THE GEOMETRY OF GAUSSIAN DOUBLE MARKOVIAN DISTRIBUTIONS

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ABSTRACT. Gaussian double Markovian models consist of covariance matrices constrained by a pair of graphs specifying zeros simultaneously in the matrix and its inverse. We study the semi-algebraic geometry of these models, in particular their dimension, smoothness and connectedness as well as algebraic and combinatorial properties.

1. INTRODUCTION

Let $N := \{1, \ldots, n\}$ and let $G$ and $H$ be two undirected, simple graphs on the vertex set $N$. Denote by $\text{PD}_n$ the set of real symmetric positive definite $n \times n$-matrices. In this paper, we study the following statistical models.

Definition 1.1. The Gaussian double Markovian model of $G$ and $H$ is

$$M(G, H) := \left\{ \Sigma \in \text{PD}_n : (\Sigma^{-1})_{ij} = 0 \text{ for all } ij \notin G, \Sigma_{kl} = 0 \text{ for all } kl \notin H \right\}.$$

Denoting the complete graph on $N$ by $K_N$, ordinary undirected Gaussian graphical models are contained in Definition 1.1 as $M(G) := M(G, K_N)$. Covariance models are contained as $M(K_N, H)$, so both model classes are unified and generalized here.

Conditional independence and graphical modeling. Conditional independence (CI) constraints are a central tool in mathematical modeling of random events. For random variables $X_1, \ldots, X_n$, basic conditional independence statements stipulate that one random variable $X_i$ is independent of another $X_j$ given a collection of remaining variables $(X_k)_{k \in K}$ where $i, j \in \{1, \ldots, n\}$ and $K \subseteq \{1, \ldots, n\} \setminus \{i, j\}$. CI constraints for discrete and normally distributed random variables translate into algebraic conditions on elementary probabilities in the discrete case and on covariance matrices in the Gaussian case. Algebraic statistics aims to understand algebraic and geometric properties of conditional independence models and to relate them to properties of statistical inference procedures.

In this paper we exclusively treat Gaussian random variables, i.e., we assume that $(X_1, \ldots, X_n)$ has a multivariate normal distribution with positive definite covariance matrix $\Sigma \in \text{PD}_n$. Since the theory of CI is insensitive to the mean, we may restrict to centered distributions.
In graphical modeling, edges and paths represent correlation or interaction and, conversely, notions of disconnectedness represent independence. Double Markovian models are conditional independence models whose CI statements are of the following two forms: either $X_i \perp \perp X_j$ (for each non-edge $ij$ of $H$) or $X_i \perp \perp X_j | X_N \setminus \{i,j\}$ (for each non-edge $ij$ of $G$). Pairwise conditional independence as in the second type is common in graphical modeling [26]. The resulting Gaussian graphical model of a simple undirected graph $G$ on $N$ with edge set $E_G$ is

$$
\mathcal{M}(G) = \mathcal{M}(G, K_N) = \{ \Sigma \in \text{PD}_n : (\Sigma^{-1})_{ij} = 0 \text{ for all } ij \notin G \}. 
$$

In words, the non-edges of $G$ specify zeros of the inverse covariance matrix $K = \Sigma^{-1}$, also called the concentration matrix. Gaussian graphical models first appeared in [35], and [41] is a modern survey containing many connections to e.g. optimization and matrix completion. Marginal independence constraints (as in the first case) also appear, for example with bidirected [12] or dashed graphs [9]. These models $\mathcal{M}(K_N, H)$ encode marginal independence constraints and are also known as covariance graph models [24, 27].

A model similar to double Markovian models appeared recently in [27, Example 3.4], where the authors consider graphical models with some entries of $K$ zero and complementary entries of $\Sigma$ nonnegative. They investigate efficient estimation procedures. These models go back to work of Kauermann [1, 24]. One way to describe them is via mixed parametrizations: the regular exponential family of all multivariate mean-zero Gaussians can be parametrized by the mean parameter $\Sigma = (\sigma_{ij})$ or the natural parameter $K = (k_{st})$. One can also employ a mixed parametrization, using $\sigma_{ij}$ and $k_{st}$ for $ij \in A$ and $st \in B$, where $A \cup B$ is a partition of the entries of an $n \times n$-symmetric matrix. Double Markovian models with $G \cup H = K_N$ arise from imposing zeros in the mixed parametrization. In general they do not form regular exponential families, though. In the terminology of [27], linear constraints on mixed parameters define mixed linear exponential families. Such models also appear in causality theory [34].

We study geometric properties of statistical models since they can imply favorable statistical properties. The asymptotic behavior of $M$-estimators like the MLE depends on properties of tangent cones that go under the name Chernoff regularity in [18]. Drton has shown that the nature of singularities determines the large sample asymptotics of likelihood ratio tests [11]. Smoothness of log-linear models for discrete random variables has been studied by examining the parametrization by marginals [16, 17]. Generally, smoothness is favorable because estimation procedures using analytical techniques like gradient descent rely on it.

In several occasions, for example in Corollary 3.21 geometric niceness results follow because either $\mathcal{M}(G, H)$ or its inverse $\mathcal{M}(H, G)$ is an ordinary graphical model and thus irreducible, connected, and smooth. In these cases one has found an effective new parametrization of $\mathcal{M}(G, H)$. This theme has occurred in the literature. For example [13] asks for a Markov equivalent directed and undirected graph to the bidirected (i.e. covariance) graph. Our geometric niceness results, however, go beyond recognizing disguised graphical models.

A systematic analysis of smoothness of Gaussian CI models has been initiated in [14]. That paper treats the $n = 4$ case in detail. It relies on similar algebraic techniques as we do here, but also on the characterization of realizable 4-gaussoids from [28]. We deal with a smaller class of models here, but achieve results independent of the number of random variables, aiming to understand how the geometry of $\mathcal{M}(G, H)$ depends on $G$ and $H$. In particular, we are
interested in dimension, smoothness, irreducible decompositions and other basic geometric facts that seem useful and interesting for inference methodology.

Algebraically, a double Markovian model \( \mathcal{M}(G, H) \) is the vanishing set inside \( \text{PD}_n \) of an ideal generated by some entries of \( \Sigma \in \text{PD}_n \) and some more of its inverse. The latter is an algebraic condition as it can be encoded as the vanishing of submaximal minors of \( \Sigma \). This puts us broadly in the framework of sparse determinantal ideals, see Definition 3.17 for the concrete class of ideals we are concerned with. The sparsity is twofold in our setting: our ideals are generated by only some minors of a sparse generic symmetric matrix, i.e., a symmetric matrix whose entries in the upper triangle are either distinct variables or zero. To our knowledge, no systematic study of these ideals has been carried out, even in the case of submaximal minors only. Minors of symmetric matrices are a classical topic in commutative algebra, see for example \([6, 8]\). Our results, in particular Theorem 3.20, can be viewed as a further step towards the study of this class of sparse determinantal ideals.

We illustrate our results on a simple preliminary example. Section 4 contains further examples.

**Example 1.2.** Let \( G = \bigtriangleup \) be a star with edge set \{12, 13, 14\} and \( H = \square \) a path with edge set \{12, 23, 34\}. To study the model \( \mathcal{M}(G, H) \), consider two indeterminate symmetric \( 4 \times 4 \)-matrices \( \Sigma = (\sigma_{ij}), K = (k_{ij}) \) representing covariance and concentration matrices. The non-edges of \( G \) dictate the zeros of \( K \) and the non-edges of \( H \) those of \( \Sigma \). Algebraically (which means ignoring the positive definiteness for a moment), the model is specified by the equations

\[
\Sigma K = 1_4, \quad k_{23} = k_{24} = k_{34} = \sigma_{13} = \sigma_{14} = \sigma_{24} = 0.
\]

These equations can be solved in \texttt{Macaulay2} \([19]\) using primary decomposition algorithms. This computation shows that the complex algebraic variety defined by (1) consists of two irreducible components. In one of the components, \( k_{22} = s_{11} = 0 \) holds. So, if this component contains covariance matrices at all, then they are of non-regular Gaussians. We do not consider this further in this example, although boundary components can be important with respect to marginalization; see Example 2.16. The other component consists of the matrices \( \Sigma \) of the form

\[
\Sigma = \begin{pmatrix}
\sigma_{11} & \sigma_{12} & 0 & 0 \\
\sigma_{12} & \sigma_{22} & 0 & 0 \\
0 & 0 & \sigma_{33} & 0 \\
0 & 0 & 0 & \sigma_{44}
\end{pmatrix}, \quad K = \begin{pmatrix}
k_{11} & k_{12} & 0 & 0 \\
k_{12} & k_{22} & 0 & 0 \\
0 & 0 & k_{33} & 0 \\
0 & 0 & 0 & k_{44}
\end{pmatrix},
\]

subject to the constraints \( \Sigma K = 1_4 \). This component is 5-dimensional and contains positive definite matrices. If one additionally normalizes the variances as \( \sigma_{ii} = 1 \) for \( i = 1, \ldots, 4 \), then \( \Sigma \) is positive definite exactly if \( \sigma_{12} \in (-1, 1) \). The (complex) singular locus of the interesting component is empty. In fact, smoothness is clear from the simple parametrization.

Several features of this example follow from results in this paper. For example, the vanishing ideal of the model is a monomial ideal by Theorem 3.20. That \( \mathcal{M}_1(G, H) \) is a curve segment is explained by Proposition 3.28. The block-diagonal structure follows from Theorem 3.23.

**Remark 1.3.** For computation it is sometimes useful to work in \((\Sigma, K)\)-space as in Example 1.2. Let \( \Sigma = (\sigma_{ij}) \) and \( K = (k_{st}) \) be generic symmetric matrices (possibly with ones on the diagonal). To computationally answer algebraic questions about constrained covariance matrices, one
Theorem A

The ring $R$ to impose equational constraints, one forms quotients by ideals generated by the equations. For example, the relation that $\Sigma K = 1_n$ is implemented by construction of the quotient ring $\mathbb{R}[\sigma_{ij}, k_{st} : i \leq j, s \leq t]/(\Sigma K - 1_n)$. Another useful trick is to impose non-vanishing or invertibility of certain polynomials, for example $\det(\Sigma)$. This is achieved by localization. The ring $\mathbb{R}[\sigma_{ij} : i \leq j]_{\det(\Sigma)}$ is an enlarged version of $\mathbb{R}[\sigma_{ij} : i \leq j]$ where now $\det(\Sigma)$ is invertible. In fact, the natural map

$$\mathbb{R}[\sigma_{ij} : i \leq j]_{\det(\Sigma)} \rightarrow \mathbb{R}[\sigma_{ij}, k_{st} : i \leq j, s \leq t]/(\Sigma K - 1_n),$$

defined by mapping $\sigma_{ij}$ to $\sigma_{ij}$ is an isomorphism, as it should be because the constraint that $K = \Sigma^{-1}$ makes all variables $k_{st}$ functions of the $\sigma_{ij}$. If $I \subseteq \mathbb{R}[\sigma_{ij} : i \leq j]$ is an ideal, then the restriction of its extension in the localization at $\det(\Sigma)$ agrees with its saturation at $\det(\Sigma)$. This provides a way to study conditional independence ideals in the ring $\mathbb{R}[\sigma_{ij}, k_{st} : i \leq j, s \leq t]/(\Sigma K - 1_n)$, where almost-principal minors of high degree are directly available as the $k_{st}$ variables. Saturation at $\det(\Sigma)$, however, is of course not equivalent to the saturation at all principal minors. We recommend [39, Chapter 3] for a general introduction to computational methods of commutative algebra with a view towards statistics.

Remark 1.4. The term double Markov property appears in [22, Lemma 1] based on [10, Exercise 16.25, p. 392] where it is called double Markovity. It describes constraints on three random variables which are in a special pair of Markov chains. This notion is unrelated to the Markovness with respect to two undirected graphs studied here. We judge the potential for confusion low enough to reuse this term.

Overview of results. The core of our work are several geometric and algebraic insights having implications for statistical procedures dealing with $\mathcal{M}(G, H)$. In these results it is often useful to restrict dimension and work with correlation matrices, which are covariance matrices with ones on the diagonal. We write $\text{PD}_{n, 1}$ for the set of positive definite matrices with ones on the diagonal. It is bounded and known as the elliptope. Then $\mathcal{M}_1(G, H) := \mathcal{M}(G, H) \cap \text{PD}_{n, 1}$ is a correlation model. Let $E_G$ denote the edge set of $G$ and $G \cap H$ the graph on $N$ with edge set $E_G \cap E_H$, and similarly $G \cup H$ the graph with edge set $E_G \cup E_H$. An important insight is that geometric and algebraic properties of double Markovian models often depend on features or the simplicity of $G \cap H$. The first result is a decomposition theorem relying on a notion of direct sum defined via block matrices in Section 2.3.

Theorem A (Theorem 3.23 and Corollary 3.24). Let $V_1, \ldots, V_r$ be a partition of $N$ such that each $V_i$ is the vertex set of a connected component of $G \cap H$. Then

$$\mathcal{M}(G, H) = \bigoplus_{i=1}^r \mathcal{M}(G|_{V_i}, H|_{V_i}),$$

i.e., every $\Sigma \in \mathcal{M}(G, H)$ has a block-diagonal structure with $r$ diagonal blocks having rows and columns indexed by the $V_i$. In particular, the correlation model satisfies $\mathcal{M}_1(G, H) = \{ 1_n \}$ if and only if $E_G \cap E_H = \emptyset$. 
The next result exhibits that also the union of $G$ and $H$ contributes. If it is complete, then the imposed constraints are simple enough to show, for example, smoothness.

