IDENTIFIABILITY IN CONTINUOUS LYAPUNOV MODELS*

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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.

1. Introduction.

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

$$M\Sigma + \Sigma M^T + C = 0, \tag{1.1}$$

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, 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 (1.1). 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 Σ, 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 $M = (m_{ij})$

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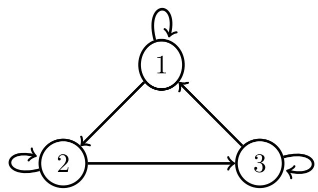

Fig. 1: The directed 3-cycle.

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 $i \to j$ is not an edge in G. In this setting our graphs will always include self-loops $i \to i$.

Example 1.1. The directed 3-cycle G with vertex set $V = \{1, 2, 3\}$ and edge set $E = \{1 \to 1, 2 \to 2, 3 \to 3, 1 \to 2, 2 \to 3, 3 \to 1\}$, 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 (1.1) 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 Σ 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 Σ? Our treatment of this question will assume that the volatility matrix C is a known positive definite matrix. The precise form of C will have no effect on our results.

Remark 1.2. Evidently, if a matrix Σ solves the Lyapunov equation for a pair (M, C) then Σ 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 1.1, we give a formal definition of graphical continuous Lyapunov models as sets of covariance matrices. We write PD_p for the cone of $p \times p$ positive-definite matrices. Recall that C is fixed to an arbitrary element of PD_p.

Definition 1.3. *Let $G = (V, E)$ be a directed graph with vertex set $V = [p]$ and an edge set E that includes all self-loops $i \to i$, $i \in [p]$. Given the fixed choice of C, the* graphical continuous Lyapunov model *of G is the set of covariance matrices*

$$\mathcal{M}_G = \left\{ \Sigma \in \mathrm{PD}_p \,:\, M\Sigma + \Sigma M^T = -C \;\; \textit{with } M \in \mathbb{R}^E \right\},$$

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 $i \to j \notin E$.

Remark 1.4. Let $\mathrm{Stab}(E) \subset \mathbb{R}^E$ be the subset of stable matrices, which is always non-empty and open. When C is positive definite, the Lyapunov equation from (1.1) has a positive definite solution Σ if and only if M is stable (Bhaya et al., 2003, Theorem 1.1). Hence, the definition of the model $\mathcal{M}_G$ remains unchanged if we replace the requirement $M \in \mathbb{R}^E$ by $M \in \mathrm{Stab}(E)$.

The identifiability question we pose asks if a covariance matrix Σ in the model $\mathcal{M}_G$ 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 parametrization map

$$\begin{aligned} \phi_G : \mathrm{Stab}(E) &\to PD_p \\ M &\mapsto \Sigma(M, C), \end{aligned} \tag{1.2}$$

where $\Sigma(M, C)$ is the unique matrix Σ that solves the Lyapunov equation given by the stable matrix M and positive definite C. See (3.1) for details on this uniqueness.

Example 1.5. By vectorization, the Lyapunov equation (1.1) is transformed into the linear equation system

$$A(\Sigma)\mathrm{vec}(M) = -\mathrm{vech}(C), \tag{1.3}$$

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

$$\begin{array}{c} \\ (1,1) \\ (1,2) \\ (1,3) \\ (2,2) \\ (2,3) \\ (3,3) \end{array} \begin{array}{c} \begin{array}{ccccccccc} 1\to1 & 1\to2 & 1\to3 & 2\to1 & 2\to2 & 2\to3 & 3\to1 & 3\to2 & 3\to3 \end{array} \\ \begin{pmatrix} 2\Sigma_{11} & 0 & 0 & 2\Sigma_{12} & 0 & 0 & 2\Sigma_{13} & 0 & 0 \\ \Sigma_{12} & \Sigma_{11} & 0 & \Sigma_{22} & \Sigma_{12} & 0 & \Sigma_{23} & \Sigma_{13} & 0 \\ \Sigma_{13} & 0 & \Sigma_{11} & \Sigma_{23} & 0 & \Sigma_{12} & \Sigma_{33} & 0 & \Sigma_{13} \\ 0 & 2\Sigma_{12} & 0 & 0 & 2\Sigma_{22} & 0 & 0 & 2\Sigma_{23} & 0 \\ 0 & \Sigma_{13} & \Sigma_{12} & 0 & \Sigma_{23} & \Sigma_{22} & 0 & \Sigma_{33} & \Sigma_{23} \\ 0 & 0 & 2\Sigma_{13} & 0 & 0 & 2\Sigma_{23} & 0 & 0 & 2\Sigma_{33} \end{pmatrix} \end{array},$$

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

Consider the 3-cycle G from Example 1.1. Then unique solvability of (1.3) for $M \in \mathbb{R}^E$ is equivalent to a submatrix of $A(\Sigma)$ being invertible, namely, the submatrix

$$A(\Sigma)_{\cdot,E} = \begin{array}{c} \\ (1,1) \\ (1,2) \\ (1,3) \\ (2,2) \\ (2,3) \\ (3,3) \end{array} \begin{array}{c} \begin{array}{cccccc} 1\to1 & 1\to2 & 2\to2 & 2\to3 & 3\to1 & 3\to3 \end{array} \\ \begin{pmatrix} 2\Sigma_{11} & 0 & 0 & 0 & 2\Sigma_{13} & 0 \\ \Sigma_{12} & \Sigma_{11} & \Sigma_{12} & 0 & \Sigma_{23} & 0 \\ \Sigma_{13} & 0 & 0 & \Sigma_{12} & \Sigma_{33} & \Sigma_{13} \\ 0 & 2\Sigma_{12} & 2\Sigma_{22} & 0 & 0 & 0 \\ 0 & \Sigma_{13} & \Sigma_{23} & \Sigma_{22} & 0 & \Sigma_{23} \\ 0 & 0 & 0 & 2\Sigma_{23} & 0 & 2\Sigma_{33} \end{pmatrix} \end{array}.$$

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

$$\det(A(\Sigma)_{\cdot,E}) = 2^3 \cdot \det(\Sigma) \cdot (\Sigma_{11}\Sigma_{22}\Sigma_{33} - \Sigma_{12}\Sigma_{13}\Sigma_{23}). \tag{1.4}$$

All displayed factors are positive when Σ 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

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

We conclude that when G is the 3-cycle, then for *all* covariance matrices $\Sigma \in \mathcal{M}_G \subseteq \mathrm{PD}_3$ there is a unique matrix $M \in \mathbb{R}^E$ such that $\Sigma = \phi_G(M)$. We will refer to this property as the 3-cycle defining a *globally identifiable* model. Note that our argument also shows that $\mathcal{M}_G = \mathrm{PD}_3$, a fact we will comment on further in Corollary 4.4.

