) = -\text{vech}(C), \tag{3}$$

where  $\text{vech}(C)$  is the half-vectorization of a fixed symmetric matrix  $C \in \text{PD}_p$ , and  $A(\Sigma)$  is a  $p(p+1)/2 \times p^2$  matrix depending on  $\Sigma$  whose form will be discussed in Section 3. In the case of  $p = 3$  variables the matrix  $A(\Sigma)$  equals

$$\begin{array}{l} (1,1) \\ (1,2) \\ (1,3) \\ (2,2) \\ (2,3) \\ (3,3) \end{array} \begin{pmatrix} 1 \rightarrow 1 & 1 \rightarrow 2 & 1 \rightarrow 3 & 2 \rightarrow 1 & 2 \rightarrow 2 & 2 \rightarrow 3 & 3 \rightarrow 1 & 3 \rightarrow 2 & 3 \rightarrow 3 \\ 2\Sigma_{11} & 0 & 0 & 2\Sigma_{12} & 0 & 0 & 2\Sigma_{13} & 0 & 0 \\ \Sigma_{12} & \Sigma_{11} & 0 & \Sigma_{22} & \Sigma_{12} & 0 & \Sigma_{23} & \Sigma_{13} & 0 \\ \Sigma_{13} & 0 & \Sigma_{11} & \Sigma_{23} & 0 & \Sigma_{12} & \Sigma_{33} & 0 & \Sigma_{13} \\ 0 & 2\Sigma_{12} & 0 & 0 & 2\Sigma_{22} & 0 & 0 & 2\Sigma_{23} & 0 \\ 0 & \Sigma_{13} & \Sigma_{12} & 0 & \Sigma_{23} & \Sigma_{22} & 0 & \Sigma_{33} & \Sigma_{23} \\ 0 & 0 & 2\Sigma_{13} & 0 & 0 & 2\Sigma_{23} & 0 & 0 & 2\Sigma_{33} \end{pmatrix}$$

where the column index  $i \rightarrow j$  corresponds to entry  $m_{ji}$  of the drift matrix  $M = (m_{ij})$ .

Consider the 3-cycle  $G$  from Example 1. Then unique solvability of (3) for  $M \in \mathbb{R}^E$  is equivalent to a submatrix of  $A(\Sigma)$  being invertible, namely, the submatrix

$$A(\Sigma)_{.,E} = \begin{matrix} & \begin{matrix} 1 \rightarrow 1 & 1 \rightarrow 2 & 2 \rightarrow 2 & 2 \rightarrow 3 & 3 \rightarrow 1 & 3 \rightarrow 3 \end{matrix} \\ \begin{matrix} (1, 1) \\ (1, 2) \\ (1, 3) \\ (2, 2) \\ (2, 3) \\ (3, 3) \end{matrix} & \left( \begin{array}{cccccc} 2\Sigma_{11} & 0 & 0 & 0 & 2\Sigma_{13} & 0 \\ \Sigma_{12} & \Sigma_{11} & \Sigma_{12} & 0 & \Sigma_{23} & 0 \\ \Sigma_{13} & 0 & 0 & \Sigma_{12} & \Sigma_{33} & \Sigma_{13} \\ 0 & 2\Sigma_{12} & 2\Sigma_{22} & 0 & 0 & 0 \\ 0 & \Sigma_{13} & \Sigma_{23} & \Sigma_{22} & 0 & \Sigma_{23} \\ 0 & 0 & 0 & 2\Sigma_{23} & 0 & 2\Sigma_{33} \end{array} \right) \end{matrix}$$

To show invertibility of  $A(\Sigma)_{.,E}$ , we may inspect its determinant, which factorizes as

$$\det(A(\Sigma)_{.,E}) = 2^3 \cdot \det(\Sigma) \cdot (\Sigma_{11}\Sigma_{22}\Sigma_{33} - \Sigma_{12}\Sigma_{13}\Sigma_{23}). \quad (4)$$

All displayed factors are positive when  $\Sigma$  is positive definite. Indeed,  $\det(\Sigma) > 0$  and the fact that  $\det(\Sigma_{ij,ij}) = \Sigma_{ii}\Sigma_{jj} - \Sigma_{ij}^2 > 0$  for all  $i \neq j$  implies that  $\Sigma_{11}^2\Sigma_{22}^2\Sigma_{33}^2 > \Sigma_{12}^2\Sigma_{13}^2\Sigma_{23}^2$ , which clarifies that the last factor is also positive. Alternatively, we can show this using the identity

$$\begin{aligned} & (\Sigma_{11}\Sigma_{22}\Sigma_{33})^2 - (\Sigma_{12}\Sigma_{13}\Sigma_{23})^2 = \\ & (\Sigma_{13}\Sigma_{23})^2 \det(\Sigma_{12,12}) + \Sigma_{11}\Sigma_{22}\Sigma_{23}^2 \det(\Sigma_{13,13}) + \Sigma_{11}^2\Sigma_{22}\Sigma_{33} \det(\Sigma_{23,23}) > 0. \end{aligned}$$

We conclude that when  $G$  is the 3-cycle, then for all covariance matrices  $\Sigma \in \mathcal{M}_{G,C} \subseteq \text{PD}_3$  there is a unique matrix  $M \in \mathbb{R}^E$  such that  $\Sigma = \phi_{G,C}(M)$ . We will refer to this property as the 3-cycle defining a globally identifiable model. Note that our argument also shows that  $\mathcal{M}_{G,C} = \text{PD}_3$ .

This small example already reveals some of the subtleties arising when analyzing identifiability of continuous Lyapunov models. The problem can be reduced to determining whether a particular submatrix that is sparsely populated with covariances has full rank (see Lemma 19 and Lemma 27) but the resulting matrices have involved graph-dependent structures. While the case of directed acyclic graphs can be approached without much effort and one obtains identifiability for all associated models (Theorem 22), cyclic graphs are more difficult to handle. For cyclic graphs, the polynomials that appear while factoring determinants, as in (4), quickly increase in complexity, and it is not easy to determine whether they are non-zero. In our main result (Theorem 31) we thus consider alternative spectral arguments that use the stability of the drift matrix  $M$  in order to derive identifiability.

## Organization and results of the paper

In Section 2 we introduce the notions of generic and global identifiability and make some preliminary observations. In Section 3, we explain the structure of the matrix  $A(\Sigma)$  that arises from (half-)vectorization of the Lyapunov equation. We also highlight how the rank of a submatrix of  $A(\Sigma)$  determines generic and global identifiability of a model. Exploiting block structure in the relevant submatrix of  $A(\Sigma)$ , we prove global identifiability for all directed acyclic graphs (DAGs) in Section 4. Our proof also yields that the models given by DAGs are closed algebraic subsets of  $\text{PD}_p$ , and that the models associated to complete DAGs are equal to  $\text{PD}_p$  (Corollary 23). In Section 5, we turn to cyclic graphs for which the relevant matrices no longer exhibit block structure. We demonstrate that for small graphs the approach studying factorizations of determinants can still

be implemented using sum of squares methods to certify that the relevant polynomials are positive on  $\text{PD}_p$ . In Section 6 we present our main result (Theorem 31), which proves that global model identifiability holds if the underlying graph is simple (i.e., does not contain any 2-cycle). If  $C$  is diagonal—the case of primary practical interest, then the requirement that the graph be simple is also necessary for global identifiability. Moreover, we are able to show that for all  $C \in \text{PD}_p$ , all simple graphs yield models  $\mathcal{M}_{G,C}$  that are closed algebraic subsets of  $\text{PD}_p$ . We discuss further the diagonal hypothesis on  $C$  in Appendix A. In Section 7, we turn to the weaker notion of generic identifiability, for which we develop a necessary criterion and computationally classify all non-simple graphs with up to 5 nodes. The paper concludes in Section 8. Some details on the structure of the matrix  $A(\Sigma)$  and the factorization of its minors are deferred to Appendix B.

The code we used for our computations is available at the repository website <https://mathrepo.mis.mpg.de/LyapunovIdentifiability>.

## 2 Notions of identifiability

We begin by recalling the concept of fibers that is useful to define the different notions of identifiability we study in subsequent sections. Let  $C \in \text{PD}_p$ , and let  $\mathcal{M}_{G,C}$  be the graphical continuous Lyapunov model associated to a directed graph  $G = (V, E)$  with vertex set  $V = [p]$  and edge set  $E$ . Let  $\phi_{G,C}$  be the parametrization from (2). The *fiber* of a matrix  $M_0 \in \text{Stab}(E)$  is the set

$$\mathcal{F}_{G,C}(M_0) = \{M \in \text{Stab}(E) : \phi_{G,C}(M) = \phi_{G,C}(M_0)\}. \quad (5)$$

In other words, a fiber comprises all drift matrices  $M \in \mathbb{R}^E$  whose Lyapunov equation (for the fixed matrix  $C \in \text{PD}_p$ ) is solved by a given covariance matrix  $\Sigma$ .

We will consider three natural notions of identifiability.

**Definition 6.** Let  $\mathcal{M}_{G,C}$  be the graphical continuous Lyapunov model given by a directed graph  $G = (V, E)$  with  $V = [p]$  and  $C \in \text{PD}_p$ . The model  $\mathcal{M}_{G,C}$  is

- (i) globally identifiable if  $\mathcal{F}_{G,C}(M_0) = \{M_0\}$  for all  $M_0 \in \text{Stab}(E)$ ;
- (ii) generically identifiable if  $\mathcal{F}_{G,C}(M_0) = \{M_0\}$  for almost all  $M_0 \in \text{Stab}(E)$ , i.e., the matrices with  $\mathcal{F}_{G,C}(M_0) \neq \{M_0\}$  form a Lebesgue null set in  $\mathbb{R}^E$ ;
- (iii) non-identifiable if  $|\mathcal{F}_{G,C}(M_0)| = \infty$  for all  $M_0 \in \text{Stab}(E)$ .