**Theorem B** (Theorems 3.8, 3.11 and 3.15). For all graphs $G$ and $H$ we have $\dim(\mathcal{M}(G, H)) \leq |E_G \cap E_H| + n$. If $G \cup H = K_N$, then $\mathcal{M}(G, H)$ is smooth of dimension $|E_G \cap E_H| + n$. Conversely, if $\mathcal{M}(G, H)$ attains this maximal dimension, its top-dimensional connected components are smooth with irreducible Zariski closure.

In Section 3.3 we initiate the study of connectedness of $\mathcal{M}(G, H)$ in the Euclidean topology. We conjecture that all double Markovian correlations models are connected (Conjecture 4.5). This contrasts with the fact that, allowing semi-definite matrices, similarly defined variants of $\mathcal{M}_1(G, H)$ can consist of isolated points as in Example 4.4. We have the following results.

**Theorem C** (Corollary 3.21, Theorem 3.22, and Propositions 3.28, 3.29 and 3.31). The double Markovian model $\mathcal{M}(G, H)$ is connected in the following cases:

1. For every non-edge $kl$ of $G$ there is at most one path $p$ in $H$ connecting $k$ and $l$ (or if this holds for $G$ and $H$ exchanged).
2. There is a vertex $i \in N$ such that for all non-edges $kl$ of $G$, every path in $H$ connecting $k$ and $l$ contains $i$ (or if this holds for $G$ and $H$ exchanged).
3. $|E_G \cap E_H| \leq 3$.

The next theorem is our main algebraic result, see Theorem 3.20 for a more general version. Here a forest is a (not necessarily connected) graph with no cycles.

**Theorem D** (Theorem 3.20). Let $G$ be any graph and $H$ a forest. Then the vanishing ideal of $\mathcal{M}_1(G, H)$ is the square-free monomial ideal

$$\mathcal{I}(\mathcal{M}_1(G, H)) = \langle \sigma_{ij}, \sigma_p : ij \notin H, p \text{ path in } H \text{ with } e(p) \notin G \rangle.$$

Here, $\sigma_p$ is the product of variables corresponding to edges in $p$, and $e(p)$ denotes its endpoints.

Finally, in Propositions 3.28 to 3.31 we give a classification up to symmetry and matrix inversion of all double Markovian models with $|E_G \cap E_H| \leq 3$.

2. Preliminaries on Conditional Independence Structures

2.1. **Gaussian conditional independence.** Gaussian graphical models as well as the double Markovian models are conditional independence models: they are sets of Gaussian distributions specified by conditional independence assumptions derived from a graph or pair of graphs. The conditional independence relations of random variables can be studied combinatorially, using abstract properties of conditional independence instead of concrete numerical data like a density function or covariance matrix. To this end, we introduce formal symbols $(ij | K)$ where $i \neq j \in N$ and $K \subseteq N \setminus \{i, j\}$. These formal symbols are subject to the efficient Matúš set notation where union is written as concatenation and singletons are written without curly braces. For example, $ijK$ is shorthand for $\{i\} \cup \{j\} \cup K$.

The symbol $(ij | K)$ shall represent the conditional independence $X_i \perp \perp X_j | X_K$ where $X_K = (X_k)_{k \in K}$. For Gaussian random variables $X_1, \ldots, X_n$, the CI statement $X_I \perp \perp X_J | X_K$ is
equivalent to \( \text{rk} \Sigma_{1K,JK} = |K| \) by [39, Proposition 4.1.9]. Using the adjoint formula for the inverse of a matrix, it can be seen that a statement \((ij)N \setminus ij\) (as it appears in the definition of a graphical model) is equivalent to \( (\Sigma^{-1})_{ij} = 0 \).

If \( I = i \) and \( J = j \) are singletons, the rank condition is equivalent to the vanishing of the determinant of the square submatrix \( \Sigma_{iK,jK} \). These determinants are almost-principal minors.

It is well-known that the statements \((ij|K)\) completely describe the entire CI relation of a random vector [30, Section 2]. The set of all conditional independence statements among \( n \) random variables is \( A_n = \{(ij|K) : i \neq j \in N, K \subseteq N \setminus ij\} \). An abstract conditional independence relation is a subset of \( A_n \). Fundamental problems in the intersection of probability, computer science and information theory concern the set of realizable subsets \( \mathcal{R} \subseteq 2^{A_n} \), meaning that for \( \mathcal{R} \in \mathcal{R} \) there is a random vector \( X \) satisfying all statements in \( \mathcal{R} \) and none of those in \( A_n \setminus \mathcal{R} \).

To each positive definite \( n \times n \)-matrix \( \Sigma \) we associate a corresponding CI relation

\[
\langle \Sigma \rangle := \{(ij|K) : \text{rk} \Sigma_{iK,jK} = |K|\} \subseteq A_n,
\]

consisting exactly of the CI statements satisfied by \( \Sigma \). Conversely, the covariance matrices satisfying all statements of a CI relation \( \mathcal{R} \) form its Gaussian conditional independence model:

\[
\mathcal{M}(\mathcal{R}) := \{\Sigma \in PD_n : \text{det}(\Sigma_{iK,jK}) = 0 \text{ for all } (ij|K) \in \mathcal{R}\} \subseteq PD_n \subseteq \text{Sym}^2(\mathbb{R}^n) \cong \mathbb{R}^{\binom{n+1}{2}}.
\]

We consider this set together with the subset topology with respect to the Euclidean topology on the set of symmetric matrices \( \text{Sym}^2(\mathbb{R}^n) \). The cone \( PD_n \) is open in \( \text{Sym}^2(\mathbb{R}^n) \) as it is the preimage of \( \mathbb{R}_{>0}^n \subseteq \mathbb{R}^n \) under the continuous map which sends \( \Sigma \in \text{Sym}^2(\mathbb{R}^n) \) to the vector in \( \mathbb{R}^n \) consisting of the determinants of all \( n \) leading principal minors, using Sylvester’s criterion. Writing \( \Sigma = (\sigma_{ij}) \), the associated correlation matrix of \( \Sigma \) has \( \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}} \) as its \( ij \)-entry.

Its diagonal consists of ones and all non-diagonal entries lie in \((-1,1)\) as \( \text{det}(\Sigma_{ij,ij}) > 0 \). Therefore, the set of correlation matrices \( PD_{n,1} \) is an intersection of \( PD_n \) with an affine linear subspace of \( \text{Sym}^2(\mathbb{R}^n) \). This yields a subspace topology and also a canonical smooth structure on \( PD_{n,1} \), making it into a smooth submanifold of \( PD_n \) of codimension \( n \). It is often convenient to work with the bounded set of correlation matrices in the model:

\[
\mathcal{M}_1(\mathcal{R}) := \{\Sigma \in PD_{n,1} : \text{det}(\Sigma_{iK,jK}) = 0 \text{ for all } (ij|K) \in \mathcal{R}\} = PD_{n,1} \cap \mathcal{M}(\mathcal{R}).
\]

Many favorable properties transfer between \( \mathcal{M}_1(\mathcal{R}) \) and \( \mathcal{M}(\mathcal{R}) \), especially if they are of differentiable nature, see Lemma 3.1. Some care is necessary when considering algebraic properties such as the number of Zariski irreducible components. \( \mathcal{M}_1(\mathcal{R}) \) is a linear section of \( \mathcal{M}(\mathcal{R}) \), so its algebraic properties may differ; see e.g. Example 4.1.

There is no finite axiomatization of the set \( \mathcal{R} \) of realizable CI relations that is valid for all \( n \). Neither in general [36] nor for Gaussians specifically [38]. Closure properties of CI relations often have cryptic names going back to the search for a finite axiomatization. In this terminology, for \( \Sigma \in PD_n \), the relation \( \langle \Sigma \rangle \) is a weakly transitive, compositional graphoid. The compound of these properties is also the definition of gaussoid [28]. Gaussoids approximate Gaussian conditional independence in a similar way to matroids approximating linear independence [4].

2.2. Undirected graphical models. If \( G \) is a graph on \( N \), then

\[
\langle G \rangle := \{(ij|K) : K \text{ separates } i \text{ and } j \text{ in } G\}
\]
denotes the CI separation statements, those that follow from separation in the graph. We refer to CI relations of the form $\langle \langle G \rangle \rangle$ as Markov relations. See [26] for all details on modeling CI by graphs. Any relation $\langle \langle G \rangle \rangle$ is realizable, meaning that it equals $\langle \langle \Sigma \rangle \rangle$ for some $\Sigma \in \text{PD}_n$ and one can even pick $\Sigma$ with all positive correlations [4, Theorem 4]. The models realizing $\langle \langle G \rangle \rangle$ are smooth as they are inverse linear spaces and thus parametrized by a diffeomorphism (see Proposition 2.2). Since the CI relation $\langle \langle G \rangle \rangle$ of any graph $G$ is realizable, it follows that $\langle \langle G \rangle \rangle$ is a gaussoid. In addition, graph separation is upward-stable, meaning that $(ij | L)$ implies $(ij | kL)$ for all $k \in N \setminus ijL$, and being an upward-stable gaussoid is even a characterization of being of the form $\langle \langle G \rangle \rangle$ for some undirected graph $G$ by [30, Proposition 2].

A pseudographoid is an abstract CI structure which satisfies the intersection property, which together with the semigraphoid axiom forms the definition of graphoid; see [28, Remark 1] for the terminology. The following lemma states that it is sufficient to verify that $\Sigma$ satisfies the maximal separation statements (which correspond to the non-edges in $G$), for it to satisfy all separation statements for $G$. In this case $\Sigma$ is Markovian for $G$.

**Lemma 2.1.** Let $G$ be an undirected graph and $\Sigma$ a complex symmetric matrix with non-vanishing principal minors and let $m = \{(ij \mid N \setminus ij) : i \neq j\}$ denote the set of maximal CI statements. Then $\langle \langle G \rangle \rangle \cap m \subseteq \langle \langle \Sigma \rangle \rangle$ implies $\langle \langle G \rangle \rangle \subseteq \langle \langle \Sigma \rangle \rangle$.

**Proof.** By [31, Corollary 1] the CI structure $\langle \langle \Sigma \rangle \rangle$ is a weakly transitive, compositional graphoid already when $\Sigma$ is a complex symmetric matrix with non-vanishing principal minors (which includes the real positive definite case). The lemma follows from [28, Lemma 3], by choosing $M = \langle \langle G \rangle \rangle \cap m$. Then $G$ is a graph with $i$ and $j$ adjacent if and only if $(ij \mid N \setminus ij) \notin M$. Since $M \subseteq \langle \langle \Sigma \rangle \rangle$ by assumption, it follows that $\langle \langle G \rangle \rangle \subseteq \langle \langle \Sigma \rangle \rangle$. □

By Lemma 2.1, $\Sigma$ is Markovian for $G$ if and only if $\langle \langle G \rangle \rangle \cap m \subseteq \langle \langle \Sigma \rangle \rangle$. The maximal CI statements $\langle \langle G \rangle \rangle \cap m$ point out precisely the non-edges in $G$ and therefore $\Sigma$ being Markovian for $G$ is equivalent to $(\Sigma^{-1})_{ij} = 0$ for all $ij \notin G$. This shows that $M(G) = M(\langle \langle G \rangle \rangle)$.

**Proposition 2.2.** Every Markov relation $\langle \langle G \rangle \rangle$ is realizable by a regular Gaussian distribution. For each graph $G$, the model $M(G)$ is irreducible and smooth.

**Proof.** Realizations for $\langle \langle G \rangle \rangle$ were constructed from (inverses of) generalized adjacency matrices in [28, Theorem 1]. By Lemma 2.1 the set $M(G)^{-1} = \{ \Sigma^{-1} : \Sigma \in M(G) \}$ is a linear subspace intersected with the cone $\text{PD}_n$. It is the interior of a spectrahedron. As such it is an irreducible semi-algebraic set and smooth. These properties are transferred to the inverse $M(G)$ by Lemmas 3.1 and 3.2 below. □

Matúš [32, Theorem 2] proved a geometric characterization of sets $M(G)^{-1}$: among all Gaussian conditional independence models, they are precisely those which are convex subsets of $\text{PD}_n$.

### 2.3. Minors, duality and direct sums
Marginalization and conditioning are natural operations on random vectors and can also be carried out on conditional independence structures. These abstract operations mimic the effect of statistical operations on a purely formal level.
Definition 2.3. Let $\mathcal{R} \subseteq \mathcal{A}_N$ and $k \in N$. The marginal and the conditional of $\mathcal{R}$ on $N \setminus k$ are, respectively,
\[
\mathcal{R} \setminus k := \{(ij|K) \in \mathcal{A}_{N \setminus k} : (ij|K) \in \mathcal{R}\}, \\
\mathcal{R} / k := \{(ij|K) \in \mathcal{A}_{N \setminus k} : (ij|K \cup k) \in \mathcal{R}\}.
\]
Any set $\mathcal{R}' \subseteq \mathcal{A}_{N'}$, $N' \subseteq N$, obtained from $\mathcal{R}$ by a sequence of marginalization and conditioning operations is a minor of $\mathcal{R}$.

On covariance matrices, marginalizing away a variable $k \in N$ is achieved by taking the principal submatrix $\Sigma \setminus k := \Sigma_{N \setminus k}$. The conditional distribution on $k$ is the Schur complement of the $k \times k$ entry $\Sigma / k := \Sigma_{N \setminus k} - \sigma_{kk}^{-1}\Sigma_{N \setminus k,k} \cdot \Sigma_{k,N \setminus k}$. This is proven in [39, Theorem 2.4.2].