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 3.3 and Theorem 5.3) but the resulting matrices have involved graph-dependent structures. While the case of directed acyclic graphs is easily handled and one obtains identifiability for all associated models (Theorem 4.3), cyclic graphs are more difficult to handle. For cyclic graphs, the polynomials that appear while factoring determinants, as in (1.4), quickly increase in complexity, and it is not easy to determine whether they are non-zero. In our main result (Theorem 6.2) 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 subsets of PD_p, and that the models associated to complete DAGs are equal to PD_p (Corollary 4.4). 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 PD_p. When feasible, such computations prove again that identifiable models are closed subsets of PD_p. In Section 6 we present our main result (Theorem 6.2), which proves that global model identifiabilty holds if and only the underlying graph is simple (i.e., does not contain any 2-cycle). In Section 7, we develop a necessary criterion for the weaker notion of generic identifiability and computationally classify all non-simple graphs with up to 5 nodes. The paper concludes in Section 8. Some details on the structure of $A(\Sigma)$ and the factorization of its minors are deferred to Appendix A.

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 $\mathcal{M}_G$ be the graphical continuous Lyapunov model associated to a directed graph $G = (V, E)$ with vertex set $V = [p]$ and edge set E. Let ϕ_G be the model's parametrization from (1.2). The *fiber* of a matrix $M_0 \in \mathrm{Stab}(E)$ is the set

$$\mathcal{F}_G(M_0) = \{M \in \mathrm{Stab}(E) : \phi_G(M) = \phi_G(M_0)\}. \tag{2.1}$$

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

We will consider three natural notions of identifiability.

DEFINITION 2.1. *Let $\mathcal{M}_G$ be the graphical continuous Lyapunov model given by a directed graph $G = (V, E)$. The model $\mathcal{M}_G$ is*

(i) globally identifiable *if $\mathcal{F}_G(M_0) = \{M_0\}$ for all $M_0 \in \mathrm{Stab}(E)$;*

(ii) generically identifiable *if $\mathcal{F}_G(M_0) = \{M_0\}$ for almost all $M_0 \in \mathrm{Stab}(E)$, i.e., the matrices with $\mathcal{F}_G(M_0) \neq \{M_0\}$ form a Lebesgue null set in $\mathbb{R}^E$;*

(iii) non-identifiable *if $|\mathcal{F}_G(M_0)| = \infty$ for all $M_0 \in \mathrm{Stab}(E)$.*

Remark 2.2. The generic properties we prove in this paper are derived by showing that they hold outside a strict subset of $\mathrm{Stab}(E)$ that is described by polynomials in the entries of the drift matrix; see e.g. Lemma 3.3. Hence, in a generically identifiable model the exception set is not merely a set of Lebesgue measure zero but rather a lower-dimensional algebraic subset of $\mathrm{Stab}(E)$.

Remark 2.3. 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 1.5 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 2.4. Consider the 2-cycle $G = (V, E)$ with $V = \{1, 2\}$ and $E = \{1 \to 1, 2 \to 2, 1 \to 2, 2 \to 1\}$. Then ϕ_G maps the 4-dimensional parameter space $\mathrm{Stab}(E)$ to the 3-dimensional 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, $\mathcal{M}_G$ is non-identifiable.

The example just given generalizes as follows:

LEMMA 2.5. *Let $G = (V, E)$ be a graph on p nodes. If $|E| > \dim(\mathcal{M}_G)$, i.e., the number of free parameters in* $\mathrm{Stab}(E)$ *is greater than the dimension of the model, then $\mathcal{M}_G$ is non-identifiable. In particular, all graphs with $|E| > p(p+1)/2$ give non-identifiable models.*

Proof. The set $\mathrm{Stab}(E)$ is open, and any one of its elements is contained in an open semialgebraic ball $S \subset \mathrm{Stab}(E)$. As $\dim(S) = |E| > \dim(\mathcal{M}_G)$, it follows that the rational map ϕ_G is generically infinite-to-one; see, e.g., Barber et al. (2022, Lemma 2.5). Apply Lemma 3.3 below to conclude that all fibers are infinite. ∎

An obvious 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 one of its subgraphs; compare Drton et al. (2011, Lemma 1) in the context of standard graphical models. Here, a graph $H = (V', E')$ is a subgraph of a graph $G = (V, E)$ if $V' \subseteq V$ and $E' \subseteq E$. We record this fact as:

PROPOSITION 2.6. *Let $\mathcal{M}_G$ be a globally identifiable model. Then $\mathcal{M}_H$ is globally identifiable for all subgraphs H of G.*

Combining this proposition with Example 2.4, we obtain that the graph of a globally identifiable model cannot contain any 2-cycles.

Definition 2.7. *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 $i \to j \in E$ and $j \to i \in E$. Otherwise, we call G non-simple.*

Proposition 2.8. *If a directed graph G defines a globally identifiable model $\mathcal{M}_G$, then G must be simple.*

A key difference when proving generic instead of global identifiability is that one may no longer argue via subgraphs. Indeed, generic identifiability may be lost but also restored when removing an edge. Example 7.4 illustrates this phenomenon.

3. Rank conditions. In this section, we discuss solving the Lyapunov equation (1.1) for the generally non-symmetric drift matrix M given the symmetric matrices Σ 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 (1.1) is uniquely solvable for the symmetric matrix Σ 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

$$(I_p \otimes M + M^\top \otimes I_p)\text{vec}(\Sigma) = -\text{vec}(C), \tag{3.1}$$

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 $I_p \otimes M + M^\top \otimes I_p$ 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 (1.1) has a unique positive definite solution Σ if and only if M is a stable matrix.