**Remark 7.** The generic properties we prove in this paper are derived by showing that they hold outside a strict subset of  $\text{Stab}(E)$  that is described by polynomials in the entries of the drift matrix; see e.g. Lemma 19. Hence, in a generically identifiable model the exception set is not merely a set of Lebesgue measure zero, but also a lower-dimensional algebraic subset of  $\text{Stab}(E)$ .

**Remark 8.** Characterizing identifiability is also a key problem for standard directed graphical models; see Drton (2018) and Sullivant (2018, Chap. 16) for a discussion of the different notions of identifiability in this context. For standard graphical models, necessary and sufficient conditions for global identifiability have been obtained (Drton et al., 2011). However, many models of interest are not globally identifiable, and much work has also gone into criteria for generic identifiability (Brito and Pearl, 2006; Drton and Weihs, 2016; Foygel et al., 2012; Kumor et al., 2019).

The 3-cycle from Example 5 is an example of global identifiability. Under global identifiability, no two distinct stable matrices may define the same covariance matrix in the model given by the graph. Unfortunately, this is not always the case.

**Example 9.** Consider the 2-cycle  $G = (V, E)$  with  $V = \{1, 2\}$  and  $E = \{1 \rightarrow 1, 2 \rightarrow 2, 1 \rightarrow 2, 2 \rightarrow 1\}$ . Then  $\phi_{G,C}$  maps the 4-dimensional parameter space  $\text{Stab}(E)$  to the 3-dimensional  $\text{PD}_2$ -cone. Hence, when computing any fiber we have to solve a linear system that is underdetermined, with 3 equations in 4 unknowns. Therefore,  $\mathcal{M}_{G,C}$  is non-identifiable, no matter the choice of  $C \in \text{PD}_2$ .

The example just given generalizes as follows:

**Lemma 10.** Let  $G = (V, E)$  be a directed graph with vertex set  $V = [p]$ , and let  $C \in \text{PD}_p$ . If  $|E| > \dim(\mathcal{M}_{G,C})$ , i.e., the number of free parameters in  $\text{Stab}(E)$  is greater than the dimension of the model, then  $\mathcal{M}_{G,C}$  is non-identifiable. In particular, all graphs with  $|E| > p(p+1)/2$  give non-identifiable models.

*Proof.* By the Hurwitz criterion, the set of sparse stable matrices  $\text{Stab}(E)$  is semialgebraic, see Horn and Johnson (1991, Theorem 2.3.3). As its dimension is  $\dim(\text{Stab}(E)) = |E| > \dim(\mathcal{M}_{G,C})$ , it follows that the rational map  $\phi_{G,C}$  defined on  $\text{Stab}(E)$  is generically infinite-to-one; see, e.g., Barber et al. (2022, Lemma 2.5). Apply lemma 19 below to conclude that all fibers are infinite.  $\square$

A straightforward but very useful fact when studying global identifiability is that if a graph  $G = (V, E)$  yields a globally identifiable model then so does every subgraph  $H = (V, E')$ ,  $E' \subseteq E$ , that is obtained by removing edges of the form  $i \rightarrow j$  with  $i \neq j$ . We record this fact as:

**Proposition 11.** Let  $\mathcal{M}_{G,C}$  be a globally identifiable model given by a directed graph  $G = (V, E)$  with  $V = [p]$  and  $C \in \text{PD}_p$ . Let  $E' \subset E$  be a subset of the edges. Then the model  $\mathcal{M}_{H,C}$  defined by the subgraph  $H = (V, E')$  is globally identifiable.

*Proof.* It holds that  $\text{Stab}(E') \subseteq \text{Stab}(E)$ . Therefore, for every matrix  $M_0 \in \text{Stab}(E')$ , we have  $\mathcal{F}_{H,C}(M_0) \subseteq \mathcal{F}_{G,C}(M_0) = \{M_0\}$ , where the last equality is due to the assumed global identifiability of  $\mathcal{M}_{G,C}$ .  $\square$

In the case where  $C$  is diagonal, further conclusions can be made.

**Proposition 12.** Let  $G = (V, E)$  be a directed graph with  $V = [p]$ . Let  $C \in \text{PD}_p$  be diagonal, and let  $I_p$  be the  $p \times p$  identity matrix. Then the models for  $C$  versus  $I_p$  are isomorphic, and so are their fibers:

- (i)  $\mathcal{M}_{G,C} = C^{1/2}\mathcal{M}_{G,I_p}C^{1/2}$ , and
- (ii)  $\mathcal{F}_{G,C}(M) = \mathcal{F}_{G,I_p}(C^{1/2}MC^{-1/2})$  for all  $M \in \text{Stab}(E)$ .

In particular,  $\mathcal{M}_{G,C}$  is globally/generically identifiable if and only if  $\mathcal{M}_{G,I_p}$  is globally/generically identifiable.

*Proof.* Since  $C$  is diagonal, the similarity transformation  $\tau_1 : M \mapsto C^{-1/2}MC^{1/2}$  is an automorphism of  $\mathbb{R}^E$ , with  $\tau_1(\text{Stab}(E)) = \text{Stab}(E)$ . Define a second linear map  $\tau_2 : \Sigma \mapsto C^{-1/2}\Sigma C^{-1/2}$ , an automorphism of the space of symmetric matrices with  $\tau_2(\text{PD}_p) = \text{PD}_p$ . Now

$$\begin{aligned} M\Sigma + \Sigma M^\top + C = 0 &\iff \\ (C^{-1/2}MC^{1/2})(C^{-1/2}\Sigma C^{-1/2}) + (C^{-1/2}\Sigma C^{-1/2})(C^{-1/2}MC^{1/2})^\top + I_p &= 0. \end{aligned}$$

Thus,  $\mathcal{M}_{G,I_p} = \tau_2(\mathcal{M}_{G,C})$  and  $\mathcal{F}_{G,I_p}(M) = \mathcal{F}_{G,C}(\tau_1^{-1}(M))$ .  $\square$

In Proposition 11 only edges are removed when forming a subgraph. When  $C$  is diagonal we may strengthen the result to subgraphs in which we also remove vertices; compare Drton et al. (2011, Lemma 1) in the context of standard graphical models.

**Proposition 13.** *Let  $G = (V, E)$  be a directed graph with  $V = [p]$ , and let  $H = (V', E')$  be a subgraph with  $V' \subseteq V$  and  $E' \subseteq E$ . If the model  $\mathcal{M}_{G,C}$  is globally identifiable for a diagonal matrix  $C \in \text{PD}_p$ , then  $\mathcal{M}_{H,C'}$  is globally identifiable for all diagonal matrices  $C' \in \text{PD}_{p'}$ , where  $p' = |V'|$ .*

*Proof.* By Proposition 11, it suffices to prove that removing an isolated vertex from  $G$  preserves global identifiability of the model for  $C$  diagonal. By Proposition 12, we may assume that  $C = I_p$  and  $C' = I_{p-1}$ , where  $p$  is an isolated node of  $G$ . Let  $M \in \text{Stab}(E)$ , and let  $M_{[p-1],[p-1]}$  be the submatrix comprising the first  $p-1$  rows and columns. Since  $p$  is isolated, the  $p$ th row and column of  $M$  is zero with the exception of the diagonal entry  $m_{pp}$ . It is not difficult to see that  $\Sigma = \phi_{G,I_p}(M)$  also has its  $p$ th row and column equal to zero except for the diagonal entry which equals  $\Sigma_{pp} = -1/(2m_{pp})$ . Hence, the entry  $m_{pp}$  is always uniquely determined by  $\Sigma$ , and we conclude that the cardinality of the fiber  $\mathcal{F}_{G,I_p}(M)$  is equal to the cardinality of  $\mathcal{F}_{H,I_{p-1}}(M_{[p-1],[p-1]})$ . Since every matrix in  $\text{Stab}(E')$  is a submatrix  $M_{[p-1],[p-1]}$  of a matrix  $M \in \text{Stab}(E)$ , the model  $\mathcal{M}_{H,I_{p-1}}$  is globally identifiable.  $\square$

Combining Proposition 13 with Example 9, we obtain that the graph of a globally identifiable model cannot contain any 2-cycles.

**Definition 14.** *A directed graph  $G = (V, E)$  is simple if it is free of 2-cycles, i.e., there do not exist two distinct nodes  $i, j \in V$  such that  $i \rightarrow j \in E$  and  $j \rightarrow i \in E$ . Otherwise, we call  $G$  non-simple.*

**Proposition 15.** *If a directed graph  $G = (V, E)$ ,  $V = [p]$ , defines a globally identifiable model  $\mathcal{M}_{G,C}$  when  $C \in \text{PD}_p$  is diagonal, then  $G$  must be simple.*

**Remark 16.** *Proposition 13 and Proposition 15 may fail for non-diagonal  $C \in \text{PD}_p$ . See Appendix A for an example.*

Unfortunately, similar subgraph arguments cannot be made for generic instead of global identifiability. Indeed, generic identifiability may be lost but also restored when removing an edge. Example 36 illustrates this phenomenon.

### 3 Rank conditions

In this section, we discuss solving the Lyapunov equation (1) for the generally non-symmetric drift matrix  $M$  given the symmetric matrices  $\Sigma$  and  $C$ . We will proceed by vectorizing the Lyapunov equation, and we will state necessary and sufficient conditions for identifiability based on the ranks of submatrices of the coefficient matrix  $A(\Sigma)$  of the vectorized Lyapunov equation.

First, recall that when the matrices  $M$  and  $C$  are given, the continuous Lyapunov equation from (1) is uniquely solvable for the symmetric matrix  $\Sigma$  if and only if no two eigenvalues of  $M$  add up to zero. This well known fact can be shown by vectorizing the equation to

$$(I_p \otimes M + M \otimes I_p)\text{vec}(\Sigma) = -\text{vec}(C), \quad (6)$$

where  $\otimes$  is the Kronecker product and  $\text{vec}(\cdot)$  is the columnwise vectorization of a matrix; see, e.g., Bernstein (2011). The coefficient matrix  $I_p \otimes M + M \otimes I_p$  is a Kronecker sum, and it follows that

its eigenvalues are the pairwise sums of the eigenvalues of  $M$ . If we now additionally assume that  $C$  is positive definite, then Lyapunov's theorem (Horn and Johnson, 1991, Theorem 2.2.1) yields that the Lyapunov equation from (1) has a unique positive definite solution  $\Sigma$  if and only if  $M$  is a stable matrix.