Lemma 2.4. For $\Sigma \in \mathbb{PD}_n$ we have $\langle \Sigma \rangle \setminus k = \langle \Sigma \setminus k \rangle$ and $\langle \Sigma \rangle / k = \langle \Sigma / k \rangle$. In particular, minors of realizable CI relations are realizable.

For any Gaussian distribution, matrix inversion exchanges the covariance and concentration matrices. The combinatorial version of this operation furnishes an involution on CI relations.

Definition 2.5. The dual of $\mathcal{R} \subseteq \mathcal{A}_N$ is $\mathcal{R}^\perp := \{(ij|N \setminus ijK) : (ij|K) \in \mathcal{R}\} \subseteq \mathcal{A}_N$.

This involution turns a covariance matrix $\Sigma$ which is Markovian for a graph $G$ into a concentration matrix $K = \Sigma^{-1}$ such that $K_{ij} = 0$ for all $ij \notin G$. It also exchanges marginal and conditional [28, Lemma 1]:

Lemma 2.6. For any $\mathcal{R} \subseteq \mathcal{A}_N$ and $k \in N$ we have $\mathcal{R}^\perp \setminus k = (\mathcal{R} / k)^\perp$. If $\Sigma$ is positive definite, then $\langle \Sigma \rangle^\perp = \langle \Sigma^{-1} \rangle$. In particular, duals of realizable CI relations are realizable.

The final operation of interest is concatenating two independent Gaussian random vectors $(X_i)_{i \in N}$ and $(Y_i)_{i \in M}$ which are indexed by disjoint ground sets $N$ and $M$. This is called direct sum in the structure theory of CI relations [29]. The corresponding CI relation is as follows.

Definition 2.7. Let $\mathcal{R}$ and $\mathcal{R}'$ be two CI structures on disjoint ground sets $N$ and $M$, respectively. Their direct sum is the CI structure
\[
\mathcal{R} \oplus \mathcal{R}' := \{(ij|K) \in \mathcal{A}_{NM} : i \in N, j \in M\} \\
\cup \{(ij|KL) \in \mathcal{A}_{NM} : (ij|K) \in \mathcal{R}, L \subseteq M\} \\
\cup \{(ij|KL) \in \mathcal{A}_{NM} : (ij|K) \in \mathcal{R}', L \subseteq N\} \subseteq \mathcal{A}_{NM}.
\]

On the level of covariance matrices, the direct sum imposes a block-diagonal structure with the summands on the diagonal. For $\Sigma \in \mathbb{PD}_N$ and $\Sigma' \in \mathbb{PD}_M$ let $\Sigma \oplus \Sigma' = \begin{pmatrix} \Sigma & 0 \\ 0 & \Sigma' \end{pmatrix}$. The following lemma is immediate.

Lemma 2.8. For $\Sigma \in \mathbb{PD}_N$ and $\Sigma' \in \mathbb{PD}_M$ we have $\langle \Sigma \oplus \Sigma' \rangle = \langle \Sigma \rangle \oplus \langle \Sigma' \rangle$. In particular, the direct sum $\mathcal{R} \oplus \mathcal{R}'$ is realizable if and only if $\mathcal{R}$ and $\mathcal{R}'$ are both realizable. Moreover, the direct sum commutes with duality and minors.
Lemma 2.9. For \( V = \mathcal{M}(\mathcal{R}) \) and \( V' = \mathcal{M}(\mathcal{R}') \) on disjoint ground sets \( N \) and \( M \), respectively, the direct sum \( U = V \oplus V' \) on \( NM \) is smooth if and only if \( V \) and \( V' \) are both smooth.

**Proof.** From the block-diagonal shape of matrices in \( U \) and Lemma 2.8 it follows that:

1. \( V \) and \( V' \) are irreducible if and only if \( U \) is irreducible,
2. \( T_{\Sigma \oplus \Sigma'} U = T_{\Sigma} V \oplus T_{\Sigma'} V' \), and
3. \( \dim U = \dim V + \dim V' \).

Given irreducibility, smoothness means equality of the tangent space dimension to the model dimension. Therefore the smoothness conditions are equivalent. \(\square\)

Remark 2.10. Any direct summand of a CI relation is a marginalization. Marginalizations in general need not preserve smoothness, as Example 2.16 below shows. But, one direction of Lemma 2.9 yields that a direct summand of a smooth model is smooth. Consequently, the non-zero entries in off-diagonal blocks are obstructions to smoothness of marginalizations.

The corresponding operations on graphs have been explained in [30]. For a graph \( G \) and a vertex \( k \), write \( G \setminus k \) for the graph \( G \) where vertex \( k \) and all incident edges are deleted and \( G / k \) for the graph \( G \) where vertex \( k \) is deleted and all vertices previously adjacent to \( k \) are connected to form a clique. The direct sum \( G \oplus G' \) of graphs \( G, G' \) on disjoint ground sets \( N, M \), respectively, consists of the disjoint unions of the vertex and edge sets of \( G \) and \( G' \) forming an undirected graph on \( NM \). The operations on CI relations, positive definite matrices and graphs are all aligned:

Lemma 2.11. Let \( G \) be a graph on vertex set \( N \) and \( k \in N \). We have \( \langle \langle G \rangle \rangle \setminus k = \langle \langle G / k \rangle \rangle \), \( \langle \langle G \rangle \rangle / k = \langle \langle G \setminus k \rangle \rangle \) and \( \langle \langle G \oplus G' \rangle \rangle = \langle \langle G \rangle \rangle \oplus \langle \langle G' \rangle \rangle \). In particular, Markov relations are closed under forming minors and direct sums.

Duality has no counterpart in undirected graphical models. If undirected graphical models are referred to as “concentration models”, their duals are “covariance models”. Sometimes they are written with bidirected edges instead of undirected ones.

2.4. Double Markovian models. In a double Markovian relation a pair of graphs \((G, H)\) specifies vanishing conditions via \( G \) on the concentration matrix and via \( H \) on the covariance matrix. This can be expressed using duality on ordinary Markov relations:

Definition 2.12. Let \( G \) and \( H \) be undirected graphs on vertex set \( N \). Their **double Markov relation** is \( \langle \langle G, H \rangle \rangle = \langle \langle G \rangle \rangle \cup \langle \langle H \rangle \rangle \).

By Lemma 2.1, \( \mathcal{M}(G, H) = \mathcal{M}(\langle \langle G, H \rangle \rangle) \) and the following is similar to Lemma 2.11.

Lemma 2.13. Let \( G \) and \( H \) be graphs on the vertex set \( N \). Then

\[ \langle \langle G, H \rangle \rangle \setminus k = \langle \langle G / k, H \setminus k \rangle \rangle, \quad \langle \langle G, H \rangle \rangle / k = \langle \langle G \setminus k, H / k \rangle \rangle. \]

Hence the class of double Markov relations is minor-closed.
All Markov relations are realizable and their models are smooth. These desirable geometric properties fail to hold for double Markov models. The CI relation \( \langle G, H \rangle \) gives only partial information about the geometry of the model. It is incomplete in the sense that \( \langle G, H \rangle \) does not contain all CI statements which are true on the model \( M(G, H) \). The remainder of this section contains examples of pathological behavior in the double Markovian setting.

Our first example of this is a double Markov relation which is not even a semigraphoid because it violates the following basic rule, which is satisfied by any probability distribution (Gaussian or not) and therefore must hold on the model \( M(G, H) \):

\[(12) \land (13|2) \Rightarrow (13) \land (12|3).\]

**Example 2.14.** Consider the two graphs \( G = \begin{array}{c}
1 \\
2 \\
3 \\
4
\end{array} \) and \( H = \begin{array}{c}
1 \\
2 \\
3 \\
\end{array} \), where the vertices are labeled \( 1, 2, 3, 4 \), clockwise starting at the top left. The vertex 4 can be replaced by any graph as long as it is not connected to 123. Because \((13) \notin \langle G \rangle \) and \((13|24) \notin \langle H \rangle \), \((13) \notin \langle G, H \rangle \). However, \((13|2)\) holds in \( G \) and \((12|L)\) holds in \( H \) for any \( L \subseteq 34 \). But \((12) \land (13|2) \) without \((13)\) in \( \langle G, H \rangle \) contradict the semigraphoid property, because by contraction \((12) \land (13|2) \Rightarrow (1,23)\) and then by decomposition \((1,23) \Rightarrow (13)\) and by weak union \((1,23) \Rightarrow (12|3)\).

The semigraphoid closure of the CI structure in Example 2.14 (with 4 being an isolated vertex) is \( A_4 \) and its model consists only of the identity matrix. As explained by Corollary 3.24, this happens because the edge sets of \( G \) and \( H \) are disjoint.

The next example uses the weak transitivity axiom \((12) \land (13|2) \Rightarrow (13) \lor (23)\) to construct a family of graph pairs \( (G, H) \) whose model is non-smooth. The basic idea is that the logical OR in the conclusion of weak transitivity produces two components of the model. We verify that the CI model of \{\((12)\), \((12|3)\)\} has two irreducible components which intersect in the positive definite cone. In particular, this model is not smooth.

**Example 2.15.** Pick \( G = H = \begin{array}{c}
1 \\
2 \\
3
\end{array} \) which connects 1 with 2 via 3. Making only small changes to the following arguments, the fourth node can be replaced by any (possibly empty) graph that is not connected to 123. The CI structure is

\[ \langle G, H \rangle = (A_4 \setminus \{(13|L) : L \subseteq 24\}) \setminus \{(23|L) : L \subseteq 14\}. \]

In particular the formula \((12) \land (12|3) \land \neg(13) \land \neg(23)\) holds for \( R = \langle G, H \rangle \), which violates weak transitivity. Because it violates weak transitivity, \( R \) is not a gaussoid and not realizable by a regular Gaussian distribution. There are two gaussoid extensions of \( R \) to consider: \( R_1 \) which adds \((13|L)\) and \( R_2 \) which adds \((23|L)\), for all \( L \), respectively, to \( R \). These extensions are isomorphic by exchanging the roles of 1 and 2. They are Markov relations corresponding to the complete graph with one edge removed. Hence, they are realizable and their models are irreducible and smooth by Proposition 2.2. However, the model of \( R \) consists of two copies of this smooth model, intersecting at the identity matrix, which makes it a singular point.

Unlike being double Markovian, being double Markovian with a smooth model is not minor-closed. Smoothness fails because marginalizations of irreducible models can be reducible.
Example 2.16. The two graphs $G = \bigg[ \bigg[ \bigg]$ and $H = \bigg\bigg[ \bigg\bigg]$ impose the following relations on a positive definite $4 \times 4$ matrix $\Sigma = (\sigma_{ij})$ in their double Markovian model:

\[
\begin{align*}
\sigma_{12} &= \sigma_{14} = \sigma_{24} = \sigma_{34} = 0, \text{ from } \langle H \rangle, \\
\sigma_{13}\sigma_{23}\sigma_{44} &= 0, \sigma_{13}\sigma_{22}\sigma_{44} = 0, \text{ from } \langle G \rangle.
\end{align*}
\]

The bounded model $\mathcal{M}_1(G, H) = \mathcal{M}(G, H) \cap \text{PD}_4$ is a curve segment parametrized by $\sigma_{23} \in (-1, 1)$ since $\sigma_{13}$ is forced to zero on $\text{PD}_4$. The marginal CI structure on $123$ is $\langle G, H \rangle \setminus 4 = \langle G / 4, H \setminus 4 \rangle = \langle N, \overline{N} \rangle$, the one from Example 2.15. Its model has two components which intersect in the identity matrix and is therefore not smooth.

To understand this phenomenon one has to distinguish the model of the marginal CI structure, $\mathcal{M}(G / 4, H \setminus 4)$, from the pointwise marginalization of $\mathcal{M}(G, H)$. What is discussed above is the former. It is reducible and properly contains the latter model as one of its two components.

The “unexpected” component of $\mathcal{M}(G / 4, H \setminus 4)$ arises from semi-definite matrices on the boundary of $\mathcal{M}(G, H)$ which become regular after marginalization. Namely, the two equations

\[
\sigma_{13}\sigma_{23}\sigma_{44} = 0, \sigma_{13}\sigma_{22}\sigma_{44} = 0
\]

imply $\sigma_{13} = 0$ on positive definite matrices, but there are semi-definite solutions to them where (1) $\sigma_{22} = 0$ and $\sigma_{23} = 0$, or (2) $\sigma_{44} = 0$, and $\sigma_{13}$ and $\sigma_{23}$ are arbitrary. Thus there are three types of solutions:

\[
\begin{pmatrix}
\sigma_{11} & 0 & 0 & 0 \\
0 & \sigma_{22} & \sigma_{23} & 0 \\
0 & \sigma_{23} & \sigma_{33} & 0 \\
0 & 0 & 0 & \sigma_{44}
\end{pmatrix},
\begin{pmatrix}
\sigma_{11} & 0 & \sigma_{13} & 0 \\
0 & 0 & 0 & 0 \\
\sigma_{13} & 0 & \sigma_{33} & 0 \\
0 & 0 & 0 & \sigma_{44}
\end{pmatrix},
\begin{pmatrix}
\sigma_{11} & 0 & \sigma_{13} & 0 \\
0 & \sigma_{22} & \sigma_{23} & 0 \\
\sigma_{13} & \sigma_{23} & \sigma_{33} & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}.
\]

The first type is visible in $\text{PD}_4$ and in $\mathcal{M}(G, H)$ and its marginalization forms one of the components of $\mathcal{M}(G / 4, H \setminus 4)$. The second type of solutions is not visible in the marginalization because it contains no $\text{PD}_3$ matrices. Marginalizing 4 from the CI structure removes the last row and column of these matrices and imposes additional constraints, in this case $\sigma_{13}\sigma_{23} = 0$. This turns the third type of solution positive definite and reduces the dimension by one. In this case, both the first and second component arise from this 2-dimensional boundary component.