However, solving for M given two symmetric (and in our context positive definite) matrices Σ 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 2.5. 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 1.5.

Lemma 3.1. *Vectorizing the Lyapunov equation (1.1), we obtain the system*

$$((\Sigma \otimes I_p) + (I_p \otimes \Sigma)K_p)\text{vec}(M) = -\text{vec}(C), \tag{3.2}$$

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

The commutation matrix K_p is the 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 3.1. It holds that

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

The Lyapunov equation (1.1) is symmetric and therefore $p(p-1)/2$ equations of the equation system (3.2) are redundant.

DEFINITION 3.2. *Given a $p \times p$ symmetric matrix Σ, 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 $k \le l$.

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

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

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

Example 1.5 displayed $A(\Sigma)$ for the case of $p = 3$. In general, the entries of $A(\Sigma)$ are given by

$$A(\Sigma)_{(k,l),i\to j} = \begin{cases} 0, & \text{if} \quad j \neq k,l; \\ \Sigma_{li}, & \text{if} \quad j = k,\ k \neq l; \\ \Sigma_{ki}, & \text{if} \quad j = l,\ l \neq k; \\ 2\Sigma_{ji}, & \text{if} \quad j = k = l. \end{cases} \tag{3.3}$$

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 $i \to j$. 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 $A(\Sigma)$. Recall that our model definition refers to a fixed choice of $C \in \mathrm{PD}_p$.

LEMMA 3.3. *Let $G = (V,E)$ be a directed graph with $V = [p]$. 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 $\mathcal{M}_G$ is*

(i) globally identifiable if and only if $A(\Sigma)_{\cdot,E}$ has full column rank $|E|$ for all $\Sigma \in \mathcal{M}_G$;

(ii) generically identifiable if and only if there exists a matrix $\Sigma \in \mathcal{M}_G$ such that $A(\Sigma)_{\cdot,E}$ has full column rank $|E|$.

If $\mathcal{M}_G$ is not generically identifiable, then it is non-identifiable.

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

$$A(\Sigma_0)_{\cdot,E}\,\mathrm{vec}(M)_E = -\mathrm{vech}(C), \tag{3.4}$$

where $\mathrm{vec}(M)_E$ is the subvector of $\mathrm{vec}(M)$ that comprises the entries indexed by (j,i) with $i \to j \in E$. Hence, $\mathcal{F}(M_0) = \{M_0\}$ precisely when $A(\Sigma_0)_{\cdot,E}$ has full column rank such that (3.4) 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 (3.1), the map ϕ_G is a rational map. Consequently, the map taking $M \in \mathrm{Stab}(E)$ to the maximal minors of $A(\phi_G(M))_{\cdot,E}$ is rational as well. Now a rational map is non-zero outside a measure zero set if and

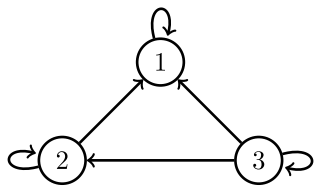

Fig. 2: The complete DAG G^* on 3 nodes.

only if there exists a single point where it is non-zero. Consequently, the existence of $\Sigma \in \mathcal{M}_G$ with $A(\Sigma)_{\cdot,E}$ of full column rank implies generic identifiability of $\mathcal{M}_G$.

Finally, if $\mathcal{M}_G$ is not generically identifiable then the column rank of $A(\Sigma)_{\cdot,E}$ is strictly smaller than $|E|$ for all $\Sigma \in \mathcal{M}_G$. From the fact that solution sets of (3.4) are not empty by definition of the model, it follows that they are positive-dimensional. Hence, $|\mathcal{F}(M_0)| = \infty$ for all $M_0 \in \mathrm{Stab}(E)$, and $\mathcal{M}_G$ is non-identifiable. ∎

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 $i \to i$, $i \in [p]$. 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 2.6, 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 4.1. *A directed simple graph $G = (V, E)$ on p nodes is* complete *if there is an edge between every pair of distinct nodes.*

A simple graph that contains all self-loops $i \to i$, $i \in [p]$, is thus complete if and only if $|E| = p(p+1)/2$. Because vertex relabelling has no impact on identifiability, we can furthermore restrict attention to a single topological ordering. In other words, it suffices to consider the single complete DAG G^* whose edge set is comprised of all edges $i \to j$ with $i \geq j$.

Example 4.2. Consider the case of $p = 3$ vertices, 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

$$\begin{array}{c} \\ (1,1) \\ (1,2) \\ (1,3) \\ (2,2) \\ (2,3) \\ (3,3) \end{array} \begin{array}{c} \begin{array}{cccccc} 1 \to 1 & 2 \to 1 & 2 \to 2 & 3 \to 1 & 3 \to 2 & 3 \to 3 \end{array} \\ \begin{pmatrix} 2\Sigma_{11} & 2\Sigma_{12} & 0 & 2\Sigma_{13} & 0 & 0 \\ \Sigma_{21} & \Sigma_{22} & \Sigma_{12} & \Sigma_{23} & \Sigma_{13} & 0 \\ \Sigma_{31} & \Sigma_{32} & 0 & \Sigma_{33} & 0 & \Sigma_{13} \\ 0 & 0 & 2\Sigma_{22} & 0 & 2\Sigma_{23} & 0 \\ 0 & 0 & \Sigma_{32} & 0 & \Sigma_{33} & \Sigma_{23} \\ 0 & 0 & 0 & 0 & 0 & 2\Sigma_{33} \end{pmatrix} \end{array}.$$

We observe that exchanging the third and the fourth column (indexed by $2 \to 2$ and $3 \to 1$, 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 Σ. Therefore, it holds for all $\Sigma \in \mathrm{PD}_3$ that

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

The block structure found in Example 4.2 generalizes and gives the main result of this section.

THEOREM 4.3. *The model $\mathcal{M}_G$ is globally identifiable for every directed acyclic graph $G = (V, E)$ on p nodes.*

Proof. As noted above, it suffices to consider the complete DAG $G^* = (V, E^*)$ whose edges are $i \to j$ for $i \geq j$. Our proof then applies Lemma 3.3, which states that model $\mathcal{M}_{G^*}$ is globally identifiable if and only if $\det(A(\Sigma)_{\cdot,E^*}) \neq 0$ for all $\Sigma \in \mathcal{M}_{G^*}$.