However, solving for  $M$  given two symmetric (and in our context positive definite) matrices  $\Sigma$  and  $C$  is a more difficult question. In general, it is not possible to have a unique solution for  $M$  due to the dimensionality problems mentioned in Lemma 10. The graphical perspective of the Lyapunov models motivates considering sparse matrices  $M$  and asking the solvability question in a new light, as we illustrated in Example 5.

**Lemma 17.** *Vectorizing the Lyapunov equation (1), we obtain the system*

$$((\Sigma \otimes I_p) + (I_p \otimes \Sigma)K_p)\text{vec}(M) = -\text{vec}(C), \quad (7)$$

where  $K_p$  is the  $p \times p$  commutation matrix.

The commutation matrix  $K_p$  is the symmetric permutation matrix that transforms the vectorization of a  $p \times p$  matrix to the vectorization of its transpose (Magnus and Neudecker, 1999, p. 54).

*Proof of Lemma 17.* It holds that

$$\begin{aligned} \text{vec}(M\Sigma + \Sigma M^\top) &= \text{vec}(M\Sigma) + \text{vec}(\Sigma M^\top) \\ &= (\Sigma^\top \otimes I_p)\text{vec}(M) + (I_p \otimes \Sigma)\text{vec}(M^\top) = ((\Sigma \otimes I_p) + (I_p \otimes \Sigma)K_p)\text{vec}(M). \end{aligned}$$

□

The Lyapunov equation (1) is symmetric and therefore  $p(p-1)/2$  equations of the equation system (7) are redundant.

**Definition 18.** *Given a  $p \times p$  symmetric matrix  $\Sigma$ , we define the  $p(p+1)/2 \times p^2$  matrix  $A(\Sigma)$  by selecting the rows of*

$$(\Sigma \otimes I_p) + (I_p \otimes \Sigma)K_p$$

*indexed by pairs  $(k, l)$  with  $k \leq l$ .*

Let  $\text{vech}(C) = (C_{kl} : k \leq l)$  be the half-vectorization of the symmetric matrix  $C$ . Then we can write the Lyapunov equation as

$$A(\Sigma)\text{vec}(M) = -\text{vech}(C).$$

As noted, we index the rows of  $A(\Sigma)$  by pairs  $(k, l)$  with  $k \leq l$ . To index the columns of  $A(\Sigma)$  we will use the potential edges  $i \rightarrow j$ , where we recall that the edge  $i \rightarrow j$  corresponds to the entry  $m_{ji}$  of the matrix  $M$ .

Example 5 displayed  $A(\Sigma)$  for the case of  $p = 3$ . In general, we have

$$A(\Sigma)_{(k,l),i \rightarrow j} = \begin{cases} 0, & \text{if } j \neq k, l; \\ \Sigma_{li}, & \text{if } j = k, k \neq l; \\ \Sigma_{ki}, & \text{if } j = l, l \neq k; \\ 2\Sigma_{ji}, & \text{if } j = k = l. \end{cases} \quad (8)$$



Any specific graphical continuous Lyapunov model assumes that  $M$  has non-zero entries only for pairs  $(j, i)$  for which the underlying graph contains the edge  $i \rightarrow j$ . We are thus led to select a subset of columns of the coefficient matrix  $A(\Sigma)$  when studying solvability of the Lyapunov equation. By the next lemma, generic and global identifiability of a graphical continuous Lyapunov model are equivalent to rank conditions on the relevant submatrix of  $A(\Sigma)$ .

**Lemma 19.** *Let  $G = (V, E)$  be a directed graph with  $V = [p]$ , and let  $C \in \text{PD}_p$ . Let  $A(\Sigma)_{\cdot, E}$  be the submatrix of  $A(\Sigma)$  obtained by selecting the columns indexed by the edges in  $E$ . Then the model  $\mathcal{M}_{G, C}$  is*

- (i) *globally identifiable if and only if  $A(\Sigma)_{\cdot, E}$  has full column rank  $|E|$  for all  $\Sigma \in \mathcal{M}_{G, C}$ ;*
- (ii) *generically identifiable if and only if there exists a matrix  $\Sigma \in \mathcal{M}_{G, C}$  such that  $A(\Sigma)_{\cdot, E}$  has full column rank  $|E|$ .*

*If  $\mathcal{M}_{G, C}$  is not generically identifiable, then it is non-identifiable.*

*Proof.* Let  $M_0 \in \text{Stab}(E)$ , and let  $\Sigma_0 = \phi_{G, C}(M_0)$  be the associated covariance matrix. The fiber  $\mathcal{F}_{G, C}(M_0)$  is the set of all matrices  $M \in \mathbb{R}^E$  with

$$A(\Sigma_0)_{\cdot, E} \text{vec}(M)_E = -\text{vech}(C), \quad (9)$$

where  $\text{vec}(M)_E$  is the subvector of  $\text{vec}(M)$  that comprises the entries indexed by  $(j, i)$  with  $i \rightarrow j \in E$ . Hence,  $\mathcal{F}_{G, C}(M_0) = \{M_0\}$  precisely when  $A(\Sigma_0)_{\cdot, E}$  has full column rank such that (9) has a unique solution. Claim (i) is now evident.

To prove (ii), note that  $A(\Sigma)_{\cdot, E}$  has full column rank if and only if the vector of all maximal minors of  $A(\Sigma)_{\cdot, E}$  is non-zero. By (6), the map  $\phi_{G, C}$  is a rational map. Consequently, the map taking  $M \in \text{Stab}(E)$  to the maximal minors of  $A(\phi_{G, C}(M))_{\cdot, E}$  is rational as well. Now a rational map is non-zero outside a measure zero set if and only if there exists a single point where it is non-zero. Consequently, the existence of  $\Sigma \in \mathcal{M}_{G, C}$  with  $A(\Sigma)_{\cdot, E}$  of full column rank implies generic identifiability of  $\mathcal{M}_{G, C}$ .

Finally, if  $\mathcal{M}_{G, C}$  is not generically identifiable then the column rank of  $A(\Sigma_0)_{\cdot, E}$  is strictly smaller than  $|E|$  for all  $\Sigma_0 = \phi_{G, C}(M_0) \in \mathcal{M}_{G, C}$ . The fiber  $\mathcal{F}_{G, C}(M_0) \subseteq \text{Stab}(E)$  is then the affine subspace of solutions to (9) of dimension  $\geq 1$ . Hence,  $|\mathcal{F}_{G, C}(M_0)| = \infty$  for all  $M_0 \in \text{Stab}(E)$ , and  $\mathcal{M}_{G, C}$  is non-identifiable.  $\square$

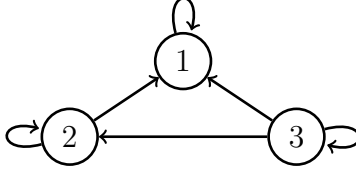
#### 4 Directed acyclic graphs

In this section, we prove that all models that are given by *directed acyclic graphs* (DAGs) are globally identifiable. In our setting, a DAG is a directed graph that does not contain any directed cycles other than the always present self-loops  $i \rightarrow i$ ,  $i \in [p]$ . This case is special in that we are able to make a simple argument based on block structure in the coefficient matrix  $A(\Sigma)$ .

By Proposition 11, in order to prove global identifiability for all DAGs it suffices to treat DAGs that are complete in the sense of the following definition.

**Definition 20.** *A directed simple graph  $G = (V, E)$  with  $V = [p]$  is complete if there is an edge between every pair of distinct nodes.*

A simple graph that also contains all self-loops  $i \rightarrow i$ ,  $i \in [p]$ , is complete if and only if  $|E| = p(p+1)/2$ . Because vertex relabelling has no impact on identifiability, we can furthermore restrict



**Figure 2:** The complete DAG  $G^*$  on 3 nodes.

attention to a single topological ordering. In other words, it suffices to consider the single complete DAG  $G^*$  whose edge set comprises all edges  $i \rightarrow j$  with  $i \geq j$ .

**Example 21.** Consider the case of  $p = 3$  nodes, for which the complete DAG  $G^* = (V, E^*)$  is shown in Figure 2. The graph encodes the drift matrix

$$M = \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ 0 & m_{22} & m_{23} \\ 0 & 0 & m_{33} \end{pmatrix},$$

and the submatrix  $A(\Sigma)_{\cdot, E^*}$  is equal to

$$\begin{matrix} & 1 \rightarrow 1 & 2 \rightarrow 1 & 2 \rightarrow 2 & 3 \rightarrow 1 & 3 \rightarrow 2 & 3 \rightarrow 3 \\ \begin{matrix} (1, 1) \\ (1, 2) \\ (1, 3) \\ (2, 2) \\ (2, 3) \\ (3, 3) \end{matrix} & \begin{pmatrix} 2\Sigma_{11} & 2\Sigma_{12} & 0 & 2\Sigma_{13} & 0 & 0 \\ \Sigma_{21} & \Sigma_{22} & \Sigma_{12} & \Sigma_{23} & \Sigma_{13} & 0 \\ \Sigma_{31} & \Sigma_{32} & 0 & \Sigma_{33} & 0 & \Sigma_{13} \\ 0 & 0 & 2\Sigma_{22} & 0 & 2\Sigma_{23} & 0 \\ 0 & 0 & \Sigma_{32} & 0 & \Sigma_{33} & \Sigma_{23} \\ 0 & 0 & 0 & 0 & 0 & 2\Sigma_{33} \end{pmatrix} \end{matrix}$$

We observe that exchanging the third and the fourth column (indexed by  $2 \rightarrow 2$  and  $3 \rightarrow 1$ , respectively) brings the matrix in a block upper-triangular form.