Next, we present a family of double Markov relations which are realizable but whose model is singular at the identity matrix. Moreover, this gives an infinite family of realizable, non-smooth models all of whose proper minors are realizable and smooth.

Example 2.17. By [14, Proposition 4.2], the model of $\mathcal{R} = \{12\}, \{12|N \setminus 12\}$ is singular at the identity matrix. It can be represented by the double Markov relation $\langle G, G \rangle$ where $G$ is the graph on $N$ whose only non-edge is 12. If $k = 1, 2$, the marginalization and conditioning of $G$ by $k$ are both the complete graph, so their double Markovian model is the entire cone $\text{PD}_n$ and smooth. If $k \in N \setminus 12$, then $G / k$ is a complete graph and $G \setminus k$ is another graph on $N \setminus k$ whose only non-edge is 12. Since a complete graph imposes no relations, we find that $\langle G, G \rangle \setminus k = \langle G \setminus k \rangle$ is a Markov relation and thus its model is smooth by Proposition 2.2.

It is clear that all further minors of these two cases yield smooth models as well. This gives infinitely many examples of minor-minimal, non-smooth double Markovian CI structures.
Explicit computation in Macaulay2 for \( n = 4, 5, 6 \) verifies that (the Zariski closure of) the model is an irreducible variety and this shows that singularities are not always caused by an intersection of irreducible components. In Example 4.2 we examine the singular locus of \( \mathcal{M}(G, G) \) further. It turns out to be another conditional independence model.

We have no general proof for the Zariski-irreducibility of the models in the preceding example when \( n \geq 7 \). It was shown in [3, Lemma 6.4] that the CI structures \( \{(12), (12|N \setminus 12)\} \) are realizable by Gaussian distributions for all \( n \geq 4 \). Thus the models are irreducible in the finite “lattice of CI relations” studied by Drton and Xiao in [14, Section 2.1]. This is a coarsening of the lattice of the usual Zariski topology induced on \( \text{PD}_n \), so CI-irreducibility provides a necessary condition for Zariski-irreducibility.

There is a Galois connection between CI structures \( \mathcal{R} \subseteq A_N \) and Gaussian CI models \( \mathcal{M}(\mathcal{R}) \subseteq \text{PD}_n \). The closed CI structures under this connection are termed complete relations by Drton and Xiao, and their [14, Theorem 2.2] characterizes them as the intersections of realizable gaussoids. The completion of a double Markovian relation \( \langle \langle G, H \rangle \rangle \) adds all CI statements which hold on every matrix in its model \( \mathcal{M}(G, H) \). For single Markovian relations \( \langle \langle G \rangle \rangle \) is always complete because it is realizable by Proposition 2.2 and its elements can be read off from \( G \).

On the other hand, Example 2.14 exhibits a pair of graphs \( G \) and \( H \) whose CI structure does not satisfy the semigraphoid property. Since the semigraphoid axiom holds for every Gaussian distribution, it follows that \( \langle \langle G, H \rangle \rangle \) need not be complete. Moreover, even if the set \( \langle \langle G, H \rangle \rangle \) is closed under the compositional graphoid axioms, which hold for all Gaussians (called semigaussoid axioms by Drton and Xiao), it may still be incomplete:

**Example 2.18.** Let \( G = \square \) and \( H = \boldsymbol{\square} \) both be 4-cycles. We have \( \langle \langle G \rangle \rangle = \{(13|24), (24|13)\} \) and \( \langle \langle H \rangle \rangle = \{(12), (34)\} \). Their union \( \mathcal{R} \) is the set of antecedents to an instance of inference rule [28, Lemma 10 (17)]:

\[
(12) \land (34) \land (13|24) \land (24|13) \Rightarrow (13)
\]

This formula is valid for all regular Gaussians. Since \( \mathcal{R} \) is not closed under this rule, it is not realizable by a positive definite matrix. It is not complete either because the inference rule (17) is a Horn clause, i.e., it has a unique consequence (13) which every realizable superset of \( \mathcal{R} \) and hence \( \mathcal{R} \) as their intersection would have to contain if it were complete.

However, \( \mathcal{R} \) is a gaussoid (therefore closed under the compositional graphoid axioms) and it is realizable by a complex matrix with non-vanishing principal minors. Consequently, working with equations in a computer algebra system like Macaulay2, one cannot deduce any further CI statements from \( \langle \langle G, H \rangle \rangle \). Positive definiteness has to be taken into account.

The completion of \( \mathcal{R} \) in the positive definite setting can be computed as its closure under the semigaussoid axioms [28, Definition 1 (7)–(9)] and the higher inference rules [28, Lemma 10 (17)–(21)] of Lněnička and Matúš. It equals \( \overline{\mathcal{R}} = A_4 \setminus \{(14|L) : L \subseteq 23\} \cup \{(23|L) : L \subseteq 14\} \). This structure is a self-dual Markov relation and hence can be written as the relation of two identical graphs \( (J, J) \) such that \( \langle \langle J \rangle \rangle = \langle \langle J \rangle \rangle^\perp \). Indeed \( J = G \cap H \) gives \( \langle \langle J \rangle \rangle = \overline{\mathcal{R}} \). This shows that nevertheless \( \mathcal{M}(G, H) = \mathcal{M}(\overline{\mathcal{R}}) = \mathcal{M}(J, J) = \mathcal{M}(G \cap H) \) is smooth.
**Question 2.19.** Is there a combinatorial criterion similar to separation in undirected graphs to derive a complete set of valid CI statements for \( \mathcal{M}(G, H) \)?

A first step is Corollary 3.24 where the triviality of the model is characterized by disjointness of the edge sets. In this case, every CI statement is a consequence of the statements in \( \langle G, H \rangle \).

3. **Geometry of the models \( \mathcal{M}(G, H) \)**

Our study of the smoothness of double Markovian models starts with the known observation that one may as well work with the bounded set of correlation matrices.

**Lemma 3.1 ([14, Lemma 3.2]).** The set \( \mathcal{M}(\mathcal{R}) \) is a smooth submanifold of \( \text{PD}_n \) if and only if \( \mathcal{M}_1(\mathcal{R}) \) is a smooth submanifold.

**Proof.** The map \( \text{PD}_n \rightarrow \mathbb{R}^n_{>0} \times \mathbb{R}^n_{>0} \times \mathcal{M}_1(\mathcal{R}) \rightarrow \mathcal{M}_1(\mathcal{R}) \rightarrow \mathcal{M}_1(\mathcal{R}) \rightarrow \mathcal{M}_1(\mathcal{R}) \rightarrow \mathcal{M}_1(\mathcal{R}) \)

sending \( \Sigma \in \mathcal{M}(\mathcal{R}) \) to its diagonal. The claim follows because for each \( \Sigma \in \mathcal{M}(\mathcal{R}) \) having only ones on the diagonal and an arbitrary positive diagonal matrix \( D \), we have \( D\Sigma D \in \mathcal{M}(\mathcal{R}) \) (by the proof of [14, Lemma 3.1]). Choosing an appropriate smooth path of diagonal matrices passing through the identity matrix, we obtain every possible tangent vector in \( T_{(1,1,\ldots,1)}\mathbb{R}^n_{>0} \).

If \( \mathcal{M}_1(\mathcal{R}) \) is a smooth submanifold of \( \text{PD}_n \), then also automatically of \( \mathcal{M}_1(\mathcal{R}) \), and the product \( \mathbb{R}^n_{>0} \times \mathcal{M}_1(\mathcal{R}) \) inherits a canonical smooth structure making the second vertical inclusion an embedding of a smooth submanifold. Then clearly the induced smooth structure on \( \mathcal{M}(\mathcal{R}) \) makes the leftmost vertical inclusion an embedding of a smooth submanifold as well. \( \square \)

The proof shows that if \( \mathcal{M}_1(\mathcal{R}) \) is a smooth submanifold of \( \text{PD}_n \), then it is in fact a smooth submanifold of \( \mathcal{M}(\mathcal{R}) \) via the inclusion. The following lemma is easily verified.

**Lemma 3.2 ([14, Lemma 3.3]).** There is a self-inverse diffeomorphism \( \text{PD}_{n,1} \rightarrow \mathcal{M}_1(\mathcal{R}) \) given by matrix inversion followed by forming the correlation matrix, mapping \( \mathcal{M}_1(\mathcal{R}) \) onto \( \mathcal{M}_1(\mathcal{R}^1) \).
In particular, \( \mathcal{M}(\mathcal{R}) \) and \( \mathcal{M}_1(\mathcal{R}) \) are smooth if and only if \( \mathcal{M}(\mathcal{R}^1) \) and \( \mathcal{M}_1(\mathcal{R}^1) \) are. As an image of a linear space under the inversion diffeomorphism any graphical model \( \mathcal{M}(G) \) is smooth, which might not be obvious from the defining \((n-1) \times (n-1)\) almost-principal minors. The (semi-)algebraic geometry of \( \mathcal{M}(\mathcal{R}) \) and \( \mathcal{M}_1(\mathcal{R}) \) can be quite different in the non-smooth case. E.g., the number of irreducible components of their Zariski closures need not always agree. However, the bijective morphism of semi-algebraic sets \( \mathbb{R}^n \to \mathcal{M}(\mathcal{R}), (D, \Sigma) \mapsto D\Sigma D \) can be used to show that their dimensions always differ by \( n \).

3.1. Basics from real algebraic geometry. We collect several foundational definitions and results from [2] and refer to this textbook for an extensive treatment.

A real algebraic set \( Z \subseteq \mathbb{R}^n \) is the vanishing set \( V(S) \) of a collection \( S \subseteq \mathbb{R}[x_1, \ldots, x_n] \) of polynomials, and \( S \) may be replaced by the ideal \( \langle S \rangle \) it generates. Real algebraic sets are the closed sets of the Zariski topology on \( \mathbb{R}^n \). If \( \Theta \subseteq \mathbb{R}^n \) is any subset, its ideal is \( \mathcal{I}(\Theta) = \{ f \in \mathbb{R}[x_1, \ldots, x_n] : f(x) = 0, \text{ for all } x \in \Theta \} \). The real algebraic set of \( \mathcal{I}(\Theta) \) is the Zariski closure \( \Theta \) of \( \Theta \). Every irreducible component of the Zariski closure of \( \Theta \) in \( \mathbb{R}^n \) intersects \( \Theta \). If \( Z \) is irreducible in this topology, \( Z \) is a real algebraic variety. A set of the form

\[
\Theta = \{ x \in \mathbb{R}^n : f_1(x) = \cdots = f_r(x) = 0, g_1(x) > 0, \ldots, g_s(x) > 0 \},
\]

where \( f_i, g_j \in \mathbb{R}[x_1, \ldots, x_n] \) are real polynomials is a basic semi-algebraic set. A finite union of basic semi-algebraic sets in a fixed \( \mathbb{R}^n \) is a semi-algebraic set. The dimension of a semi-algebraic set \( \Theta \subseteq \mathbb{R}^n \) is the Krull dimension of its coordinate ring \( \mathbb{R}[x_1, \ldots, x_n]/\mathcal{I}(\Theta) \). The dimension of \( \Theta \) then equals the dimension of its Zariski closure as \( \mathcal{I}(\Theta) = \mathcal{I}(\Theta) \). A semi-algebraic set \( \Theta \subseteq \mathbb{R}^n \) is semi-algebraically connected if for every two disjoint semi-algebraic subsets \( A, B \subseteq \Theta \) which are closed in \( \Theta \) and satisfy \( A \cup B = \Theta \), one has \( A = \Theta \) or \( B = \Theta \). According to [2, Theorem 2.4.5], a semi-algebraic set \( \Theta \subseteq \mathbb{R}^n \) is semi-algebraically connected if and only if it is connected with respect to the Euclidean topology on \( \mathbb{R}^n \).

**Definition 3.3.** For a real algebraic set \( V \subseteq \mathbb{R}^n \) with vanishing ideal \( \mathcal{I}(V) = \langle f_1, \ldots, f_r \rangle \), the Zariski tangent space \( T_pV \) at \( p \in V \) is the kernel of the Jacobian matrix

\[
J_p = \left( \frac{\partial f_i}{\partial x_j}(p) \right)_{i=1,\ldots,r \atop j=1,\ldots,n}.
\]

The algebraic set \( V \) is smooth at \( p \in V \) if it is irreducible and \( \dim(T_pV) = \dim(V) \) or, equivalently, \( \text{rk}(J_p) = n - \dim(V) \). Finally, \( V \) is smooth if it is smooth at every point \( p \in V \).

Assume \( V \) is an irreducible real algebraic set. Krull’s principal ideal theorem implies that the rank of the Jacobian is at most \( n - \dim(V) \) or equivalently \( \dim(T_pV) \geq \dim(V) \). Moreover, the rank does not depend on the set of generators of \( \mathcal{I}(V) \). This follows from the fact that adding an element of the ideal \( \mathcal{I}(V) \) to a list of generators does not change the rank as the gradient of the additional polynomial is linearly dependent on the gradients of the generators at every point \( p \in V \). This reasoning also proves the following:
Lemma 3.4. Let $V \subseteq \mathbb{R}^n$ be a real algebraic set with generators $f_1, \ldots, f_r$ of $\mathcal{I}(V)$ and let $g_1, \ldots, g_s \in \mathcal{I}(V)$ be arbitrary. Then for all $p \in V$ we have
\[
\text{rk} \left( \frac{\partial f_i}{\partial x_j} (p) \right)_{i=1,\ldots,r, \atop j=1,\ldots,n} \geq \text{rk} \left( \frac{\partial g_i}{\partial x_j} (p) \right)_{i=1,\ldots,s, \atop j=1,\ldots,n}.
\]
The natural application of Lemma 3.4 is to bound the $\dim(V)$ when $\mathcal{I}(V)$ is not known.