In what follows, let $\Sigma \in \mathrm{PD}_p$. Partition the edge set as $E^* = E_1^* \cup E_2^* \cup \cdots \cup E_p^*$, where $E_i^* = \{j \to i : j \geq i\}$. Similarly, partition the row index set of $A(\Sigma)$ into the disjoint union of the sets $R_k = \{(k, l) : l \geq k\}$, $k = 1, \ldots, p$. Inspecting (3.3), 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

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

Inspecting again (3.3), we find that $A(\Sigma)_{R_i,E_i^*}$ is equal to the principal submatrix $P(\Sigma)_{\geq i} := \Sigma_{\{i,\ldots,p\},\{i,\ldots,p\}}$ 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 Σ are positive, we obtain that

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

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

The proof of Theorem 4.3 shows that for any complete DAG $G = (V, E)$ the matrix $A(\Sigma)_{\cdot,E}$ is invertible for all $\Sigma \in \mathrm{PD}_p$. Using this fact, the proof of the theorem reveals more information about Lyapunov models arising from DAGs.

COROLLARY 4.4. *Let $G = (V, E)$ be a DAG on p nodes. Then $\mathcal{M}_G$ is an algebraic and thus closed subset of PD_p. Moreover, if G is complete then $\mathcal{M}_G = \mathrm{PD}_p$.*

Proof. Let G be a complete DAG. By Theorem 4.3, the square matrix $A(\Sigma)_{\cdot,E}$ has full rank for all $\Sigma \in \mathrm{PD}_p$. Therefore, the solution $\mathrm{vec}(M)$ to the vectorized Lyapunov equation (3.4) exists uniquely for all $\Sigma \in \mathrm{PD}_p$. The resulting drift matrix M has the right support by construction, hence $\mathcal{M}_G = \mathrm{PD}_p$.

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 $\Sigma \in \mathrm{PD}_p$ the same is true for $A(\Sigma)_{\cdot,E}$; recall Proposition 2.6. Hence, a matrix $\Sigma \in \mathrm{PD}_p$ is in $\mathcal{M}_G$ if and only if $\mathrm{vech}(C)$ is in the column span of $A(\Sigma)_{\cdot,E}$ if and only if the $(|E| + 1)$-minors of the augmented matrix $(A(\Sigma)_{\cdot,E} \mid \mathrm{vech}(C))$ vanish. The model $\mathcal{M}_G$ is thus an algebraic subset: it is the set of positive definite matrices at which these minors vanish. ∎

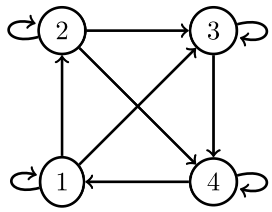

Fig. 3: A completion of the 4-cycle.

5. Sums of squares decompositions and finer rank conditions. The presence of directed cycles in the graph breaks the block-diagonal structure found for DAGs (Theorem 4.3) and makes it far more difficult to study the rank of $A(\Sigma)$. In this section we show that small cyclic graphs can nevertheless be handled by applying sums of squares decompositions to certify positivity of subdeterminants of $A(\Sigma)$. Moreover, we show that we may place our rank conditions on a smaller matrix containing a basis for the kernel of $A(\Sigma)$.

In Example 1.5, 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 PD_3. We were able to argue this via the positivity of 2×2 principal minors of Σ. However, a direct extension of this approach to cyclic graphs with a larger number of vertices is difficult. Nevertheless, some headway can be made by exploiting the positive-definiteness of Σ via its Cholesky decomposition.

Example 5.1. Let $G = (V, E)$ be the completion of the 4-cycle given by $E = \{1 \to 1, 2 \to 2, 3 \to 3, 4 \to 4, 1 \to 2,\ 1 \to 3,\ 2 \to 3, 2 \to 4,\ 3 \to 4,\ 4 \to 1\}$ and displayed in Figure 3. Let $\Sigma = LL^T$ be the Cholesky decomposition of $\Sigma \in \mathrm{PD}_4$ 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

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

where the key factor is

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

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 $\mathcal{M}_G$ is globally identifiable.

Remark 5.2. 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 1.5, Example 4.2, and Example 5.1). This phenomenon actually occurs for any complete simple graph (see Corollary A.2 in the Appendix), and it suggests that identifiability of the models should be encoded in a smaller matrix. Indeed, this information is carried by a specific row restriction of $H(\Sigma)$, a $p^2 \times p(p-1)/2$ matrix whose columns form a basis of the kernel of $A(\Sigma)$. Details about the kernel and an explicit description of a basis can be found in Theorem A.1.

THEOREM 5.3. *Let $G = (V, E)$ be a directed graph with $V = [p]$. Let $H(\Sigma)$ be a matrix whose columns form a basis of the kernel of $A(\Sigma)$ and let $H(\Sigma)_{E^c,\cdot}$ be the submatrix obtained by restriction to rows corresponding to non-edges E^c of G. Then the associated model $\mathcal{M}_G$ is*

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

Proof. Recall from Lemma 3.3 that (3.4) has a unique solution for any $\Sigma_0 \in \mathcal{M}_G$ if and only if $A(\Sigma_0)_{\cdot,E}$ has linearly independent columns. The latter condition can be rephrased as follows: the kernel of $A(\Sigma_0)$ does not contain any element $\mathrm{vec}(M) \neq 0$ such that $M \in \mathbb{R}^E$.

Note that $H(\Sigma)$ has linearly independent columns for any $\Sigma \in \mathrm{PD}_p$. Indeed, it can be checked that the rows corresponding to the non-edges of a DAG on p nodes form a maximal minor of $H(\Sigma)$ with a block structure consisting of principal minors of Σ. Therefore, the absence of non-trivial kernel elements with the right support is equivalent to the linear independence of the columns of the extended matrix $(H(\Sigma_0) \mid \mathrm{vec}(M))$ for any non-trivial $M \in \mathbb{R}^E$. It only remains to be proven that this is equivalent to the $|E^c| \times p(p-1)/2$ submatrix $H(\Sigma_0)_{E^c,\cdot}$ having rank $p(p-1)/2$.