Up to some rows being scaled by 2, the three diagonal blocks are principal minors of the positive definite matrix  $\Sigma$ . Therefore, it holds for all  $\Sigma \in \text{PD}_3$  that

$$\begin{aligned} |\det A(\Sigma)_{\cdot, E^*}| &= \begin{vmatrix} 2\Sigma_{11} & 2\Sigma_{12} & 2\Sigma_{13} \\ \Sigma_{12} & \Sigma_{22} & \Sigma_{23} \\ \Sigma_{13} & \Sigma_{23} & \Sigma_{33} \end{vmatrix} \cdot \begin{vmatrix} 2\Sigma_{22} & 2\Sigma_{23} \\ \Sigma_{23} & \Sigma_{33} \end{vmatrix} \cdot |2\Sigma_{33}| \\ &= 2^3 \cdot \det(\Sigma) \cdot \det(\Sigma_{23,23}) \cdot \Sigma_{33} > 0. \end{aligned}$$

The block structure found in Example 21 generalizes and gives the main result of this section.

**Theorem 22.** Let  $G = (V, E)$  be a DAG with  $V = [p]$ . Then the model  $\mathcal{M}_{G,C}$  is globally identifiable for every matrix  $C \in \text{PD}_p$ .

*Proof.* As noted above, it suffices to consider the complete DAG  $G^* = (V, E^*)$  whose edges are  $i \rightarrow j$  for  $i \geq j$ . Our proof then applies Lemma 19, which states that model  $\mathcal{M}_{G^*,C}$  is globally identifiable if and only if  $\det(A(\Sigma)_{\cdot, E^*}) \neq 0$  for all  $\Sigma \in \mathcal{M}_{G^*,C}$ .

In what follows, let  $\Sigma \in \text{PD}_p$ . Partition the edge set as  $E^* = E_1^* \cup E_2^* \cup \dots \cup E_p^*$ , where  $E_i^* = \{j \rightarrow i : j \geq i\}$ . Similarly, partition the row index set of  $A(\Sigma)$  into the disjoint union of the

sets  $R_k = \{(k, l) : l \geq k\}$ ,  $k = 1, \dots, p$ . Inspecting (8), we see that the submatrix

$$A(\Sigma)_{R_k, E_i^*} = 0 \quad \text{if } k > i.$$

Hence, the matrix  $A(\Sigma)$  can be arranged in block upper-triangular form, and

$$\det(A(\Sigma)_{\cdot, E^*}) = \prod_{i=1}^p \det(A(\Sigma)_{R_i, E_i^*}).$$

Inspecting again (8), we find that  $A(\Sigma)_{R_i, E_i^*}$  is equal to the principal submatrix  $P(\Sigma)_{\geq i} := \Sigma_{\{i, \dots, p\}, \{i, \dots, p\}}$  but with the first row of  $P(\Sigma)_{\geq i}$  (the one indexed by  $i$ ) being multiplied by 2 in  $A(\Sigma)_{R_i, E_i^*}$ . Since all principal minors of a positive definite matrix  $\Sigma$  are positive, we obtain that

$$|\det(A(\Sigma)_{\cdot, E^*})| = 2^p \prod_{i=1}^p \det(P(\Sigma)_{\geq i}) > 0 \quad \text{for all } \Sigma \in \text{PD}_p.$$

In particular,  $A(\Sigma)_{\cdot, E^*}$  has non-vanishing determinant for all  $\Sigma \in \mathcal{M}_{G^*, C}$ .  $\square$

The proof of Theorem 22 shows that for any complete DAG  $G = (V, E)$  the matrix  $A(\Sigma)_{\cdot, E}$  is invertible for all  $\Sigma \in \text{PD}_p$ . Using this fact, the proof of the theorem reveals more information about Lyapunov models arising from DAGs.

**Corollary 23.** *Let  $G = (V, E)$  be a DAG with  $V = [p]$ . Then  $\mathcal{M}_{G, C}$  is an algebraic and thus closed subset of  $\text{PD}_p$ . If  $G$  is complete then  $\mathcal{M}_{G, C} = \text{PD}_p$ .*

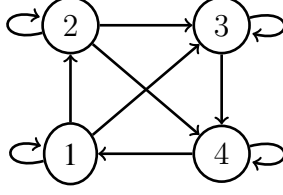
*Proof.* Let  $G$  be a complete DAG. By Theorem 22, the square matrix  $A(\Sigma)_{\cdot, E}$  has full rank for all  $\Sigma \in \text{PD}_p$ . Therefore, the solution  $\text{vec}(M)$  to the vectorized Lyapunov equation (9) exists uniquely for all  $\Sigma \in \text{PD}_p$ . The resulting drift matrix  $M$  has the right support by construction, hence  $\mathcal{M}_{G, C} = \text{PD}_p$ .

If  $G$  is a non-complete DAG, then we may add edges to obtain a complete DAG  $\bar{G} = (V, \bar{E})$ . As  $A(\Sigma)_{\cdot, \bar{E}}$  has full column rank for all  $\Sigma \in \text{PD}_p$  the same is true for  $A(\Sigma)_{\cdot, E}$ ; recall Proposition 11. Hence, a matrix  $\Sigma \in \text{PD}_p$  is in  $\mathcal{M}_{G, C}$  if and only if  $\text{vech}(C)$  is in the column span of  $A(\Sigma)_{\cdot, E}$  if and only if the  $(|E| + 1)$ -minors of the augmented matrix  $(A(\Sigma)_{\cdot, E} \mid \text{vech}(C))$  vanish. The model  $\mathcal{M}_{G, C}$  is thus an algebraic subset: it is the set of positive definite matrices at which these minors vanish.  $\square$

## 5 Sums of squares decompositions and finer rank conditions

Directed cycles break the block-diagonal structure found for DAGs (Theorem 22) making it difficult to check rank conditions on  $A(\Sigma)$ . In this section we show that small cyclic graphs can nevertheless be handled by applying sums of squares decompositions to certify positivity of sub-determinants. Moreover, we show that our rank conditions may be placed on a smaller matrix containing a basis for the kernel of  $A(\Sigma)$ .

In Example 5, we proved global identifiability for the 3-cycle by showing that the key factor  $\Sigma_{11}\Sigma_{22}\Sigma_{33} - \Sigma_{12}\Sigma_{13}\Sigma_{23}$  in the determinant of  $A(\Sigma)_{\cdot, E}$  is positive on  $\text{PD}_3$ . We were able to argue this via the positivity of  $2 \times 2$  principal minors of  $\Sigma$ . However, a direct extension of this approach to cyclic graphs with a larger number of nodes is difficult. Nevertheless, some headway can be made by exploiting the positive-definiteness of  $\Sigma$  via its Cholesky decomposition.



**Figure 3:** A completion of the 4-cycle.

**Example 24.** Let  $G = (V, E)$  be the completion of the 4-cycle with  $V = [4]$  and  $E = \{1 \rightarrow 1, 2 \rightarrow 2, 3 \rightarrow 3, 4 \rightarrow 4, 1 \rightarrow 2, 1 \rightarrow 3, 2 \rightarrow 3, 2 \rightarrow 4, 3 \rightarrow 4, 4 \rightarrow 1\}$ . It is displayed in Figure 3. Let  $\Sigma = LL^\top$  be the Cholesky decomposition of  $\Sigma \in \text{PD}_4$  in terms of the lower-triangular matrix

$$L = \begin{pmatrix} l_{11} & 0 & 0 & 0 \\ l_{12} & l_{22} & 0 & 0 \\ l_{13} & l_{23} & l_{33} & 0 \\ l_{14} & l_{24} & l_{34} & l_{44} \end{pmatrix}$$

with  $l_{11}, l_{22}, l_{33}, l_{44} > 0$ . Then

$$|\det(A(LL^\top)_{\cdot, E})| = 16 l_{44}^2 l_{33}^2 l_{22}^4 l_{11}^6 \cdot |f(L)|,$$

where the key factor is

$$\begin{aligned} f(L) = & l_{14}^2 l_{22}^2 l_{33}^2 - l_{12} l_{14} l_{22} l_{24} l_{33}^2 + l_{12}^2 l_{24}^2 l_{33}^2 + l_{22}^2 l_{24}^2 l_{33}^2 - l_{13} l_{14} l_{22}^2 l_{33} l_{34} \\ & + l_{12} l_{14} l_{22} l_{23} l_{33} l_{34} + l_{12} l_{13} l_{22} l_{24} l_{33} l_{34} - l_{12}^2 l_{23} l_{24} l_{33} l_{34} + l_{13}^2 l_{22}^2 l_{34}^2 \\ & - 2l_{12} l_{13} l_{22} l_{23} l_{34}^2 + l_{12}^2 l_{23}^2 l_{34}^2 + l_{12}^2 l_{33}^2 l_{34}^2 + l_{22}^2 l_{33}^2 l_{34}^2 + l_{13}^2 l_{22}^2 l_{44}^2 \\ & - 2l_{12} l_{13} l_{22} l_{23} l_{44}^2 + l_{12}^2 l_{23}^2 l_{44}^2 + l_{12}^2 l_{33}^2 l_{44}^2 + l_{22}^2 l_{33}^2 l_{44}^2. \end{aligned}$$

A computer algebra system such as *Macaulay2* with the package from Cifuentes et al. (2020) quickly finds a sum of squares (SOS) decomposition for  $f$  as

$$\begin{aligned} f(L) = & \left( \frac{1}{2} l_{14} l_{22} l_{33} - \frac{1}{2} l_{12} l_{24} l_{33} - l_{13} l_{22} l_{34} + l_{12} l_{23} l_{34} \right)^2 \\ & + (-l_{13} l_{22} l_{44} + l_{12} l_{23} l_{44})^2 + (l_{12} l_{33} l_{34})^2 + (l_{12} l_{33} l_{44})^2 + (l_{22} l_{24} l_{33})^2 \\ & + (l_{22} l_{33} l_{34})^2 + (l_{22} l_{33} l_{44})^2 + \frac{3}{4} \left( l_{14} l_{22} l_{33} - \frac{1}{3} l_{12} l_{24} l_{33} \right)^2 + \frac{2}{3} (l_{12} l_{24} l_{33})^2. \end{aligned}$$

Since  $l_{22} l_{33} l_{44} > 0$ , it follows that  $f$  is strictly positive for any Cholesky factor  $L$ . Therefore,  $|\det(A(\Sigma)_{\cdot, E})| > 0$  and we conclude that  $\mathcal{M}_{G,C}$  is globally identifiable, no matter the choice of  $C \in \text{PD}_4$ .