A semi-algebraic set $\Theta \subseteq \mathbb{R}^n$ is smooth at $p \in \Theta$ if $p$ is contained in a unique irreducible component $Z$ of the Zariski closure of $\Theta$ and $p$ is a smooth point of $Z$. If $\Theta$ is smooth at every point, then $\Theta$ is smooth. The set of smooth points of $\Theta$ is its smooth locus, denoted $\Theta_{\text{sm}}$. The smooth locus of a non-empty real algebraic set $V$ is a non-empty Zariski-open subset of $V$ by [2, Proposition 3.3.14]. If $V$ is irreducible, $V_{\text{sm}}$ is a Zariski-dense open subset. The smooth locus $V_{\text{sm}}$ of a real algebraic variety $V$ is a smooth submanifold of $\mathbb{R}^n$ by [2, Proposition 3.3.11]. From this it follows that, if $\Theta \subseteq \mathbb{R}^n$ is a basic semi-algebraic set such that its Zariski closure is irreducible, then $\Theta_{\text{sm}}$ is a smooth submanifold of $\mathbb{R}^n$ by viewing $\Theta_{\text{sm}}$ as an open subset (in the Euclidean topology) of $\overline{\Theta}_{\text{sm}}$.

3.2. Smoothness of the models $\mathcal{M}(G, H)$. The geometry of double Markovian models is best understood in terms of semi-algebraic sets. We can identify
\[
\mathcal{M}(G, H) = \mathcal{M}(G) \cap \mathcal{M}(H)^{-1}
\]
with
\[
\hat{\mathcal{M}(G, H)} := \left\{ (\Sigma, \Sigma^{-1}) : \Sigma_{ij} = 0 \text{ for all } ij \notin H \text{ and } (\Sigma^{-1})_{kl} = 0 \text{ for all } kl \notin G \right\},
\]
and the latter is a smooth submanifold of $\text{PD}_n \times \text{PD}_n$ if and only if $\mathcal{M}(G, H)$ is a smooth submanifold of $\text{PD}_n$, as follows from the diagram:
\[
\begin{array}{ccc}
\text{PD}_n & \xrightarrow{\text{id} \times \text{inv}} & \text{PD}_n \times \text{PD}_n \\
\uparrow & & \uparrow \\
\mathcal{M}(G, H) & \cong & \hat{\mathcal{M}(G, H)}.
\end{array}
\]
Because of this, it suffices to study the smoothness of $\mathcal{M}(G, H)$.

Both $\mathcal{M}_G$ and $\mathcal{M}_H^{-1}$ are smooth submanifolds of $\text{PD}_n$. It is sufficient for the intersection to be smooth that the intersection be transverse at every point [20, Chapter 1 §5], meaning that the dimensions of tangent spaces add up to that of the ambient manifold. This criterion yields Theorem 3.8, once we have computed the tangent spaces.

Proposition 3.5. A basis of the tangent space $T_p \mathcal{M}(G)$ is given by the matrices
\[
M^{ij} := P^i \cdot P_j + P_j \cdot P_i, \quad \text{for } i = j \text{ or } ij \in E_G,
\]
where $P_i$ is the $i$-th column of $P$ and $P_j$ is the $j$-th row of $P$. A basis of the tangent space $T_p \mathcal{M}(H)^{-1}$ consists of $E^{ij} := E_{ij} + E_{ji}$ for $i = j$ or $ij \in E_H$, where $E_{ij}$ is the $n \times n$ matrix having a 1 at the $(i,j)$-th position and zeros everywhere else.
Theorem 3.8. with mean parameter

The following theorem was suggested to us by Piotr Zwiernik. It was the starting point of our

we use the differential of the matrix inversion

vanishing of the

zero constraints on both mean and natural parameters are imposed, the result is in general

such that the non-edges of

∪

G

is a valid parametrization for the exponential family. In the situation of Theorem 3.8, when

Remark 3.9. Multivariate centered Gaussian random vectors form a regular exponential family

with mean parameter Σ and natural parameter K = Σ⁻¹ [40, Chapter 3]. According to [40, Corollary 3.17], a mixed parametrization (σ_{ij}, k_{st})_{ij \in A, st \in B} with A ∪ B = E_{KN} and A ∩ B = ∅ is a valid parametrization for the exponential family. In the situation of Theorem 3.8, when

G ∪ H = K_N, the non-edges of G and H are disjoint. Therefore one could pick A, B ⊆ E_{KN} such that the non-edges of G are contained in B and the non-edges of H in A. However, when zero constraints on both mean and natural parameters are imposed, the result is in general not a regular exponential family. Therefore smoothness results like Theorem 3.8 do not simply follow from general theory.
Theorem 3.11. \( \dim(\mathcal{M}(G, H)) = \dim(\mathcal{M}(G)) + \dim(\mathcal{M}(H)) \) and so, regarding dimensions, by Remark 3.6
\[
\dim(\mathcal{M}(G, H)) = \frac{n^2 + n}{2} - \left( \frac{n^2 - n}{2} - |E_G| + \frac{n^2 - n}{2} - |E_H| \right)
= |E_G| + |E_H| - \frac{n^2 - 3n}{2}
= |E_G \cap E_H| + n,
\]
where we have used \( |E_G| + |E_H| = \binom{n}{2} + |E_G \cap E_H| \). The intersection with \( \text{PD}_{n,1} \) satisfies
\[
\dim(M_1(G, H)) = \dim(M(G, H) \cap \text{PD}_{n,1}) = \dim(M(G, H)) - n = |E_G \cap E_H|.
\]
If one is not in the favorable situation \( G \cup H = K_N \), the dimension computation becomes more involved. Let \( G \) and \( H \) now be arbitrary graphs on \( N \), and denote by \( E_G^c \) the edge complement \( \binom{N}{2} \setminus E_G \) and similarly for \( E_H \). The following lemma is a technical core for dimension bounds.

Lemma 3.10. With \( \Sigma = (\sigma_{st})_{st \in \binom{N+1}{2}} \), let \( f_{ij} = \sigma_{ij} \) for \( i j \in E_H^c \) and \( g_{kl} = \det(\Sigma_{N \setminus k, N \setminus l}) \) for \( k l \in E_G^c \). Consider the differentials
\[
J_H = \left( \frac{\partial f_{ij}}{\partial \sigma_{st}} \right)_{ij \in E_H^c, st \in \binom{N+1}{2}} \quad \text{and} \quad J_G = \left( \frac{\partial g_{kl}}{\partial \sigma_{st}} \right)_{kl \in E_G^c, st \in \binom{N+1}{2}}.
\]
For every \( \Sigma \in \mathcal{M}(G, H) \), define \(|E_G^c| + |E_H^c| \) matrix \( \tilde{J}_\Sigma \) by stacking \( J_G \) and \( J_H \):
\[
\tilde{J}_\Sigma := \begin{pmatrix} J_G \\ J_H \end{pmatrix}.
\]
Then \( \text{rk} \tilde{J}_\Sigma \geq \binom{n}{2} - |E_G \cap E_H| \).

Proof. The kernel of \( \tilde{J}_\Sigma \) is the intersection of the kernels of \( J_G \) and \( J_H \). The Zariski closures \( \overline{\mathcal{M}(G)} \) and \( \overline{\mathcal{M}(H)^{-1}} \) in \( \text{Sym}^2(\mathbb{R}^n) \cap \text{GL}(\mathbb{R}^n) \) of \( \mathcal{M}(G) \) and \( \mathcal{M}(H)^{-1} \) are both irreducible smooth varieties, \( \overline{\mathcal{M}(G)} \) by Proposition 2.2 and \( \overline{\mathcal{M}(H)^{-1}} \) because it is a linear space. The Zariski tangent spaces have been computed in Proposition 3.5. Using \( \dim(U \cap V) = \dim(U) + \dim(V) - \dim(U + V) \) for finite-dimensional vector spaces \( U \) and \( V \) inside a common vector space, we compute
\[
\dim(\text{ker}(\tilde{J}_\Sigma)) = \dim(\text{span}(E_{ij} : i j \in E_H \text{ or } i = j) \cap \text{span}(M^{kl} : k l \in E_G \text{ or } k = l))
= (|E_G| + n) + (|E_H| + n)
- \dim(\text{span}(E_{ij} : i j \in E_H \text{ or } i = j) + \text{span}(M^{kl} : k l \in E_G \text{ or } k = l))
\leq |E_G \cap E_H| + n.
\]
In the last step we used that the dimension of the sum of the two vector spaces is at least \( |E_H \cup (E_G \setminus E_H)| + n = |E_G \cup E_H| + n \) because the matrix \( (M^{kl}_{st})_{kl,st \in E_G \setminus E_H} \) is a principal submatrix of the inverse of the information matrix and therefore invertible. \( \Box \)

Theorem 3.11. We have \( \dim(\mathcal{M}(G, H)) \leq |E_G \cap E_H| + n. \)
Proof. The polynomials \( f_{ij} \) and \( g_{kl} \) from Lemma 3.10 lie in the vanishing ideal \( \mathcal{I}(\mathcal{M}(G, H)) \subseteq \mathbb{R}[\sigma_{st} : st \in \binom{N+1}{2}] \), and hence in the prime ideal of every irreducible component \( Z \) of the Zariski closure \( \mathcal{V}(\mathcal{I}(\mathcal{M}(G, H))) \) inside the affine space \( \text{Sym}^2(\mathbb{R}^n) \). Then the Jacobian matrix \( J_\Sigma \) at \( \Sigma \in \mathcal{M}(Z) \) of a generating set of \( \mathcal{I}(Z) \) satisfies \( \text{rk} J_\Sigma \geq \text{rk} \bar{J}_\Sigma \) by Lemma 3.4. By Lemma 3.10, for \( \Sigma \in \mathcal{M}(G, H) \), \( \text{rk} \bar{J}_\Sigma \geq \binom{n}{2} - |E_G \cap E_H| \). Then Krull’s principal ideal theorem implies that the Zariski tangent space satisfies \( \dim(T_\Sigma Z) \geq \dim(Z) \), and so

\[
\dim(Z) \leq \dim(T_\Sigma Z) = \left(\frac{n+1}{2}\right) - \text{rk}(J_\Sigma) \leq \left(\frac{n+1}{2}\right) - \text{rk}(\bar{J}_\Sigma) \leq |E_G \cap E_H| + n. \quad \square
\]

Corollary 3.12. We have \( \dim(\mathcal{M}_1(G, H)) \leq |E_G \cap E_H| \).

Remark 3.13. The inequalities in Corollary 3.12 and Theorem 3.11 can be strict. Example 2.15 contains a model \( \mathcal{M}_1(G, H) \) of dimension 1 with \( |E_G \cap E_H| = 2 \). It is reducible with two irreducible components which intersect only in the identity matrix \( 1_4 \).

Using the dimension bound we can show that \( E_G \cap E_H = \emptyset \) if \( \mathcal{M}_1(G, H) \) is zero-dimensional, i.e., a union of finitely many points (including \( 1_n \)). Indeed, if \( E_G \cap E_H \neq \emptyset \), then \( \dim(\mathcal{M}_1(G, H)) \geq 1 \) because after some permutation of \( N \) one can assume that \( 12 \in E_G \cap E_H \). Then

\[
\Sigma = \begin{pmatrix}
1 & \sigma_12 & 0 & \ldots & 0 \\
\sigma_12 & 1 & 0 & \ldots & 0 \\
0 & 0 & 1 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \ldots & 1
\end{pmatrix}
\]

lies in \( \mathcal{M}_1(G, H) \) for any \( \sigma_{12} \in (-1, 1) \). Corollary 3.24 below strengthens this further. In fact, \( E_G \cap E_H = \emptyset \) if and only if the model consists only of \( 1_n \).

Lemma 3.14. Let \( V := \overline{\mathcal{M}(G, H)} \) and \( \Sigma \in \mathcal{M}(G, H) \). Then \( \dim(T_\Sigma V) \leq |E_G \cap E_H| + n. \)

Proof. The Zariski tangent space \( T_\Sigma V \) is the kernel of the Jacobian matrix \( J_\Sigma \) at \( \Sigma \in \mathcal{M}(G, H) \) of a generating set of \( \mathcal{I}(V) \). By Lemma 3.4 and Lemma 3.10, we have \( \text{rk} J_\Sigma \geq \text{rk} \bar{J}_\Sigma \geq \binom{n}{2} - |E_G \cap E_H| \) which yields the claimed inequality. \( \square \)

Theorem 3.15. Every connected component of \( \mathcal{M}(G, H) \) of dimension \( |E_G \cap E_H| + n \) is smooth and has irreducible Zariski closure.