Assume that $H(\Sigma_0)_{E^c,\cdot}$ has rank $p(p-1)/2$ and consider one of its non-vanishing maximal minors. It can always be extended to a non-vanishing maximal minor of $(H(\Sigma_0) \mid \mathrm{vec}(M))$ by adding one of the rows corresponding to $m_{ji} \neq 0$. Therefore, the extended matrix has full rank.

The converse implication can be directly proven by contrapositive. Indeed, if $H(\Sigma_0)_{E^c,\cdot}$ has rank strictly less than $p(p-1)/2$, then there exists a (not unique) non-trivial $M_0 \in \mathbb{R}^E$ such that $\mathrm{vec}(M_0)$ belongs to the kernel of $A(\Sigma_0)$. ∎

Example 5.4. Consider the 6×9 matrix $A(\Sigma)$ in Example 1.5 corresponding to $p = 3$ and set $H(\Sigma) = \ker A(\Sigma)$. Then

$$H(\Sigma) = \begin{array}{cc} \begin{pmatrix} -\Sigma_{12} & 0 & -\Sigma_{13} \\ -\Sigma_{22} & 0 & -\Sigma_{23} \\ -\Sigma_{23} & 0 & -\Sigma_{33} \\ \Sigma_{11} & -\Sigma_{13} & 0 \\ \Sigma_{12} & -\Sigma_{23} & 0 \\ \Sigma_{13} & -\Sigma_{33} & 0 \\ 0 & \Sigma_{12} & \Sigma_{11} \\ 0 & \Sigma_{22} & \Sigma_{12} \\ 0 & \Sigma_{23} & \Sigma_{13} \end{pmatrix} & \begin{array}{c} 1 \to 1 \\ 1 \to 2 \\ 1 \to 3 \\ 2 \to 1 \\ 2 \to 2 \\ 2 \to 3 \\ 3 \to 1 \\ 3 \to 2 \\ 3 \to 3 \end{array} \end{array},$$

where the row labels refer to columns in $A(\Sigma)$ and are therefore indexed by all possible edges (including self-loops) of a graph on 3 nodes.

Consider the DAG on 3 nodes given in Figure 2 and take its set of non-edges $E^c = \{1 \to 2, 1 \to 3, 2 \to 3\}$. 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 Σ, as expected from Theorem 4.3.

Now let $E^c = \{1 \to 3, 2 \to 1, 3 \to 2\}$ be the set of non-edges of the 3-cycle given in 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 (1.4). See Example 7.1 for an illustration of generic identifiability in the case of a non-simple graph on 3 nodes.

Although we have a very explicit description of $H(\Sigma)$ and its restriction to rows corresponding to non-edges E^c of a graph, a combinatorial statement on when those determinants vanish eludes our current knowledge.

Following Example 5.1, 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 Σ. However, this procedure is already computationally challenging for some cyclic graphs on 5 nodes.

Despite the limitations displayed, this approach is worth our attention because it provides information of the model beyond identifiability. Similarly to the case of complete DAGs in Corollary 4.4, whenever the determinant is indeed a non-vanishing SOS, it follows that $\mathcal{M}_G = \mathrm{PD}_p$. Our computational experiments prove this fact on a small number of nodes.

PROPOSITION 5.5. *Let $G = (V, E)$ be a simple cyclic graph with $p \leq 5$ nodes except the graphs displayed in Figure 4 and any of their subgraphs that are not subgraphs of other complete graphs. Then $\mathcal{M}_G$ is an algebraic and thus closed subset of PD_p. Moreover, if G is complete then $\mathcal{M}_G = \mathrm{PD}_p$.*

Our attempts to find an SOS decomposition with Macaulay2 and Matlab for the graphs in Figure 4 have not succeeded so far. However, we have no evidence that such

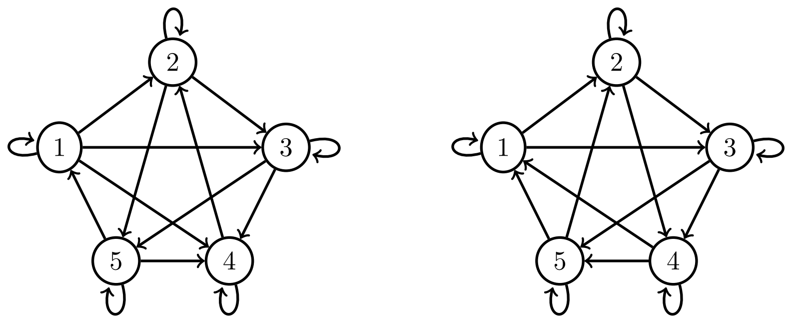

Fig. 4: The two simple cyclic graphs on 5 nodes, for which the result of Proposition 5.5 has not been established so far.

a decomposition does not exist and, even if this was the case, it still does not imply that the polynomial vanishes.

Conjecture 5.6. The statement in Proposition 5.5 holds for all simple graphs.

6. Simple cyclic graphs. In this section we establish our main result: Global identifiability of Lyapunov models given by simple cyclic graphs. Our proof exploits a parametrization of stable matrices M that are solutions to the Lyapunov equation in terms of skew-symmetric matrices (matrices K with $K^T = -K$). The following result can be found in Barnett and Storey (1967).

LEMMA 6.1. *Consider the continuous Lyapunov equation from* (1.1) *for given* $\Sigma, C \in \mathrm{PD}_p$. *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*

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

THEOREM 6.2. *A model* $\mathcal{M}_G$ *is globally identifiable if and only if* G *is a simple graph.*

Proof. ($\Longrightarrow$): This was shown in Proposition 2.8.

($\Longleftarrow$): Let $G = (V, E)$ be a simple graph on p nodes. Let $M_1, M_2 \in \mathrm{Stab}(E)$ be any two matrices that solve the Lyapunov equation (1.1) for the same $\Sigma \in \mathcal{M}_G$ and $C \in \mathrm{PD}_p$. According to Lemma 6.1 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

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

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 Σ^{-1}.

Consider now the square M^2. We have

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

As Σ 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 $\operatorname{tr}(M^2) \leq 0$.

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

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

which implies that $m_{ii}^2 = 0$ for all $i \in 1, \ldots, p$. Therefore, $\operatorname{tr}(M^2) = 0$.