**Remark 25.** A polynomial being a sum of squares is a stronger requirement than the polynomial being non-zero. Therefore, we could have a non-vanishing determinant even if the considered polynomial factor failed the SOS test. However, we do not know of an example where this might be the case.

Observe that  $\det(\Sigma) = (\det L)^2 = l_{11}^2 l_{22}^2 l_{33}^2 l_{44}^2$  appears as a factor of  $\det(A(\Sigma)_{\cdot, E})$  in all our examples so far (recall Example 5, Example 21, and Example 24). This phenomenon actually occurs

for any complete simple graph (see Corollary 43 in the Appendix) and suggests that identifiability should be encoded in a smaller matrix. Indeed, this information is carried by a specific row restriction of a matrix whose columns form a basis of the kernel of  $A(\Sigma)$ .

The kernel of  $A(\Sigma)$  is described by the following fact, straightforward to verify; see also Barnett and Storey (1967). It parametrizes the stable matrices  $M$  that are solutions to the Lyapunov equation in terms of skew-symmetric matrices (matrices  $K$  with  $K^\top = -K$ ).

**Lemma 26.** *Consider the continuous Lyapunov equation from (1) for given  $\Sigma, C \in \text{PD}_p$ . Then a matrix  $M \in \mathbb{R}^{p \times p}$  solves the Lyapunov equation if and only if there exists a skew-symmetric matrix  $K$  such that*

$$M = \left( K - \frac{1}{2}C \right) \Sigma^{-1}.$$

The space of skew-symmetric matrices has dimension  $p(p-1)/2$ . Hence, for  $\Sigma \in \text{PD}_p$ , the kernel of  $A(\Sigma)$  also has dimension  $p(p-1)/2$ . We give further details about the spectral properties of  $A(\Sigma)$  in Theorem 42. The following result now gives simplified rank conditions for identifiability.

**Lemma 27.** *Let  $G = (V, E)$  be a directed graph with  $V = [p]$ , and let  $C \in \text{PD}_p$ . For every  $\Sigma \in \text{PD}_p$ , let  $H(\Sigma)$  be a  $p^2 \times p(p-1)/2$  matrix whose columns form a basis of the kernel of  $A(\Sigma)$ , and let  $H(\Sigma)_{E^c}$  be the submatrix obtained by restriction to rows corresponding to non-edges  $E^c$  of  $G$ . Then the associated model  $\mathcal{M}_{G,C}$  is*

- (i) *globally identifiable if and only if  $H(\Sigma)_{E^c}$  has full column rank  $p(p-1)/2$  for all  $\Sigma \in \mathcal{M}_{G,C}$ ;*
- (ii) *generically identifiable if and only if there exists a matrix  $\Sigma \in \mathcal{M}_{G,C}$  such that  $H(\Sigma)_{E^c}$  has full column rank  $p(p-1)/2$ .*

*Proof.* Recall from Lemma 19 that the elements of the fiber are solutions of the equation system (9), which has a unique solution for a given (positive definite) matrix  $\Sigma \in \mathcal{M}_{G,C}$  if and only if  $A(\Sigma)_{\cdot, E}$  has linearly independent columns. The latter condition can be rephrased as follows: the kernel of  $A(\Sigma)$  does not contain any element  $\text{vec}(M) \neq 0$  such that  $M \in \mathbb{R}^E$ . Put differently, (9) admits a unique solution if and only if the column span of  $H(\Sigma)$  does not contain any element  $\text{vec}(M) \neq 0$  for  $M \in \mathbb{R}^E$ . As  $H(\Sigma)$  has linearly independent columns, this latter condition is equivalent to the linear independence of the columns of the extended matrix  $(H(\Sigma) \mid \text{vec}(M))$  for any non-trivial  $M \in \mathbb{R}^E$ . It remains to be proven that this, in turn, is equivalent to the  $|E^c| \times p(p-1)/2$  submatrix  $H(\Sigma)_{E^c}$  having rank  $p(p-1)/2$ .

Assume that  $H(\Sigma)_{E^c}$  has rank  $p(p-1)/2$ , and consider one of its non-vanishing maximal minors. This minor can always be extended to a non-vanishing maximal minor of  $(H(\Sigma) \mid \text{vec}(M))$  by adding one of the rows corresponding to  $m_{ji} \neq 0$ . Therefore, the extended matrix has full rank.

For the converse implication, note that if  $H(\Sigma)_{E^c}$  has rank strictly less than  $p(p-1)/2$ , then there exists a (not unique) non-trivial  $M \in \mathbb{R}^E$  such that  $\text{vec}(M)$  belongs to the kernel of  $A(\Sigma)$ .  $\square$

For a convenient choice of a basis of the kernel of  $A(\Sigma)$  we may appeal to the following fact.

**Lemma 28.** *For a matrix  $\Sigma \in \text{PD}_p$ , the kernel of  $A(\Sigma)$  equals*

$$\begin{aligned} \ker A(\Sigma) &= \{ \text{vec}(K\Sigma^{-1}) : K \text{ skew-symmetric} \} \\ &= \{ \text{vec}(\Sigma K) : K \text{ skew-symmetric} \}. \end{aligned}$$

*Proof.* The first equality holds by Lemma 26. The second equality follows from the fact that  $K$  is skew-symmetric if and only if  $\Sigma K \Sigma$  is skew-symmetric.  $\square$

For  $1 \leq k, l \leq p$ , let  $K^{(k,l)} = e_k \otimes e_l - e_l \otimes e_k$  be the skew-symmetric matrix whose only non-zero entries are 1 in place  $(k, l)$  and  $-1$  in place  $(l, k)$ . Then the set  $\{K^{(k,l)} : k < l\}$  is a basis of the space of  $p \times p$  skew-symmetric matrices and, thus, the set  $\{\text{vec}(\Sigma K^{(k,l)}) : k < l\}$  is a basis of  $\ker A(\Sigma)$ . We may thus choose the matrix  $H(\Sigma)$  in Lemma 28 as the matrix with entries

$$H(\Sigma)_{i \rightarrow j, (k,l)} = \text{vec}(\Sigma K^{(k,l)})_{ji} = \begin{cases} -\Sigma_{lj} & \text{if } i = k, \\ \Sigma_{kj} & \text{if } i = l, \\ 0 & \text{otherwise.} \end{cases} \quad (10)$$

Note that we index the rows of  $H(\Sigma)$  by all possible edges of a directed graph (including self-loops), in accordance with the indexing of the columns of  $A(\Sigma)$ .

**Example 29.** Consider the  $6 \times 9$  matrix  $A(\Sigma)$  in Example 5 corresponding to  $p = 3$ . Then the matrix from (10) is

$$H(\Sigma) = \begin{pmatrix} -\Sigma_{12} & 0 & -\Sigma_{13} \\ -\Sigma_{22} & 0 & -\Sigma_{23} \\ -\Sigma_{23} & 0 & -\Sigma_{33} \\ \Sigma_{11} & -\Sigma_{13} & 0 \\ \Sigma_{12} & -\Sigma_{23} & 0 \\ \Sigma_{13} & -\Sigma_{33} & 0 \\ 0 & \Sigma_{12} & \Sigma_{11} \\ 0 & \Sigma_{22} & \Sigma_{12} \\ 0 & \Sigma_{23} & \Sigma_{13} \end{pmatrix} \begin{matrix} 1 \rightarrow 1 \\ 1 \rightarrow 2 \\ 1 \rightarrow 3 \\ 2 \rightarrow 1 \\ 2 \rightarrow 2 \\ 2 \rightarrow 3 \\ 3 \rightarrow 1 \\ 3 \rightarrow 2 \\ 3 \rightarrow 3 \end{matrix}.$$

Consider the DAG on 3 nodes given in Figure 2, for which the set of non-edges is  $E^c = \{1 \rightarrow 2, 1 \rightarrow 3, 2 \rightarrow 3\}$ . Then

$$|\det H(\Sigma)_{E^c, \cdot}| = \left| \det \begin{pmatrix} -\Sigma_{22} & 0 & -\Sigma_{23} \\ -\Sigma_{23} & 0 & -\Sigma_{33} \\ \Sigma_{13} & -\Sigma_{33} & 0 \end{pmatrix} \right| = \Sigma_{33}(\Sigma_{22}\Sigma_{33} - \Sigma_{23}^2)$$

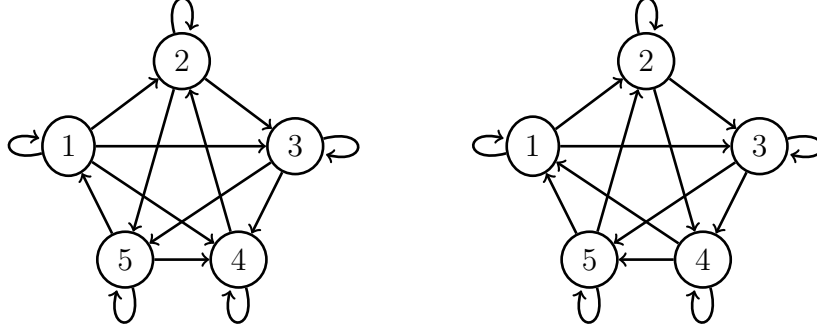
is a product of two principal minors of  $\Sigma$ , as expected from Theorem 22.

Next, let  $E^c = \{1 \rightarrow 3, 2 \rightarrow 1, 3 \rightarrow 2\}$  be the set of non-edges of the 3-cycle from Figure 1. Then

$$|\det H(\Sigma)_{E^c, \cdot}| = \left| \det \begin{pmatrix} -\Sigma_{23} & 0 & -\Sigma_{33} \\ \Sigma_{11} & -\Sigma_{13} & 0 \\ 0 & \Sigma_{22} & \Sigma_{12} \end{pmatrix} \right| = \Sigma_{11}\Sigma_{22}\Sigma_{33} - \Sigma_{12}\Sigma_{13}\Sigma_{23},$$

which is what we obtained in (4).