Proof. Let \( V := \overline{\mathcal{M}(G, H)} \subseteq \text{Sym}^2(\mathbb{R}^n) \). Let \( M \) be a connected component of \( \mathcal{M}(G, H) \) and \( Z \) an irreducible component of its Zariski closure \( \overline{M} \) with \( \dim(Z) = |E_G \cap E_H| + n \). Then at every point \( \Sigma \in \mathcal{M}(M \cap Z) \), we have

\[
|E_G \cap E_H| + n = \dim(Z) \leq \dim(T_\Sigma Z) \leq \dim(T_\Sigma V) \leq |E_G \cap E_H| + n,
\]

hence all inequalities are equalities, proving that the local rings \( \mathcal{O}_{V, \Sigma} \) with \( \Sigma \in \mathcal{M}(M \cap Z) \) are regular. Regular local rings are integral domains by [25, Corollary 13.6]. Hence, for every \( \Sigma \in \mathcal{M}(M \cap Z) \), there is only one irreducible component of \( \overline{M} \) containing \( \Sigma \), so \( Z \) does not intersect any other irreducible component of \( \overline{M} \) inside \( M \). Therefore, as \( M \) is connected, \( \overline{M} = Z \) is irreducible, and \( M = M \cap Z \) is smooth. \( \square \)
**Remark 3.16.** The proof of Theorem 3.15 also shows that a connected component of \( \mathcal{M}_1(G, H) \) of dimension \(|E_G \cap E_H|\) is smooth and has irreducible Zariski closure. Proposition 3.31 (8) contains a smooth model \( \mathcal{M}_1(G, H) \) on 4 vertices of dimension 3 = |E_G \cap E_H| with \( G \cup H \neq K_4 \), so the converse of Theorem 3.8 is false. Even when \( G \cup H \neq K_N \), Theorem 3.15 still provides a sufficient criterion for smoothness. In fact, we know of no example of a smooth model \( \mathcal{M}(G, H) \) (resp. \( \mathcal{M}_1(G, H) \)) having dimension less than \(|E_G \cap E_H| + n \) (resp. \(|E_G \cap E_H|\)).

We now move on to the vanishing ideal \( I(\mathcal{M}_1(G, H)) \) of double Markovian models. Ordinary Gaussian graphical models have rational parametrizations and their vanishing ideals are prime. Vanishing ideals of double Markovian models need not be prime. They arise from conditional independence ideals by removing components whose varieties do not intersect PD_n and taking the radical. We do not expect double Markovian CI ideals to be radical. In the discrete case, radicality fails even for ideals defined by the global Markov condition [23, Example 4.9]. The Vámos gaussoid from [4, Example 13] yields a Gaussian CI ideal which is not radical (in the ring \( \mathbb{C}[\sigma_{ij} : i < j] \) where the diagonal of \( \Sigma \) is not normalized).

For the rest of the section we mostly restrict to the normalized variance case, that is \( \mathcal{M}_1(G, H) \) as opposed to \( \mathcal{M}(G, H) \). This removes duplication from the statements. In most cases only small changes are necessary to change a result for \( \mathcal{M}_1(G, H) \) into one for \( \mathcal{M}(G, H) \).

**Definition 3.17.** Let \( G \) and \( H \) be two graphs on \( N \) and \( \Sigma = (\sigma_{ij}) \) a generic symmetric matrix with ones on the diagonal. The **saturated conditional independence ideal** \( \text{CI}_{G,H} \subseteq \mathbb{R}[\sigma_{ij} : i < j] \) is the saturation of the ideal \( \langle \sigma_{ij}, \det(\Sigma_{k\in C}) : ij \in E^*_H, kl \in E^*_G \rangle \) at the product of all principal minors of \( \Sigma \). Similarly, the **simplified saturated conditional independence ideal** \( \text{SCI}_{G,H} \subseteq \mathbb{R}[\sigma_{ij} : i < j] \) is the saturation of \( \langle \sigma_{ij}, \det(\Sigma_{N\setminus I,N\setminus K}) : ij \in E^*_H, kl \in E^*_G \rangle \) at the product of all principal minors of \( \Sigma \).

Clearly, \( \text{SCI}_{G,H} \subseteq \text{CI}_{G,H} \) and their varieties in the affine space of symmetric matrices with ones on the diagonal agree over both \( \mathbb{R} \) and \( \mathbb{C} \) by Lemma 2.1. The ideals \( \text{SCI}_{G,H} \) and \( \text{CI}_{G,H} \) are saturations of determinantal ideals of symmetric matrices. The latter have been featured in the work of Conca [5, 6, 7], but little seems to be known in general (at least in comparison to ordinary determinantal ideals). Double Markovian models might provide an incentive to further study ideals generated by collections of minors of sparse symmetric matrices.

In the following lemma we consider for a moment the scheme of \( \text{CI}_{G,H} \), including the multiplicity information stored in the coordinate ring. The dual of the Zariski tangent space at the identity \( 1_n \) is \( m/(\text{CI}_{G,H} + m^2) \) where \( m := \langle \sigma_{st} : s < t \rangle \) is the maximal ideal in \( A := \mathbb{R}[\sigma_{st} : s < t] \) corresponding to \( 1_n \). Its dimension is also known as the embedding dimension of \( (A/\text{CI}_{G,H} m)_m \), denoted \( \text{edim}(A/\text{CI}_{G,H} m) \) and equals the dimension of the tangent space at the identity.

**Lemma 3.18.** Let \( V := \nu(\text{CI}_{G,H}) \) as a subscheme of the affine space of symmetric \( n \times n \) matrices with ones on the diagonal. Then the embedding dimension of \( V \) at \( 1_n \) is \(|E_G \cap E_H|\).

**Proof.** The short exact sequence

\[
0 \to (\text{CI}_{G,H} + m^2)/m^2 \to m/m^2 \to m/(\text{CI}_{G,H} + m^2) \to 0
\]
With all this in place we can express almost-principal minors in terms of path products. This formula appears first in [21]. We include a quick proof disregarding the signs which we do not use in the sequel.

The lemma states \( \dim(T_{1,n} V) = |E_G \cap E_H| \), and similarly one shows \( \dim(T_{1,n} V) = |E_G \cap E_H| + n \) if \( V = V(\CI_{G,H}) \) consists of all symmetric \( n \times n \) matrices with no restriction on the diagonals, considering \( \CI_{G,H} \) as an ideal in \( \mathbb{R}[\sigma_{st} : s \leq t] \). The lemma also shows that, when \( \CI_{G,H} \) equals the vanishing ideal and \( V \) is smooth at \( \mathbb{1}_n \), then \( \dim(M_1(G,H)) = |E_G \cap E_H| \) and \( \dim(M(G,H)) = |E_G \cap E_H| + n \).

The next proposition expresses almost-principal minors of symmetric matrices via paths in a graph. Here we use the conventions from [26]. A path \( p \) traverses no vertex more than once and \( V(p) \subseteq N \) denotes this set of vertices, \( e(p) = kl \) the endpoints of \( p \), and \( \sigma_p = \prod_{ij \in p} \sigma_{ij} \) the product over the variables corresponding to edges of \( p \). The sign of \( p \) is \( \text{sgn}(p) := (-1)^{|V(p)| - 1} \).

All with this in place we can express almost-principal minors in terms of path products.

**Proposition 3.19.** Let \( H \) be a graph on the vertex set \( N \) and let \( \Sigma = (\sigma_{ij}) \) be a generic \( n \times n \) symmetric matrix with \( \sigma_{ij} = 0 \) for all \( ij \notin E_H \). Then

\[
(-1)^{k+l} \det(\Sigma_{N \setminus k,N \setminus l}) = \sum_{\substack{\text{path in } H, \\ e(p) = kl}} \text{sgn}(p) \cdot \det(\Sigma_{N \setminus V(p),N \setminus V(p)}) \cdot \sigma_p.
\]

This formula appears first in [21]. We include a quick proof disregarding the signs which we do not use in the sequel.

**Proof.** By the Leibniz formula, \( \det(\Sigma_{N \setminus l,N \setminus k}) = \sum_{\tau} \text{sgn}(\tau) \prod_{i \in N \setminus l} \sigma_{i,\tau(i)} \), where the sum is over all bijective \( \tau : N \setminus l \to N \setminus k \). The summand corresponding to \( \tau \) is non-zero if and only if each \( \{i, \tau(i)\} \) with \( \tau(i) \neq i \) is an edge of \( H \). Starting at the vertex \( k \), the sequence \( k, \tau(k), \tau^2(k), \ldots \) is a path from \( k \) to \( l \) in \( H \), showing that

\[
\det(\Sigma_{N \setminus l,N \setminus k}) = \sum_{\substack{\text{path in } H, \\ e(p) = kl}} \pm \sigma_p \cdot \sum_{\tau' : N \setminus V(p) \to N \setminus V(p)} \text{sgn}(\tau') \prod_{i \in N \setminus V(p)} \sigma_{i,\tau'(i)}
\]

\[
= \sum_{\substack{\text{path in } H, \\ e(p) = kl}} \pm \sigma_p \cdot \det(\Sigma_{N \setminus V(p),N \setminus V(p)}). \quad \square
\]

If all but one term in \( \det(\Sigma_{N \setminus l,N \setminus k}) \) vanish, the CI ideal ought to be a monomial ideal. Taking care of details like saturation, it also follows that it agrees with the vanishing ideal.

**Theorem 3.20.** Let \( G \) and \( H \) be graphs on \( N \) such that for every non-edge \( kl \) of \( G \), there is at most one path \( p \) in \( H \) connecting \( k \) and \( l \). Then

\[
\SCI_{G,H} = \CI_{G,H} = \langle \mathcal{M}_1(G,H) \rangle = \langle \sigma_{ij} : ij \notin E_H, \ p \text{ a path in } H \text{ such that } e(p) \notin E_G \rangle.
\]
Theorem 3.22. Theorem 3.20, irreducibility implies that the square-free monomial ideal with respect to the identity matrix and thus connected. Therefore, having the maximal hypothesis of Theorem 3.20 may seem restrictive but, for example, it includes the case To show that this (radical) ideal equals the vanishing ideal, it suffices to see that each of vertices where \( \sigma \) agrees with its saturation at the product of all principal minors of \( M \) that for all non-edges \( e \in E \) inside \( H \), then \( \det(\Sigma_{N_{\setminus k,N_{\setminus l}}}) = \pm \det(\Sigma_{N_{\setminus V(p),N_{\setminus V(p)}}}) \cdot \sigma_p \), so \( \sigma_p \) lies in the saturated simplified conditional independence ideal. If there exists no such path, this almost-principal minor vanishes. Since the square-free monomial ideal \( \langle \sigma_{ij}, \sigma_p : ij \notin E_H, p \text{ a path in } H \text{ such that } e(p) \notin E_G \rangle \) agrees with its saturation at the product of all principal minors of \( \Sigma \), it equals \( \text{SCI}_{G,H} \).

Proof. Let \( \Sigma \) be the generic symmetric matrix with ones on the diagonal and zeros corresponding to non-edges of \( H \). If \( ij \notin E_H \), all terms of almost-principal minors of \( \Sigma \) which contain \( \sigma_{ij} \) can be neglected since \( \sigma_{ij} \in \text{SCI}_{G,H} \subseteq \text{CI}_{G,H} \). By Proposition 3.19, if \( p \) is the unique path connecting \( k \) and \( l \) inside \( H \), then \( \det(\Sigma_{N_{\setminus k,N_{\setminus l}}}) = \pm \det(\Sigma_{N_{\setminus V(p),N_{\setminus V(p)}}}) \cdot \sigma_p \), so \( \sigma_p \) lies in the connectedness.

The hypothesis of Theorem 3.20 may seem restrictive but, for example, it includes the case that \( H \) is a forest and \( G \) is arbitrary. On the other hand, it is easy to find an example on four vertices where \( H \) is a cycle and \( \text{SCI}_{G,H} \) is not a monomial ideal.

Determining vanishing ideals of ordinary Gaussian graphical models can already be complicated, see for example [33]. However, it seems plausible that a divide-and-conquer approach based on toric fiber products as in [15, 37] is applicable for some suitably decomposable graph pairs \( G, H \).

3.3. Connectedness. In this subsection we study connectedness of \( \mathcal{M}(G, H) \) in the real topology. If the vanishing ideal is known and simple enough, the results are easy as in the next corollary. Theorem 3.22 contains a sufficient condition based on connectedness in \( G \) and \( H \).

Corollary 3.21. Under the hypotheses of Theorem 3.20, the model \( \mathcal{M}(G, H) \) is connected. Moreover the following are equivalent.

1. \( \mathcal{M}(G, H) \) is smooth.
2. \( \mathcal{M}(G, H) \) is irreducible.
3. \( \mathcal{M}(G, H) \) has the maximal dimension \( |E_G \cap E_H| + n \).

In this case, \( \mathcal{M}(G, H) = \mathcal{M}(G \cap H)^{-1} \) is an inverse graphical model, hence a spectrahedron.

Proof. As a union of coordinate subspaces intersected PD, \( \mathcal{M}(G, H) \) is star-shaped with respect to the identity matrix and thus connected. Therefore, having the maximal dimension implies smoothness by Theorem 3.15, and smoothness together with connectedness implies irreducibility because regular local rings are integral domains [25, Corollary 13.6]. By Theorem 3.20, irreducibility implies that the square-free monomial ideal \( \text{SCI}_{G,H} \) is prime. This is equivalent to the condition that for a path \( p \) inside \( H \) with \( e(p) = kl \in E_G \) there exists an edge \( ij \in p \cap E_G \). Thus, if \( G' \) is the graph on \( N \) which is obtained from \( G \) by adding all edges in \( E_G \cap E_H \), then \( \mathcal{M}(G, H) = \mathcal{M}(G', H) = \mathcal{M}(G \cap H)^{-1} \), in particular \( \mathcal{M}(G, H) \) has dimension \( |E_G \cap E_H| + n \).