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

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

which implies that $\lambda_i^2 = 0$ for all $i \in 1, \ldots, p$. But this is only true if $\lambda_i = 0$ for all $i = 1, \ldots, p$. 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 Lyapunov equation admits a unique sparse solution. ∎

While Theorem 6.2 solves the problem of characterizing global identifiability, our proof starts with the assumption that $\Sigma \in \mathcal{M}_G$ and does not solve Conjecture 5.6 for complete simple cyclic graphs. This is in contrast of our earlier proof of Theorem 4.3 and Corollary 4.4.

7. Non-simple graphs. In this section, we consider directed graphs $G = (V, E)$ that are allowed to have two-cycles, i.e., may be non-simple. By Proposition 2.8 we know that models given by non-simple graphs can never be globally identifiable. However, non-simple graphs with at most $p(p+1)/2$ edges may still give generically identifiable models (Definition 2.1, Lemma 2.5). We are able to provide a combinatorial condition that is necessary for generic identifiability, and we computationally classify all graphs with up to 5 nodes. The computational study reveals examples for which generic identifiability depends in subtle ways on the pattern of edges.

We begin with a small example.

Example 7.1. Let $G = (V, E)$ be the graph from Figure 5, a 2-cycle with an additional edge pointing to a third node. To inspect identifiability of $\mathcal{M}_G$, we may use the kernel basis of Example 5.4 with the set of non-edges $E^c = \{1 \to 3, 3 \to 1, 3 \to 2\}$.

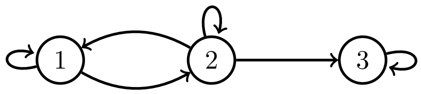

Fig. 5: Non-simple graph on 3 nodes.

We find

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

Since $\mathcal{M}_G$ contains positive definite matrices with $\Sigma_{23} \neq 0$, we conclude that $\mathcal{M}_G$ is generically (but not globally) identifiable.

If the fixed volatility matrix $C \in \mathrm{PD}_3$ is diagonal, then the matrices in $\mathcal{M}_G$ with $\Sigma_{23} = 0$ are obtained precisely from the drift matrices in the lower-dimensional set $\{M \in \mathrm{Stab}(E) : m_{32} = 0\}$. Indeed, if $m_{32} = 0$, then the situation is as if the $2 \to 3$ edge were removed, and we will see in Proposition 7.3 that this implies $\Sigma_{23} = 0$ when C is diagonal. Conversely, when solving for Σ given a drift matrix $M \in \mathbb{R}^E$ we find that Σ_{23} is a rational function of (M, C) whose numerator is

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

For $C \in \mathrm{PD}_3$ and M stable, the second factor is negative. Thus, if $\Sigma = \Sigma(M, C)$ is a positive definite matrix in $\mathcal{M}_G$, then $\Sigma_{23} = 0$ implies $m_{32} = 0$.

By Lemma 2.5, $|E| \leq p(p+1)/2$ 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.

Definition 7.2. *A* trek *is 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 also treks.

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

Proposition 7.3. *Suppose the fixed volatility matrix $C \in \mathrm{PD}_p$ is diagonal and $\Sigma \in \mathcal{M}_G$. If there is no trek from i to j in G, then $\Sigma_{ij} = 0$.*

Example 7.4. 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 2.6. But why is $\mathcal{M}_{G_2}$ 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 7.3 yields $\Sigma_{24} = \Sigma_{34} = 0$ when C is diagonal. Although the PD_4-cone has dimension $\binom{4+1}{2} = 10$, the existence of the constraints $\Sigma_{24} = \Sigma_{34} = 0$ implies that $\dim(\mathcal{M}_{G_2}) \leq 10 - 2 = 8$. Since $|E_2| = 9 > 8$, non-identifiability follows from by Lemma 2.5. The argument refers to C diagonal, but the identifiability status of a model does not change when it is defined with respect to another fixed matrix C.

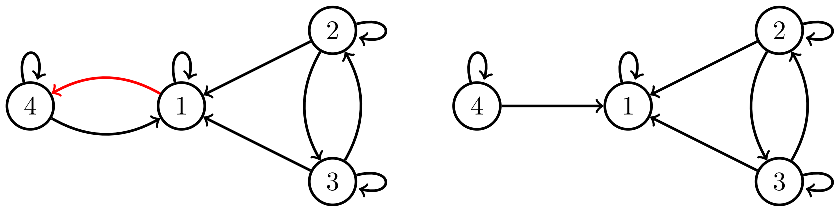

Fig. 6: Left: G_1, generically identifiable graph on 4 nodes. Right: G_2, non-identifiable subgraph of G_1.

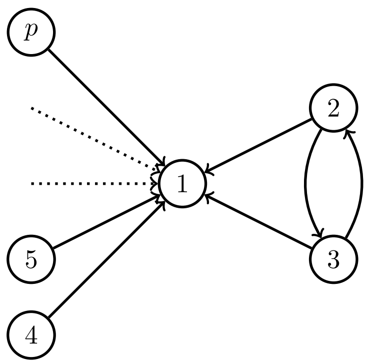

Fig. 7: Directed graph that is not identifiable. We omit the self-loops in this picture.

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

The ideas in Example 7.4 can be generalized into a sharper necessary condition for identifiability.

Corollary 7.5. *Let $G = (V, E)$ be a directed graph on p nodes. For G to be generically identifiable it has to hold that*

$$|E| \leq p(p+1)/2 - \#\{\text{pairs } i, j \in V \text{ with no trek}\}. \tag{7.1}$$

Proof. The claim follows from Lemma 2.5 and Proposition 7.3 and the fact that generic identifiability does not depend on which matrix $C \in \mathrm{PD}_p$ is fixed as volatility matrix $C \in \mathrm{PD}_p$. ∎

An interesting consequence of this criterion is that it can be applied to construct graphs of arbitrary size with fewer than $p(p+1)/2$ edges that are not identifiable. Example 7.4 can be generalized to such a family.