Following Example 24, we can establish global identifiability by computing an SOS decomposition of the determinant of the restricted kernel  $H(\Sigma)_{E^c, \cdot}$  using the Cholesky decomposition of  $\Sigma$ . Such computations allowed us to establish:



**Figure 4:** The two simple cyclic graphs on 5 nodes, for which a sum of squares decomposition of the determinant of interest is computationally difficult.

**Proposition 30.** *Let  $G = (V, E)$  be a simple graph with  $V = [p]$ , and let  $C \in \text{PD}_p$ . Let  $L \in \mathbb{R}^{p \times p}$  be lower-triangular. If  $p \leq 4$ , then there exists a permutation matrix  $P$  such that  $\det H(PLL^\top P^\top)_{E^c}$  is an everywhere positive sum of squares in the entries of  $L$ , implying that  $\mathcal{M}_{G,C}$  is globally identifiable. The same is true for  $p = 5$  with the exception of two computationally intractable types of graphs, which are depicted in Figure 4.*

For our computer proof of the claims in the proposition, we applied the computer algebra system Macaulay2. For the graphs in Figure 4, we additionally employed Matlab toolboxes, but our computations did not terminate. It is natural to conjecture that Proposition 30 holds for all graphs with  $p = 5$ , and even all simple graphs.

## 6 Simple cyclic graphs

In this section we establish our main result: global identifiability of all Lyapunov models given by simple cyclic graphs. Moreover, we can show that simple cyclic graphs give models that are algebraic subsets of the positive definite cone. Our proofs exploit the parametrization of stable matrices  $M$  that are solutions to the Lyapunov equation in terms of skew-symmetric matrices (matrices  $K$  with  $K^\top = -K$ ); recall Lemma 26.

**Theorem 31.** *Let  $G = (V, E)$  be a directed graph with  $V = [p]$ .*

- (i) *If  $G$  is simple, then the model  $\mathcal{M}_{G,C}$  is globally identifiable for all  $C \in \text{PD}_p$ .*
- (ii) *If  $C \in \text{PD}_p$  is diagonal, then the model  $\mathcal{M}_{G,C}$  is globally identifiable if and only if  $G$  is simple.*

*Proof.* It suffices to prove (i), as (ii) then follows from Proposition 15.

To prove (i), suppose  $G$  is indeed simple. Let  $M_1, M_2 \in \text{Stab}(E)$  be any two matrices that solve the Lyapunov equation (1) for the same  $\Sigma \in \mathcal{M}_{G,C}$ . According to Lemma 26 there exist two skew-symmetric matrices  $K_1$  and  $K_2$  such that  $M_1 = (K_1 - \frac{1}{2}C)\Sigma^{-1}$  and  $M_2 = (K_2 - \frac{1}{2}C)\Sigma^{-1}$ . For the difference we obtain

$$M := M_1 - M_2 = (K_1 - \frac{1}{2}C)\Sigma^{-1} - (K_2 - \frac{1}{2}C)\Sigma^{-1} = (K_1 - K_2)\Sigma^{-1}.$$

The difference  $K = K_1 - K_2$  is again skew-symmetric, so that  $M$  is the product of a skew-symmetric matrix  $K$  and the positive definite matrix  $\Sigma^{-1}$ .

Consider now the square  $M^2$ . We have

$$M^2 = K\Sigma^{-1}K\Sigma^{-1}.$$

As  $\Sigma$  is positive definite, the square root  $\Sigma^{\frac{1}{2}}$  exists, and  $M^2$  is similar to

$$\Sigma^{-\frac{1}{2}}M^2\Sigma^{\frac{1}{2}} = \Sigma^{-\frac{1}{2}}K\Sigma^{-1}K\Sigma^{-\frac{1}{2}}.$$

As  $K$  is skew-symmetric,

$$\Sigma^{-\frac{1}{2}}K\Sigma^{-1}K\Sigma^{-\frac{1}{2}} = -(\Sigma^{-\frac{1}{2}}K)\Sigma^{-1}\left(\Sigma^{-\frac{1}{2}}K\right)^\top.$$

We observe that  $M^2$  is similar to a symmetric and negative semi-definite matrix. Therefore, the eigenvalues of  $M^2$  are non-positive and  $\text{tr}(M^2) \leq 0$ .

As  $M$  is supported over a simple graph, it holds for all pairs of indices  $i \neq j$  that  $m_{ij} \neq 0$  implies that  $m_{ji} = 0$ . Hence, the diagonal of  $M^2$  is given by the squared diagonal elements of  $M$ , i.e.,  $(M^2)_{ii} = m_{ii}^2$ . It follows that

$$0 \leq \sum_{i=1}^p m_{ii}^2 = \text{tr}(M^2) \leq 0,$$

which implies that  $\text{tr}(M^2) = 0$ .

Let  $\lambda_1, \dots, \lambda_p \in \mathbb{C}$  be the eigenvalues of  $M$ . The eigenvalues of  $M^2$  are then  $\lambda_1^2, \dots, \lambda_p^2$ . Since  $M^2$  is similar to a negative semi-definite matrix, all its eigenvalues satisfy  $\lambda_1^2, \dots, \lambda_p^2 \leq 0$ . Then,

$$0 = \text{tr}(M^2) = \sum_{i=1}^p \lambda_i^2 \leq 0,$$

which implies that  $\lambda_i^2 = 0$  for all  $i \in 1, \dots, p$ . But this is only true if  $\lambda_i = 0$  for all  $i = 1, \dots, p$ . Therefore, all eigenvalues of  $M$  are zero.

Observe that  $M = K\Sigma^{-1}$  is similar to  $\tilde{M} = \Sigma^{-\frac{1}{2}}K\Sigma^{-1}\Sigma^{\frac{1}{2}}$ , which is skew-symmetric since

$$\tilde{M}^\top = (\Sigma^{-\frac{1}{2}}K\Sigma^{-\frac{1}{2}})^\top = \Sigma^{-\frac{1}{2}}K^\top\Sigma^{-\frac{1}{2}} = -\Sigma^{-\frac{1}{2}}K\Sigma^{-\frac{1}{2}} = -\tilde{M}.$$

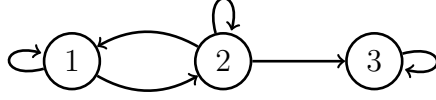
Skew-symmetric matrices are diagonalizable, and we deduce that  $M$  is similar to the zero matrix. But then  $M = 0$  and consequently  $M_1 = M_2$ , which shows that the Lyapunov equation admits a unique sparse solution.  $\square$

In addition to global identifiability, we have a generalization of Corollary 23 to general simple graphs.

**Corollary 32.** *Let  $G = (V, E)$  be a simple graph with  $V = [p]$ . Then  $\mathcal{M}_{G,C}$  is an algebraic and thus closed subset of  $\text{PD}_p$ . If  $G$  is complete then  $\mathcal{M}_{G,C} = \text{PD}_p$ .*

*Proof.* Consider first the case where  $G$  is complete (with an edge between every pair of nodes). Let  $\Sigma_0 \in \text{PD}_p$  be an arbitrary positive definite matrix. Choosing  $M = -I_p$ , the negated identity matrix, shows that  $\Sigma_0$  belongs to the model  $\mathcal{M}_{G,C_0}$  for  $C_0 = 2\Sigma_0$ . By Theorem 31 and Lemma 19, we obtain that the determinant of  $A(\Sigma)_{\cdot,E}$  is non-zero at every matrix in  $\mathcal{M}_{G,C_0}$  and, in particular,





**Figure 5:** Non-simple graph on 3 nodes.

at  $\Sigma_0$ . We conclude that  $\det(A(\Sigma)_{\cdot, E}) \neq 0$  on all of  $\text{PD}_p$ . As in the proof of Corollary 23, we deduce that  $\mathcal{M}_{G,C} = \text{PD}_p$  for all  $C \in \text{PD}_p$ .

If  $G$  is not complete, then it can be augmented to a complete graph  $\bar{G} = (V, \bar{E})$ , and we may complete the proof in analogy to the proof of Corollary 23.  $\square$

## 7 Non-simple graphs

In this section, we consider directed graphs  $G = (V, E)$  that are allowed to be non-simple, i.e., may contain a two-cycle. In our study, we restrict attention to the case where  $C \in \text{PD}_p$  is diagonal. Proposition 15 tells us that, for  $C$  diagonal, a model  $\mathcal{M}_{G,C}$  given by a non-simple graph  $G$  can never be globally identifiable. However, non-simple graphs with at most  $p(p+1)/2$  edges may still give generically identifiable models (Definition 6, Lemma 10). We are able to provide a combinatorial condition that is necessary for generic identifiability, and we computationally classify all graphs with  $p \leq 5$  nodes. Our study reveals examples for which generic identifiability depends in subtle ways on the pattern of edges.

We begin with a small example.

**Example 33.** Let  $G = (V, E)$  be the graph from Figure 5, a 2-cycle with an additional edge pointing to a third node, and let  $C \in \text{PD}_3$  be a diagonal matrix. To inspect identifiability of  $\mathcal{M}_{G,C}$ , we may use the kernel basis of Example 29 with the set of non-edges  $E^c = \{1 \rightarrow 3, 3 \rightarrow 1, 3 \rightarrow 2\}$ . We find

$$\det H(\Sigma)_{E^c} = \det \begin{pmatrix} -\Sigma_{23} & 0 & -\Sigma_{33} \\ 0 & \Sigma_{12} & \Sigma_{11} \\ 0 & \Sigma_{22} & \Sigma_{12} \end{pmatrix} = \Sigma_{23} (\Sigma_{11}\Sigma_{22} - \Sigma_{12}^2).$$

Since  $\mathcal{M}_{G,C}$  contains positive definite matrices with both vanishing and non-vanishing  $\Sigma_{23}$ , we conclude that  $\mathcal{M}_{G,C}$  is generically (but not globally) identifiable.