Theorem 3.22. Let \( G \) and \( H \) be graphs on \( N \) with the property that there exists \( i \in N \) such that for all non-edges \( kl \in E_G \), every path in \( H \) connecting \( k \) and \( l \) contains \( i \). Then the model \( \mathcal{M}(G, H) \) is connected.
Proof. In this proof we denote by \( H \setminus i \) the graph on \( N \) obtained from \( H \) by deleting all edges incident with \( i \) but keeping \( i \) as a vertex. The model \( \mathcal{M}(H \setminus i)^{-1} \) is connected as it is the intersection of a linear space with the convex set \( \text{PD}_n \), and the intersection of convex sets is convex, hence connected. Clearly, \( \Sigma \in \mathcal{M}(H \setminus i)^{-1} \) if and only if \( \Sigma \in \mathcal{M}(H)^{-1} \) and \( \sigma_{ij} = 0 \) for all \( j \neq i \). The determinantal identity of Proposition 3.19, and the assumptions on \( G \) and \( H \) imply \( \mathcal{M}(H \setminus i)^{-1} \subseteq \mathcal{M}(G, H) \). Now, let \( \Sigma \in \mathcal{M}(G, H) \) be arbitrary. It suffices to find a path from \( \Sigma \) to some matrix in \( \mathcal{M}(H \setminus i)^{-1} \).

For \( \varepsilon \in [0, 1] \) consider

\[
\Sigma^\varepsilon := \Sigma \odot \begin{pmatrix}
1 & \ldots & 1 & \varepsilon & 1 & \ldots & 1 \\
\vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
1 & \ldots & 1 & \varepsilon & 1 & \ldots & 1 \\
\varepsilon & \varepsilon & 1 & \varepsilon & \varepsilon & \ldots & \varepsilon \\
1 & \ldots & 1 & \varepsilon & 1 & \ldots & 1 \\
\vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
1 & \ldots & 1 & \varepsilon & 1 & \ldots & 1
\end{pmatrix},
\]

where the second factor has entries \( \varepsilon \) in the \( i \)-th row and column, but 1 in entry \( ii \). The symbol \( \odot \) denotes the Hadamard product which multiplies matrices entry-wise. Then \( \Sigma^\varepsilon \) is symmetric and positive definite for all \( \varepsilon \in [0, 1] \) as it is the Hadamard product of a positive definite matrix and a positive semi-definite matrix with strictly positive diagonal entries. Moreover, \( \Sigma^1 = \Sigma \) and \( \Sigma^0 \in \mathcal{M}(H \setminus i)^{-1} \), so it suffices to show that \( \Sigma^\varepsilon \in \mathcal{M}(G, H) \) for all \( \varepsilon \in [0, 1] \). This follows from the assumptions on \( G \) and \( H \) as for all \( kl \in E_G \) with \( k \neq i \neq l \) we have

\[
\det((\Sigma^\varepsilon)_{N \setminus k, N \setminus l}) = \sum_{p \text{ path in } G} \sgn(p) \cdot \sigma^\varepsilon_p \cdot \det((\Sigma^\varepsilon)_{N \setminus V(p), N \setminus V(p)})
\]

\[
= \varepsilon^2 \cdot \sum_{p \text{ path in } G} \sgn(p) \cdot \sigma_p \cdot \det((\Sigma)_{N \setminus V(p), N \setminus V(p)})
\]

\[
= \varepsilon^2 \cdot \det((\Sigma)_{N \setminus k, N \setminus l}) = 0,
\]

using in the second step that, by assumption, \( i \in V(p) \) for all occurring paths \( p \), so that the occurring principal minors of \( \Sigma^\varepsilon \) agree with the corresponding principal minors of \( \Sigma \). Moreover, each monomial \( \sigma^\varepsilon_p \) contains exactly two variables that are scaled by \( \varepsilon \). If one of \( k \) and \( l \) agrees with \( i \), the same calculation works with \( \varepsilon \) instead of \( \varepsilon^2 \). \( \square \)

3.4. The decomposition theorem. Section 3.5 contains a classification of models with small \( |E_G \cap E_H| \). This is based on the following decomposition theorem, whose proof also works for complex hermitian positive definite matrices.

**Theorem 3.23.** Let \( G, H \) be two graphs on the vertex set \( N \). Let \( V_1, \ldots, V_r \) be a partition of \( N \) such that each \( V_i \) is the vertex set of a connected component of \( G \cap H \), considered as the
Therefore, we have equality in the Cauchy–Schwarz inequality on the space of real symmetric matrices, implying the middle cancels out. Since the trace is cyclic, we have

\[
\sum_{w \in W} \Sigma_{vw} (\Sigma^{-1})_{vw} = 0 = \sum_{w \in W} 0.
\]

In particular, \( \text{tr}(\Sigma_W (\Sigma^{-1})_W^t) = 0 \). As \( \Sigma_V \) and \( \Sigma_W \) are positive definite, there exist symmetric square roots \( A_V \) and \( A_W \) such that \( A_V^t = \Sigma_V \) and \( A_W^t = \Sigma_W \). We now define

\[
\Sigma' := \begin{pmatrix} A_V^{-1} & 0 \\ 0 & A_W^{-1} \end{pmatrix} \cdot \Sigma \cdot \begin{pmatrix} A_V^{-1} & 0 \\ 0 & A_W^{-1} \end{pmatrix} = \begin{pmatrix} 1_V & A_V^{-1} \Sigma_W A_W^{-1} \\ A_W \Sigma_V A_V^{-1} & 1_W \end{pmatrix}.
\]

Clearly, \( \text{tr}(\Sigma') = |V| + |W| = n \). For the inverse matrix we have

\[
\Sigma'^{-1} = \begin{pmatrix} A_V & 0 \\ 0 & A_W \end{pmatrix} \cdot \Sigma^{-1} \cdot \begin{pmatrix} A_V & 0 \\ 0 & A_W \end{pmatrix} = \begin{pmatrix} (\Sigma^{-1})_V & 0 \\ A_W (\Sigma^{-1})_W^t A_V & (\Sigma^{-1})_W^t \end{pmatrix}.
\]

Now observe that \( \Sigma'_W (\Sigma'^{-1})_W^t = A_W^{-1} \Sigma_W (\Sigma^{-1})_W^t A_V \) as the product \( A_W^{-1} A_V = 1_W \) in the middle cancels out. Since the trace is cyclic, we have

\[
\text{tr}(\Sigma'_W (\Sigma'^{-1})_W^t) = \text{tr}(A_W^{-1} \Sigma_W (\Sigma^{-1})_W^t A_V) = \text{tr}(\Sigma_W (\Sigma^{-1})_W^t A_V A_W^{-1}) = 0.
\]

Moreover,

\[
1_V = (\Sigma' \Sigma'^{-1})_V = (\Sigma^{-1})_V + \Sigma'_W (\Sigma'^{-1})_W^t,
\]

implying \( \text{tr}((\Sigma'^{-1})_V) = \text{tr}(1_V) = |V| \). Similarly, \( \text{tr}((\Sigma'^{-1})_W) = |W| \), so \( \text{tr}(\Sigma'^{-1}) = |V| + |W| = n \). As \( \Sigma' \) is real symmetric positive definite there exists a symmetric square root \( T \) with \( T^2 = \Sigma' \) and thus also \( T^{-2} = \Sigma^{-1} \). Using the inner product \( \langle X, Y \rangle = \text{tr}(XY) = \sum_{i,j=1}^n x_{ij} y_{ij} \) on the space of real symmetric matrices,

\[
\langle T, T \rangle = \text{tr}(T^2) = \text{tr}(\Sigma') = n,
\]

\[
\langle T^{-1}, T^{-1} \rangle = \text{tr}(T^{-2}) = \text{tr}(\Sigma'^{-1}) = n,
\]

\[
\langle T, T^{-1} \rangle = \text{tr}(1_n) = n.
\]

Therefore, we have equality in the Cauchy–Schwarz inequality

\[
n^2 = \langle T, T^{-1} \rangle^2 \leq \langle T, T \rangle \cdot \langle T^{-1}, T^{-1} \rangle = n^2,
\]
implying that $T$ and $T^{-1}$ are linearly dependent as matrices, i.e., $T = \lambda T^{-1}$ for some $\lambda \in \mathbb{R}$. This implies $\Sigma' = T^2 = \lambda \mathbb{1}_n$. In particular, $0 = \Sigma'_{VW} = A_{V}^{-1} \Sigma_{VW} A_{W}^{-1}$ as matrices. But this is equivalent to $\Sigma_{VW} = 0$, as desired. \hfill \square

If all $V_i$ are single vertices we get the following.

**Corollary 3.24.** We have $\mathcal{M}_1(G, H) = \{1_n\}$ if and only if $E_G \cap E_H = \emptyset$.

In other words, if $\Sigma$ is a symmetric positive definite $(n \times n)$-matrix with the property that every off-diagonal entry vanishes either in $\Sigma$ or in $\Sigma^{-1}$ (or both), then $\Sigma$ is a diagonal matrix. We have not found this result in the literature.

**Remark 3.25.** A natural question is whether the assumption of positive definiteness in Theorem 3.23 is necessary. Example 4.4 shows that Corollary 3.24 does not hold for positive semi-definite matrices, and Example 3.27 below shows that Theorem 3.23 does not hold for principally regular matrices, that is, matrices whose principal minors do not vanish. We do not know if Corollary 3.24 holds in this case.

**Remark 3.26.** A simpler variant of Theorem 3.23 can be proven by recursive direct sum decomposition and duality: To every pair of graphs $(G, H)$ on $N$ there exists a partition $V_1, \ldots, V_r$ of $N$ such that

1. $G_i = G|_{V_i}$ and $H_i = H|_{V_i}$ are connected.
2. $\mathcal{M}(G, H)$ is smooth if and only if all $\mathcal{M}(G_i, H_i)$ are smooth.
3. $\mathcal{M}(G, H)$ is connected if and only if all $\mathcal{M}(G_i, H_i)$ are connected.

The merit of this simpler assertion is that it does not require positive definiteness. It also holds for principally regular models of $\langle G, H \rangle$ over $\mathbb{C}$ because the proof uses only elementary operations on CI relations introduced in Section 2.3.

**Example 3.27.** Consider the graph in Fig. 1. We study the variety of $\langle G, H \rangle$ in Macaulay2:

\[
R = \mathbb{Q}[x_{11}, x_{12}, x_{13}, x_{14}, x_{15}, x_{16}, x_{22}, x_{23}, x_{24}, x_{25}, x_{26}, x_{33}, x_{34}, x_{35}, x_{36}, x_{44}, x_{45}, x_{46}, x_{55}, x_{56}, x_{66}]
\]
\[
X = \text{genericSymmetricMatrix}(R,x11,6)
\]

-- Impose the relations from \( H \) directly on the matrix
\[
X = \text{sub}(X, \{ x16=>0, x24=>0, x25=>0, x26=>0, x35=>0 \})
\]

-- Pick an affine slice of the model which is likely to contain
-- positive definite matrices by diagonal dominance
\[
X = \text{sub}(X, \{
    x11=>10, x22=>10, x33=>10, x44=>10, x55=>10, x66=>10,
    x12=>1, x13=>1, x23=>1, x45=>1, x46=>1, x56=>1
\})
\]

\[
\begin{pmatrix}
10 & 1 & 1 & x_{14} & x_{15} & 0 \\
1 & 10 & 1 & 0 & 0 & 0 \\
1 & 1 & 10 & x_{34} & 0 & x_{36} \\
x_{14} & 0 & x_{34} & 10 & 1 & 1 \\
x_{15} & 0 & 0 & 1 & 10 & 1 \\
0 & 0 & x_{36} & 1 & 1 & 10
\end{pmatrix}
\]

Some of the variables are specified to ensure quick termination of the following computations. If Theorem 3.23 held for principally regular matrices, \( x_{14} \), \( x_{15} \), \( x_{34} \) and \( x_{36} \) would vanish on every principally regular matrix satisfying the equations of \( \langle \langle G \rangle \rangle \).

-- The relations imposed by \( G \)
\[
 I = \text{radical ideal}(
    \text{det submatrix}'(X, \{0\}, \{3\}), \quad -- \text{14}
    \text{det submatrix}'(X, \{0\}, \{4\}), \quad -- \text{15}
    \text{det submatrix}'(X, \{2\}, \{3\}), \quad -- \text{34}
    \text{det submatrix}'(X, \{2\}, \{5\}) \quad -- \text{36}
)
\]

-- Saturation at each of the principal minors
\[
J = \text{fold}((I,f) \rightarrow I : f, I, \text{subsets(numRows}(X)) / (K \rightarrow \text{det } X_K^K))
\]
decompose \( J \)

\[
\langle x_{14}, x_{15}, x_{34}, x_{36} \rangle \\
\cap (1210x_{14}^2 - 999, -11x_{14} + x_{15}, -x_{14} + x_{34}, -11x_{14} + x_{36}) \\
\cap (1210x_{14}^2 - 981, -11x_{14} + x_{15}, x_{14} + x_{34}, 11x_{14} + x_{36})
\]

The first component has the desired block structure of \( K_{123} \oplus K_{456} \), but the other components contain real points as well. Consider the last component. It consists of two real points:

\[
x_{14} = \pm \sqrt{\frac{981}{1210}}, \quad x_{15} = 11x_{14}, \quad x_{34} = -x_{14}, \quad x_{36} = -11x_{14}.
\]

This yields a real matrix satisfying the equations of \( \langle \langle G, H \rangle \rangle \) and whose principal minors are non-zero. However, the determinant of the entire matrix equals \( -\frac{4374}{55} \), which is not positive.
This shows that $\{G, H\}$ has real, principally regular solutions without block-diagonal structure. The positive definite matrices in the affine slice $J$ of the model all fall into the first component and do have the block structure. A purely algebraic computation, without taking positive definiteness into account, would not be able to prove Theorem 3.23.