Corollary 7.6. *Consider the graph $G = (V, E)$ with $p \geq 4$ nodes displayed in Figure 7. The model $\mathcal{M}_G$ is non-identifiable.*

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

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

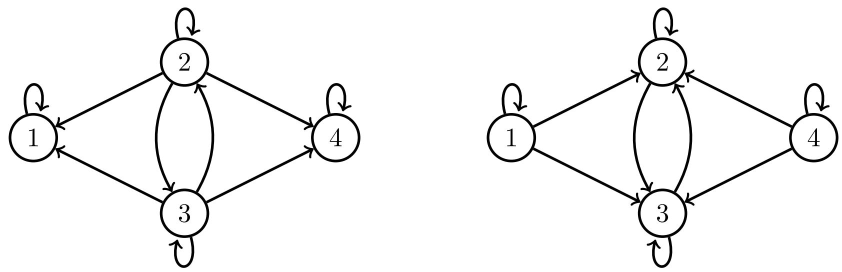

Fig. 8: Left: non-identifiable graph that fulfills the necessary criterion in Corollary 7.5. Right: Reversing edges retains non-identifiability, but now due to Corollary 7.5 as $\Sigma_{14} = 0$.

There are no treks between any pair of nodes $\{2, \ldots, p\}$ except for the pair $(2, 3)$. This results in $\binom{p-1}{2} - 1$ pairs of nodes with no trek. Corollary 7.5 implies that

$$\dim(\mathcal{M}_G) \leq \frac{p(p+1)}{2} - \binom{p-1}{2} + 1 = 2p. \qquad \square$$

Unfortunately, the criterion in Corollary 7.5 is not sufficient.

Example 7.7. Consider the left graph $G_1 = (V, E)$ as in Figure 8. Graph G_1 fulfills the necessary condition of Corollary 7.5 as the number of parameters is $6+4 = 10$ and all pairs of vertices are connected with a trek, which is why the right side of equation (7.1) is also $\binom{4+1}{2} = 10$. However, $A(\Sigma)_{\cdot,E} \in \mathbb{R}^{10\times 10}$ does not have full rank because the columns of $A(\Sigma)$ may be linearly combined to

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

Therefore, graph G_1 is not identifiable despite fulfilling the necessary criterion. The right graph G_2 is simply not identifiable as the necessary condition of Corollary 7.5 is violated due to the absence of a trek between node 1 and 4.

For smaller examples, we may check generic identifiability by choosing random drift matrices and determining whether the resulting matrix Σ satisfies the rank condition from Lemma 3.3. 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 Theorem 5.3 is rank-deficient, thus implying non-identifiability. We implemented this strategy for all non-simple graphs up to 5 nodes with less than $p(p+1)/2$ parameters. 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.

nodes	total non-simple	non-identifiable	non-identifiable satisfying (7.1)
3	2	0	0
4	80	3	2
5	4862	68	37

Table 1: Classification of models with $p = 3, 4, 5$ nodes. The last column displays the number of non-identifiable graphs for which the necessary criterion for generic identifiability in Corollary 7.5 holds.

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 is a complete characterization of globally identifiable models as those arising from simple graphs. Moreover, we provide a necessary condition for generic identifiability of models arising from non-simple graphs and obtain a computational classification of graphs with up to 5 vertices.

Our analysis of directed acyclic graphs (DAGs) exploits block structure in the coefficient matrix for the Lyapunov equation. This leads to a proof of global identifiability and implies that DAG models are closed algebraic subsets of the positive definite cone. In particular, the models of complete DAGs equal the entire positive definite cone. We are unable to draw these same conclusions for cyclic simple graphs, for which the coefficient matrix no longer exhibits block structure. Nevertheless, we conjecture that cyclic simple graphs also define closed algebraic subsets. This conjecture is based on sum of squares computations for graphs with up to 5 vertices.

While we were able to solve the problem of characterizing global identifiability, we know less about generic identifiability of graphical Lyapunov models. Our results include a necessary but not sufficient graphical criterion for non-simple graphs to be generically identifiable. We hope that future research will lead to an improved understanding of generic identifiability of the models we considered.

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Appendix A. Spectral description, kernel and factorization.

Throughout this paper we emphasized the relevance of having access to as much information as possible regarding the matrix $A(\Sigma)$. In this appendix, we consider its square version $\tilde{A}(\Sigma)$, for which we derive a full spectral characterization in Theorem A.1. Along the way, we give a description of the kernel $H(\Sigma)$ of $A(\Sigma)$. An immediate consequence is that $\det(\Sigma)$ is a factor of $\det(A(\Sigma)_{\cdot,E})$ for $|E| = p(p+1)/2$, see Corollary A.2.

THEOREM A.1. *Let $\tilde{A}(\Sigma) = \Sigma\otimes I_p + (I_p\otimes\Sigma)K_p$ and let $(\lambda_i)_{i\in[p]}$ be the eigenvalues of Σ with corresponding eigenvectors $(z_i)_{i\in[p]}$. The matrices $\tilde{A}(\Sigma)$ and $\tilde{A}(\Sigma)^\top$ have $p(p+1)/2$ not necessarily distinct eigenvalues $\lambda_i+\lambda_j$ with eigenvectors $z_i\otimes z_j + z_j\otimes z_i$, where $1\le i\le j\le p$. The remaining $p(p-1)/2$ eigenvalues of the matrices are zero. The vectors in*

$$H(\Sigma) = \begin{pmatrix} v^{(12)} & v^{(13)} & \dots & v^{(1p)} & v^{(23)} & \dots v^{(2p)} & \dots & v^{((p-1)p)} \end{pmatrix},$$

where $v^{(ij)}$ are vectors of length p^2 with

$$\begin{aligned} v^{(ij)}_{(i,1),\dots,(i,p)} &= -\Sigma_{\cdot,j}, \\ v^{(ij)}_{(j,1),\cdots,(j,p)} &= \Sigma_{\cdot,i}, \\ v^{(ij)} &= 0 \quad \textit{otherwise}, \end{aligned}$$

form a basis of the kernel of $\tilde{A}(\Sigma)$. In particular, this is also a basis of the kernel of $A(\Sigma)$. The vectors

$$\tilde{H}_\top(\Sigma) = \begin{pmatrix} w^{(12)} & w^{(13)} & \dots & w^{(1p)} & w^{(23)} & \dots w^{(2p)} & \dots & w^{(p-1p)} \end{pmatrix},$$

where $w^{(ij)}$ are vectors of length p^2 with

$$\begin{aligned} w^{(ij)}_{(i,j)} &= -1, \\ w^{(ij)}_{(j,i)} &= 1, \\ w^{(ij)} &= 0 \quad \textit{otherwise}, \end{aligned}$$

form a basis of the kernel of $\tilde{A}(\Sigma)^\top$.