Note that the matrices  $\Sigma \in \mathcal{M}_{G,C}$  with  $\Sigma_{23} = 0$  are obtained precisely from the drift matrices in the lower-dimensional set  $\{M \in \text{Stab}(E) : m_{32} = 0\}$ . Indeed, if  $m_{32} = 0$ , then the situation is as if the  $2 \rightarrow 3$  edge were removed, and we will see in Proposition 35 that this implies  $\Sigma_{23} = 0$  when  $C$  is diagonal. Conversely, when solving for  $\Sigma$  given a drift matrix  $M \in \mathbb{R}^E$  we find that  $\Sigma_{23}$  is a rational function of  $(M, C)$  whose numerator is

$$m_{32} (c_{11}m_{21}^2 \text{tr}(M) + c_{22}m_{11}^2 \text{tr}(M) + c_{22} \det(M)).$$

As  $C$  is positive definite and  $M$  stable, the second factor is negative. Thus, if  $\Sigma = \Sigma(M, C)$  is a positive definite matrix in  $\mathcal{M}_{G,C}$ , then  $\Sigma_{23} = 0$  implies  $m_{32} = 0$ .

By Lemma 10,  $|E| \leq p(p+1)/2$  is a necessary condition for generic identifiability of the model of a graph  $G = (V, E)$ . We now show how this bound may be improved by accounting for knowledge about vanishing covariances.



**Figure 6:** Left: graph  $G_1$  on 4 nodes with  $\mathcal{M}_{G_1, C}$  generically identifiable. Right: subgraph  $G_2$  of  $G_1$  such that  $\mathcal{M}_{G_2, C}$  is non-identifiable.  $C \in \text{PD}_4$  is diagonal.

**Definition 34.** A trek is a sequence of edges of the form

$$l_m \leftarrow l_{m-1} \leftarrow \cdots \leftarrow l_1 \leftarrow t \rightarrow r_1 \rightarrow \cdots \rightarrow r_{n-1} \rightarrow r_n.$$

The node  $t$  is the top node of the trek. The directed paths  $l_m \leftarrow l_{m-1} \leftarrow \cdots \leftarrow l_1$  and  $r_1 \rightarrow \cdots \rightarrow r_{n-1} \rightarrow r_n$  are the left and the right side of the trek, respectively. The definition allows for one or both sides to be trivial, so directed paths and also single nodes are treks.

From Varando and Hansen (2020, Corollary 2.3), we deduce the following fact.

**Proposition 35.** Let  $G = (V, E)$  be a directed graph with  $V = [p]$ , and let  $C \in \text{PD}_p$  be diagonal. If there is no trek from  $i$  to  $j$  in  $G$ , then  $\Sigma_{ij} = 0$  in all matrices  $\Sigma \in \mathcal{M}_{G, C}$ .

**Example 36.** Let  $C \in \text{PD}_4$  be diagonal. Then the left graph  $G_1 = (V, E_1)$  in Figure 6 defines a generically identifiable model but its subgraph  $G_2 = (V, E_2)$  does not. This example stresses that global identifiability is needed in Proposition 11. But why is  $\mathcal{M}_{G_2, C}$  non-identifiable despite  $G_2$  having fewer edges? We observe that  $G_2$  contains no trek between 2 and 4 and no trek between 3 and 4. Proposition 35 yields  $\Sigma_{24} = \Sigma_{34} = 0$ . Although the  $\text{PD}_4$ -cone has dimension  $\binom{4+1}{2} = 10$ , the existence of the constraints  $\Sigma_{24} = \Sigma_{34} = 0$  implies that  $\dim(\mathcal{M}_{G_2, C}) \leq 10 - 2 = 8$ . Since  $|E_2| = 9 > 8$ , non-identifiability follows from by Lemma 10.

As a last subtlety, we emphasize that if we remove one of the edges  $2 \rightarrow 1$ ,  $3 \rightarrow 1$ , or  $4 \rightarrow 1$  of  $G_2$ , we are left again with a generically identifiable model.

The ideas in Example 36 can be generalized into a sharper necessary condition for identifiability that is a consequence of Lemma 10 and Proposition 35.

**Corollary 37.** Let  $G = (V, E)$  be a directed graph with  $V = [p]$ . If  $\mathcal{M}_{G, C}$  is generically identifiable for a diagonal matrix  $C \in \text{PD}_p$ , then it has to hold that

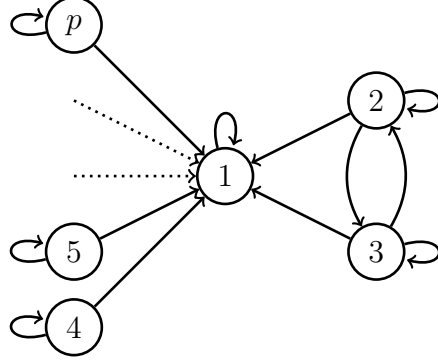
$$|E| \leq \frac{p(p+1)}{2} - \#\{ \{i, j\} : i, j \in V \text{ with no trek between them} \}. \quad (11)$$

With this criterion in hand, we can construct graphs of arbitrary size  $p$  and fewer than  $p(p+1)/2$  edges that yield non-identifiable models.

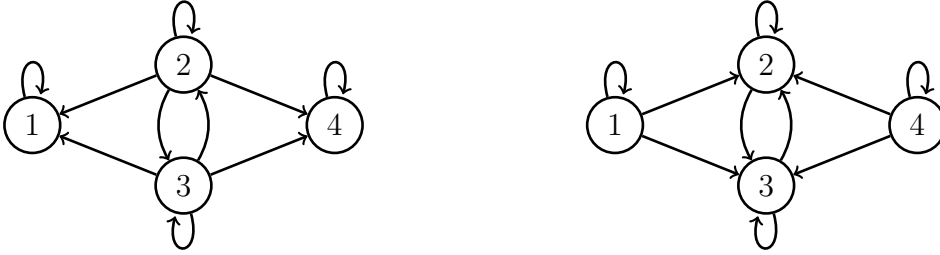
**Corollary 38.** Consider the graph  $G = (V, E)$  with  $p \geq 4$  nodes displayed in Figure 7. The model  $\mathcal{M}_{G, C}$  is non-identifiable for any diagonal  $C \in \text{PD}_p$ .

*Proof.* The number of parameters  $|E|$  is

$$\begin{aligned} & 2 \text{ (edges from 2-cycle)} + p - 1 \text{ (edges pointing to node 1)} \\ & + p \text{ (parameters due to the selfloops)} = 2p + 1. \end{aligned}$$



**Figure 7:** Graph  $G$  with  $V = [p]$  such that  $\mathcal{M}_{G,C}$  is non-identifiable for diagonal  $C \in \text{PD}_p$ .



**Figure 8:** Left: graph fulfilling the criterion in Corollary 37, yet yields a non-identifiable model. Right: Reversing edges retains non-identifiability, due to Corollary 37, as  $\Sigma_{14} = 0$ .

There are no treks between any pair of nodes  $\{2, \dots, p\}$  except for the pair  $(2, 3)$ . This results in  $\binom{p-1}{2} - 1$  (unordered) pairs of nodes with no trek. Corollary 37 implies that

$$\dim(\mathcal{M}_{G,C}) \leq \frac{p(p+1)}{2} - \binom{p-1}{2} + 1 = 2p.$$

□

Unfortunately, the criterion in Corollary 37 is not sufficient.

**Example 39.** Let  $G_1 = (V, E)$  be the left graph in Figure 8. Graph  $G_1$  fulfills the necessary condition of Corollary 37 as the number of parameters is  $6 + 4 = 10$  and all pairs of nodes are connected with a trek, which is why the right side of equation (11) is also  $\binom{4+1}{2} = 10$ . However,  $A(\Sigma)_{.,E} \in \mathbb{R}^{10 \times 10}$  does not have full rank because the columns of  $A(\Sigma)$  may be linearly combined to

$$\begin{aligned} & \Sigma_{13}A(\Sigma)_{.,2 \rightarrow 1} + \Sigma_{23}A(\Sigma)_{.,2 \rightarrow 2} + \Sigma_{33}A(\Sigma)_{.,2 \rightarrow 3} + \Sigma_{34}A(\Sigma)_{.,2 \rightarrow 4} \\ & - \Sigma_{12}A(\Sigma)_{.,3 \rightarrow 1} - \Sigma_{22}A(\Sigma)_{.,3 \rightarrow 2} - \Sigma_{23}A(\Sigma)_{.,3 \rightarrow 3} - \Sigma_{24}A(\Sigma)_{.,3 \rightarrow 4} = 0. \end{aligned}$$

Therefore, the model  $\mathcal{M}_{G_1,C}$  is non-identifiable for  $C$  diagonal despite fulfilling the necessary criterion. The right graph in Figure 8 yields a non-identifiable model for the simple reason that the necessary condition of Corollary 37 is violated due to the absence of a trek between nodes 1 and 4.

For smaller examples, we may check generic identifiability by choosing random drift matrices and determining whether the resulting matrix  $\Sigma$  satisfies the rank condition from Lemma 19. When

this does not succeed we can check symbolically whether the corresponding restriction of the coefficient matrix  $A(\Sigma)$  or the restricted kernel basis  $H(\Sigma)$  from Lemma 27 is rank-deficient, thus implying non-identifiability. We implemented this strategy for all non-simple graphs with  $p \leq 5$  nodes and less than  $p(p+1)/2$  parameters. As justified by Proposition 12, we took  $C = I_p$  in our computations. This led to the results displayed in Table 1, which shows that the majority of graphs are generically identifiable. The details of the computations can be found at <https://mathrepo.mis.mpg.de/LyapunovIdentifiability>.

**Table 1:** Classification of models with  $p = 3, 4, 5$  nodes and  $C = I_p$ . The last column displays the number of non-identifiable models whose underlying graphs satisfy the necessary criterion for generic identifiability in Corollary 37.

nodes	total non-simple	non-identifiable	non-identifiable satisfying (11)
3	2	0	0
4	80	3	2
5	4862	68	37

## 8 Conclusion

Graphical continuous Lyapunov models offer a new perspective on modeling the covariance structure of multivariate data by relating each observation to an underlying continuous-time dynamic process. The resulting covariance structure is determined by the continuous Lyapunov equation. Our work addresses the fundamental problem of whether, up to joint scaling, the parameters of the dynamic process can be identified from the covariance matrix of the cross-sectional equilibrium observations. Our main contribution shows that simple graphs yield globally identifiable models, and that the graph being simple is necessary and sufficient for global identifiability in the case where the volatility matrix  $C$  is diagonal. Moreover, we are able to show that the models of simple graphs are closed algebraic subsets of the positive definite cone. In particular, the models of complete simple graphs equal the entire positive definite cone.

Our analysis of directed acyclic graphs (DAGs) highlights block structure in the coefficient matrix for the Lyapunov equation. This leads to a straightforward proof of global identifiability and also reveals that the determinant studied in our rank conditions is a positive sum of squares in the entries of a Cholesky factor. This sum of squares property was also observed in small cyclic graphs.

While we were able to characterize global identifiability, we know less about generic identifiability of graphical Lyapunov models. Our results include an effective necessary but not sufficient graphical criterion for non-simple graphs to be generically identifiable. We also obtain a computational classification of graphs with up to 5 nodes, and we hope that future research will lead to an improved understanding of generic identifiability of the models we considered.

## Acknowledgements

This project has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No 883818). The first author further acknowledges support from the Hanns-Seidel Foundation.

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## A Volatility matrix: diagonal vs. non-diagonal PD matrix

This section aims at providing insight into the need of the diagonality constraint on the volatility matrix  $C \in \text{PD}_p$  of the Lyapunov equation to ensure that some of the stronger results of the paper hold.

**Example 40.** Let  $G$  be the 2-cycle with an additional third node, so  $V = [3]$  and  $E = \{1 \rightarrow 1, 1 \rightarrow 2, 2 \rightarrow 1, 2 \rightarrow 2, 3 \rightarrow 3\}$ , which encodes drift matrices

$$M = \begin{pmatrix} m_{11} & m_{12} & 0 \\ m_{21} & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix}.$$

Let  $C = (c_{ij}) \in \text{PD}_3$ . Clearly, the graph does not contain any treks between nodes 1 and 3, nor between nodes 2 and 3. However, a matrix  $\Sigma = \phi_{G,C}(M)$  has

$$\Sigma_{13} = \frac{c_{23}m_{12} - c_{13}(m_{22} + m_{33})}{(m_{11}m_{22} - m_{12}m_{21}) + m_{33}(m_{11} + m_{22} + m_{33})},$$

with a denominator that is positive on  $\text{Stab}(E)$  and a numerator that is constant zero only if  $c_{13} = c_{23} = 0$ . The same holds for  $\Sigma_{23}$  by symmetry. This example serves to highlight that Proposition 35 may be false when  $C$  is not diagonal. Indeed, the treks would need to be allowed to move along new edges that reflect presence of non-zero diagonal entries in  $C$ ; compare Varando and Hansen (2020).

**Example 41.** Consider again the 2-cycle with an additional third node from the previous example. Again, consider an arbitrary matrix  $C = (c_{ij}) \in \text{PD}_3$ . The kernel basis of Example 29 restricted to the set of non-edges  $E^c = \{1 \rightarrow 3, 2 \rightarrow 3, 3 \rightarrow 1, 3 \rightarrow 2\}$ , namely

$$H(\Sigma)_{E^c, \cdot} = \begin{pmatrix} -\Sigma_{23} & 0 & -\Sigma_{33} \\ \Sigma_{13} & -\Sigma_{33} & 0 \\ 0 & \Sigma_{12} & \Sigma_{11} \\ 0 & \Sigma_{22} & \Sigma_{12} \end{pmatrix},$$

is rank deficient for any  $\Sigma \in \text{PD}_3$  if and only if  $\Sigma_{13} = \Sigma_{23} = 0$ . Adding this constraint to the Lyapunov equation yields  $c_{13} = c_{23} = 0$ . Therefore, it follows from Lemma 27 that  $\mathcal{M}_{G,C}$  is globally identifiable for any  $C = (c_{ij}) \in \text{PD}_3$  in which  $c_{13}$  and  $c_{23}$  do not vanish simultaneously.

Observe that this provides a counterexample to Proposition 15 and Proposition 13 when dropping the diagonality assumption. To begin with, such  $\mathcal{M}_{G,C}$  is an instance of a globally identifiable model associated to a non-simple graph. Moreover, the subgraph  $H$  obtained by removing node 3 from  $G$  defines a non-identifiable model for all positive definite volatility matrices by Lemma 10.

For the sake of completeness, note that, by Example 40,  $c_{13} = c_{23} = 0$  completely describes when the rank of  $H(\Sigma)_{E^c, \cdot}$  drops for all  $\Sigma \in \mathcal{M}_{G,C}$ . In other words, the model is non-identifiable if and only if  $c_{13} = c_{23} = 0$  and globally identifiable otherwise.

## B Spectral description, kernel and factorization

Here, we collect spectral properties of  $A(\Sigma)$ , derived more conveniently for its square  $p \times p$  version

$$\tilde{A}(\Sigma) = \Sigma \otimes I_p + (I_p \otimes \Sigma)K_p,$$

which features in Lemma 17. We will then use this information to clarify that  $\det(\Sigma)$  is a factor of  $\det(A(\Sigma)_{.,E})$  for complete graphs which have edge sets of size  $|E| = p(p+1)/2$ ; see Corollary 43.

**Theorem 42.** *Let  $\Sigma \in \text{PD}_p$ , and let  $(\lambda_i)_{i \in [p]}$  be its eigenvalues with corresponding orthogonal eigenvectors  $(z_i)_{i \in [p]}$ .*

- (i) *The matrix  $\tilde{A}(\Sigma)$  has rank  $p(p+1)/2$ , and (10) gives a basis for its kernel.*
- (ii) *The transposed matrix  $\tilde{A}(\Sigma)^\top$  has rank  $p(p+1)/2$ , and a basis for its kernel is given by  $\text{vec}(e_i \otimes e_j - e_j \otimes e_i)$  for  $1 \leq i < j \leq p$ .*
- (iii) *Counting with multiplicities, the  $p(p+1)/2$  non-zero eigenvalues of  $\tilde{A}(\Sigma)$  and of  $\tilde{A}(\Sigma)^\top$  are given by the sums  $\lambda_i + \lambda_j$  for  $1 \leq i \leq j \leq p$  and for either matrix the associated set of orthogonal eigenvectors is  $\text{vec}(z_i \otimes z_j + z_j \otimes z_i)$  for  $1 \leq i \leq j \leq p$ .*

*Proof.* (i) follows from (10), and (ii) follows from the symmetry of the Lyapunov (matrix) equation.

For (iii), the claim about  $\tilde{A}(\Sigma)$  follows from the calculation

$$\begin{aligned} & (z_i \otimes z_j + z_j \otimes z_i)\Sigma + \Sigma(z_i \otimes z_j + z_j \otimes z_i)^\top \\ &= [\lambda_j(z_i \otimes z_j) + \lambda_i(z_j \otimes z_i)] + [\lambda_i(z_i \otimes z_j) + \lambda_j(z_j \otimes z_i)] \\ &= (\lambda_i + \lambda_j)(z_i \otimes z_j + z_j \otimes z_i). \end{aligned}$$

The transpose  $\tilde{A}(\Sigma)^\top = \Sigma \otimes I_p + K_p(I_p \otimes \Sigma)$  encodes the Lyapunov equation with  $M$  replaced by  $M^\top$  and the claim about  $\tilde{A}(\Sigma)^\top$  follows from the symmetry of the matrices  $z_i \otimes z_j + z_j \otimes z_i$ . The orthogonality of the eigenvectors holds because

$$\text{tr}((z_i \otimes z_j + z_j \otimes z_i)(z_k \otimes z_l + z_l \otimes z_k)) = 0$$

unless  $\{i, j\} = \{k, l\}$ . □

As a consequence of Theorem 42, we can conclude information regarding the factorization of the determinant of  $A(\Sigma)_{.,E}$  when  $|E| = p(p+1)/2$  such that  $A(\Sigma)_{.,E}$  is a square matrix.

**Corollary 43.** *Let  $G = (V, E)$  be a directed graph with  $V = [p]$  and  $|E| = p(p+1)/2$ . The polynomials  $\det(\Sigma)$  and  $\det(H(\Sigma)_{E^c, \cdot})$  are factors of  $\det(A(\Sigma)_{.,E})$ .*

*Proof.* The zero set of the determinant  $\det(\Sigma)$  is the set of singular symmetric matrices. Since  $\det(\Sigma)$  is an irreducible polynomial, every polynomial that vanishes at all singular matrices must be a polynomial multiple of  $\det(\Sigma)$ . Hence, it suffices to show that  $\det(A(\Sigma)_{.,E}) = 0$  for all singular matrices  $\Sigma$ . So let  $\Sigma$  be a singular matrix. Then there exists an eigenvalue  $\lambda_i = 0$  with  $i \in [p]$ . Using Theorem 42 this implies that the eigenvalue  $\lambda_i + \lambda_i$  of  $\tilde{A}(\Sigma)$  is zero (the theorem is written for  $\Sigma$  positive definite but the fact we used also holds for  $\Sigma$  singular). Hence,  $\text{rank}(\tilde{A}(\Sigma)) \leq p(p+1)/2 - 1$  which implies that  $\text{rank}(A(\Sigma)_{.,E}) \leq p(p+1)/2 - 1$  and thus  $\det(A(\Sigma)_{.,E}) = 0$ .

The fact that  $\det(H(\Sigma)_{E^c, \cdot})$  is a factor of  $\det(A(\Sigma)_{.,E})$  follows from the proof of Lemma 27. □