Proof. For $1\le i\le j\le p$, consider the vectors $\tilde{z}_{ij} = z_i\otimes z_j + z_j\otimes z_i$. Since z_i and z_j are eigenvectors, the vector $\tilde{z}_{ij}$ cannot be the zero vector. Consider the indices $j\ge i$ and $l\ge k$ where not both $i=k$ and $j=l$. The vector $\tilde{z}_{ij}$ consists of blocks of length p of linear combinations of the vectors z_i and z_j. The same applies for $\tilde{z}_{kl}$. As the eigenvectors of Σ are all linearly independent we also have that $\tilde{z}_{ij}$ and $\tilde{z}_{kl}$ are linearly independent. We calculate

$$\tilde{A}(\Sigma)\tilde{z}_{ij} = (\Sigma\otimes I_p + (I_p\otimes\Sigma)K_p)(z_i\otimes z_j + z_j\otimes z_i)$$

in two steps. Firstly,

$$\begin{aligned} (\Sigma\otimes I_p)\tilde{z}_{ij} &= (\Sigma\otimes I_p)(z_i\otimes z_j) + (\Sigma\otimes I_p)(z_j\otimes z_i) \\ &= \Sigma z_i\otimes z_j + \Sigma z_j\otimes z_i = \lambda_i(z_i\otimes z_j) + \lambda_j(z_j\otimes z_i). \end{aligned}$$

Secondly, we obtain

$$\begin{aligned}(I_p \otimes \Sigma)K_p\tilde{z}_{ij} =&(I_p \otimes \Sigma)K_p(z_i \otimes z_j) + (I_p \otimes \Sigma)\\ =&(I_p \otimes \Sigma)(z_j \otimes z_i) + (I_p \otimes \Sigma)(z_i \otimes z_j) = z_j \otimes \Sigma z_i + z_i \otimes \Sigma z_j\\ =&\lambda_i(z_j \otimes z_i) + \lambda_j(z_i \otimes z_j).\end{aligned}$$

We conclude that

$$\tilde{A}(\Sigma)\tilde{z}_{ij} = (\lambda_i + \lambda_j)\tilde{z}_{ij},$$

with $\tilde{z}_{ij} \neq 0$. Hence $\lambda_i + \lambda_j$ is an eigenvalue of $\tilde{A}(\Sigma)$ with eigenvector $\tilde{z}_{ij}$. Due to the symmetry of the Lyapunov equation, the matrix $\tilde{A}(\Sigma)$ has $p(p-1)/2$ linearly dependent rows. As such, the zero eigenvalue appears with multiplicity $p(p-1)/2$. On the other hand, $\tilde{A}(\Sigma)$ and $\tilde{A}(\Sigma)^\top$ share the same spectrum. Their eigenvectors for non-zero eigenvalues are related by changing the position of the commutation matrix

$$(\Sigma \otimes I_p + (I_p \otimes \Sigma)K_p)^\top = \Sigma \otimes I_p + K_p(I_p \otimes \Sigma).$$

Now we focus on the eigenvectors of the zero eigenvalue of $\tilde{A}(\Sigma)$. That the vectors $v^{(ij)}$ belong to the kernel of $A(\Sigma)$ follows from the remarks regarding the structure of $A(\Sigma)$ in Section 3. Now, consider the maximal minor $M_{H(\Sigma)}$ of $H(\Sigma)$ obtained by restricting to rows indexed by $\{1 \to 2, 1 \to 3, \dots, 1 \to p, 2 \to 3, 2 \to 4. \dots, 2 \to p, \dots, p-1 \to p\}$. Note that this set corresponds to the non-edges of a complete DAG. Using similar arguments as in Theorem 4.3 we see that $\det(M_{H(\Sigma)}) \neq 0$, and hence $\operatorname{rank}(H(\Sigma)) = p(p-1)/2$. Since the class of DAGs is globally identifiable by Theorem 4.3, we know that the dimension of $\operatorname{im}(A(\Sigma))$ is $p(p+1)/2$. By the rank-nullity theorem, $\dim(\ker(A(\Sigma)))$ must be $p(p-1)/2$ and the column vectors $v^{(ij)}$ of $H(\Sigma)$ form a basis of the kernel. Finally, regarding the kernel of $\tilde{A}(\Sigma)^\top$, the vectors $w^{(ij)}$ belong to it as they cancel out columns that are duplicates of each other. As the vectors $w^{(ij)}$ with $i < j$ always have their non-zero entries in different position, we have that $\operatorname{rank}(H_\top(\Sigma)) = p(p-1)/2$ and that the column vectors $w^{(ij)}$ of $H_\top(\Sigma)$ form a basis of the kernel of $\tilde{A}(\Sigma)^\top$. ∎

As a consequence of Theorem A.1, we can conclude information regarding the factorization of the determinant of $A(\Sigma)_{\cdot,E}$. Note that this only makes sense for a square matrix, namely $|E| = p(p+1)/2$.

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

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 $\det(A(\Sigma)_{\cdot,E}) = 0$ for all singular matrices Σ. Let Σ be singular, then there exists an eigenvalue $\lambda_i = 0$ with $i \in [p]$. Using Theorem A.1 this implies that the eigenvalue $\lambda_i + \lambda_i$ of $\tilde{A}(\Sigma)$ is zero. Then, it holds that $\operatorname{rank}(\tilde{A}(\Sigma)) \leq p(p+1)/2 - 1$ which implies that $\operatorname{rank}(A(\Sigma)_{\cdot,E}) \leq p(p+1)/2 - 1$ and thus $\det(A(\Sigma)_{\cdot,E}) = 0$.

The fact that $\det(H(\Sigma)_{E^c,\cdot})$ is a factor of $\det(A(\Sigma)_{\cdot,E})$ follows from the proof of Theorem 5.3. ∎