3.5. Classification of the models $\mathcal{M}(G, H)$ with $|E_G \cap E_H| \leq 3$. Theorem 3.11 bounds the model dimension in terms of $|E_G \cap E_H|$. We finish our analysis of the geometry of $\mathcal{M}(G, H)$ with a classification of models with small intersections of the edge sets. In view of Theorem 3.23 we can restrict to the cases where $E_G \cap E_H$ defines a connected graph on the subset of vertices of $N$ incident to some edge in $E_G \cap E_H$. For any $N' \subseteq N$, we also write $PD_{N'}$ for the set of positive definite matrices with rows and columns indexed by $N'$. For disjoint subsets $N'$ and $N''$, a direct sum $PD_{N'} \oplus PD_{N''}$ indicates the set of block-diagonal positive definite matrices inside $PD_{N' \cup N''}$ with the rows and columns of the two blocks indexed, respectively, by $N'$ and $N''$, and similarly for $PD_{N',1} \oplus PD_{N'',1}$ if we restrict to ones on the diagonal.

Proposition 3.28. Let $E_G \cap E_H = \{ij\}$ consist of a single edge. Then

$$\mathcal{M}(G, H) = PD_{ij}. $$

In particular, $\mathcal{M}_1(G, H)$ is connected and smooth of the maximal dimension $|E_G \cap E_H| = 1$.

Proof. Immediate from Theorem 3.23 and the definitions.

Proposition 3.29. Let $|E_G \cap E_H| = 2$ and so $E_G \cap E_H = \{ij, jk\}$ with distinct $i, j, k$.

(1) If $ik \in E_G \setminus E_H$, then $\mathcal{M}(G, H) = \mathcal{M}(G \cap H)^{-1}$ is an inverse graphical model.

(2) In case $ik \in E_H \setminus E_G$, symmetrically $\mathcal{M}(G, H) = \mathcal{M}(G \cap H)$ is a graphical model.

(3) If $ik \notin E_G \cup E_H$, then $\mathcal{M}_1(G, H)$ decomposes as

$$\mathcal{M}_1(G, H) = \{1_n + tE^{ij} : t \in (-1, 1)\} \cup \{1_n + tE^{jk} : t \in (-1, 1)\}. $$

The Zariski closure of $\mathcal{M}_1(G, H)$ is a pair of lines intersecting in $1_n$. Thus $\mathcal{M}_1(G, H)$ is connected of dimension one, with reducible Zariski closure.

Proof. After a suitable permutation of $N$, we assume $ij = 12$ and $jk = 23$. Any $\Sigma \in \mathcal{M}_1(G, H)$ has the block-diagonal form consisting of an upper left $(3 \times 3)$-block and an identity matrix. Therefore we can assume $N = 123$. Then, in the first case, we have

$$\Sigma = \begin{pmatrix} 1 & \sigma_{12} & 0 \\ \sigma_{12} & 1 & \sigma_{23} \\ 0 & \sigma_{23} & 1 \end{pmatrix}, \quad \text{adj}(\Sigma) = \begin{pmatrix} 1 - \sigma_{23}^2 & -\sigma_{12} & \sigma_{12}\sigma_{23} \\ -\sigma_{12} & 1 & -\sigma_{23} \\ \sigma_{12}\sigma_{23} & -\sigma_{23} & 1 - \sigma_{12}^2 \end{pmatrix}. $$

As $13 \in E_G$, we have that $G = K_3$ is complete, so there are no further restrictions and we obtain $\mathcal{M}(G, H) = \mathcal{M}(G \cap H)^{-1}$. In the second case, the same is true if we replace $\Sigma$ by $\Sigma^{-1}$ everywhere, so $\mathcal{M}(G, H) = \mathcal{M}(G \cap H)$. Finally, in the third case, $13 \notin E_G \cup E_H$, so we additionally get $\sigma_{12} = 0$ or $\sigma_{23} = 0$, obtaining the union of two line segments, as desired.
Remark 3.30. Proposition 3.29 shows that in some non-obvious cases double Markovian models are graphical or inverse graphical models. This theme has occurred in the literature. For example, in [13, Proposition 12] it is shown that the only way that a covariance graph model $\mathcal{M}(K_N, H)$ is a graphical model $\mathcal{M}(G, K_N)$ is if covariance and concentration matrices have aligned block structures and the model is a product of $\text{PD}$ cones (in particular, $G = H$ is a disjoint union of cliques).

The same ideas also prove the following via direct computations.\footnote{Proposition 3.31 differs slightly from the published version doi:10.1111/sjos.12604 because the latter did not include the case where $E_G \cap E_H$ forms a star.}

Proposition 3.31. Let $|E_G \cap E_H| = 3$. If $E_G \cap E_H = \{ij, ik, jk\}$ forms a 3-clique, then $\mathcal{M}(G, H) = \text{PD}_{ij}$. Otherwise $E_G \cap E_H = \{ij, jk, kl\}$ with distinct $i, j, k, l$ forms a path or $E_G \cap E_H = \{ij, ik, il\}$ is a star. Up to swapping $G$ and $H$, we can restrict to the case where $H_{ijkl}$ has equally many or more non-edges than $G_{ijkl}$ (i.e., at least as many prescribed zeros in the covariance matrix as in the concentration matrix). We can restrict moreover to $n = 4$ and assume $(i, j, k, l) = (1, 2, 3, 4)$. If $E_G \cap E_H = \{12, 23, 34\}$ is a path, we have the following cases up to symmetry and inversion:

1. $E_H = E_G \cap E_H$ and $E_G = K_{1234}$. Here, $\mathcal{M}(G, H) = \mathcal{M}(G \cap H)^{-1}$.
2. $E_H = E_G \cap E_H$ and $E_G = K_{1234 \setminus \{13\}}$. Here, $\mathcal{M}(G, H) = (\text{PD}_{12} \oplus \text{PD}_{34}) \cup \mathcal{M}(\{23, 34\})^{-1}$.
3. $E_H = E_G \cap E_H$ and $E_G = K_{1234 \setminus \{14\}}$. Here, $\mathcal{M}(G, H) = (\text{PD}_{12} \oplus \text{PD}_{34}) \cup \mathcal{M}(\{12, 23\})^{-1} \cup \mathcal{M}(\{23, 34\})^{-1}$.
4. $E_H = E_G \cap E_H$ and $E_G = K_{1234 \setminus \{13, 14\}}$. Here, $\mathcal{M}(G, H)$ is as in the previous case.
5. $E_H = E_G \cap E_H$ and $E_G = K_{1234 \setminus \{13, 24\}}$. Here, $\mathcal{M}(G, H) = (\text{PD}_{12} \oplus \text{PD}_{34}) \cup \text{PD}_{23}$.
6. $E_G = E_H = E_G \cap E_H$. Here, $\mathcal{M}(G, H)$ is as in the previous case.
7. $E_H = (E_G \cap E_H) \cup \{13\}$ and $E_G = K_{1234 \setminus \{13\}}$. Here,

$$\mathcal{M}_1(G, H) = \begin{pmatrix}
1 & \sigma_{12} & \sigma_{12}\sigma_{23} & 0 \\
\sigma_{12} & 1 & \sigma_{23} & 0 \\
\sigma_{12}\sigma_{23} & \sigma_{23} & 1 & \sigma_{34} \\
0 & 0 & \sigma_{34} & 1
\end{pmatrix} : \sigma_{12} \in (-1, 1), \sigma_{23}^2 + \sigma_{34}^2 < 1
$$

8. $E_H = (E_G \cap E_H) \cup \{13\}$ and $E_G = K_{1234 \setminus \{13, 14\}}$. Here, $\mathcal{M}_1(G, H)$ is as in the previous case.
9. $E_H = (E_G \cap E_H) \cup \{13\}$ and $E_G = K_{1234 \setminus \{13, 24\}}$. Here,

$$\mathcal{M}_1(G, H) = (\text{PD}_{\{12\}, 1} \oplus \text{PD}_{\{34\}, 1})$$

$$\cup \begin{pmatrix}
1 & \sigma_{12} & \sigma_{12}\sigma_{23} & 0 \\
\sigma_{12} & 1 & \sigma_{23} & 0 \\
\sigma_{12}\sigma_{23} & \sigma_{23} & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix} : \sigma_{12}, \sigma_{23} \in (-1, 1)
$$
(10) $E_H = (E_G \cap E_H) \cup \{14\}$ and $E_G = K_{1234} \setminus \{14\}$. Here,

$$M_1(G, H) = \begin{cases} 1 \sigma_{12} 0 & \frac{-\sigma_{12} \sigma_{23} \sigma_{34}}{1 - \sigma_{23}^2} \\ \sigma_{12} & 1 \\ 0 & \sigma_{23} & 1 \\ \frac{-\sigma_{12} \sigma_{23} \sigma_{34}}{1 - \sigma_{23}^2} & 0 & \sigma_{34} \end{cases} : \sigma_{12}^2 + \sigma_{23}^2 < 1, \sigma_{23}^2 + \sigma_{34}^2 < 1. $$

(11) $E_H = (E_G \cap E_H) \cup \{14\}$ and $E_G = K_{1234} \setminus \{13, 14\}$. Here,

$$M_1(G, H) = (PD_{\{12, 1\}} \oplus PD_{\{34, 1\}}) \cup \begin{cases} 1 \sigma_{12} 0 & 0 \\ 0 & \sigma_{23} & 0 \\ 0 & 0 & \sigma_{34} \end{cases} : \sigma_{23}^2 + \sigma_{34}^2 < 1. $$

If $E_G \cap E_H = \{12, 13, 14\}$ is a star, we have the following cases up to symmetry and inversion:

(1) $E_H = E_G \cap E_H$ and $E_G = K_{1234}$. Here, $M(G, H) = M(G \cap H)^{-1}$.

(2) $E_H = E_G \cap E_H$ and $E_G = K_{1234} \setminus \{23\}$. Then

$$M_1(G, H) = \begin{cases} 1 \sigma_{12} \sigma_{14} \\ \sigma_{12} & 1 \\ \sigma_{13} & 0 \sigma_{14} \end{cases} : \sigma_{13}^2 + \sigma_{14}^2 < 1,$$

a union of two discs intersecting in a line segment.

(3) $E_H = (E_G \cap E_H) \cup \{23\}$ and $E_G = K_{1234} \setminus \{23\}$. Then

$$M_1(G, H) = \begin{cases} 1 \sigma_{12} \sigma_{14} \\ \sigma_{12} & 1 \\ \sigma_{12}^2 \sigma_{14} \sigma_{23} \sigma_{34} \end{cases} : \sigma_{12} \in (-1, 1),$$

(4) $E_H = E_G \cap E_H$ and $E_G = K_{1234} \setminus \{23, 24\}$. Then

$$M_1(G, H) = \begin{cases} 1 \sigma_{12} 0 & 0 \\ \sigma_{12} & 1 \\ 0 & 0 \sigma_{14} \end{cases} : \sigma_{13}^2 + \sigma_{14}^2 < 1.$$
\( E_H = (E_G \cap E_H) \cup \{23\} \) and \( E_G = K_{1234} \setminus \{23, 24\} \). Then

\[
M_1(G, H) = \begin{cases} 
\left\{ \begin{pmatrix} 1 & \sigma_{12} & \sigma_{13} & 0 \\
\sigma_{12} & 1 & \sigma_{12}\sigma_{13} & 0 \\
\sigma_{13} & \sigma_{12}\sigma_{13} & 1 & 0 \\
0 & 0 & 0 & 1 \end{pmatrix} : \sigma_{12}, \sigma_{13} \in (-1, 1) \right\} \\
\cup \left\{ \begin{pmatrix} 1 & 0 & \sigma_{13} & \sigma_{14} \\
0 & 1 & 0 & 0 \\
\sigma_{13} & 0 & 1 & 0 \\
\sigma_{14} & 0 & 0 & 1 \end{pmatrix} : \sigma_{13}^2 + \sigma_{14}^2 < 1 \right\} 
\end{cases}
\]

(6) \( E_G = E_H = E_G \cap E_H \). Then \( M_1(G, H) \) is the union of the three coordinate line segments parametrized by \( \sigma_{12}, \sigma_{13} \) and \( \sigma_{14} \), all contained in \((-1, 1)\).

In particular, for \(|E_G \cap E_H| \leq 3\) the models \( M(G, H) \) are connected in the Euclidean topology. Moreover, \( M(G, H) \) is smooth if and only if its Zariski closure is irreducible if and only if \( \dim(M_1(G, H)) = |E_G \cap E_H| \) is maximal. However, Example 4.2 below shows that there exist irreducible but singular double Markovian models on four vertices. Proposition 3.31 also shows that double Markovian models need not be equi-dimensional.

**Remark 3.32.** The preceding classification for \(|E_G \cap E_H| \leq 3\) and computer-aided computations on \( n \leq 4 \) vertices show that in this range for every smooth model \( M(G, H) \) with \( G \cap H \) connected, there exist graphs \( G', H' \) such that \( M(G, H) = M(G', H') \) and \( G' \cup H' = K_N \), thus the smoothness of the geometric model follows from Theorem 3.8. It is unknown whether there are smooth models without this property.

**Remark 3.33.** Any classification project would profit from a complete list of models of double Markovian CI structures or equivalently the set of completions of relations \( \langle G, H \rangle \). There is no efficient, combinatorial algorithm to compute the completion of \( \langle G, H \rangle \), although computing the completion can be reduced to invocations of the Positivstellensatz and thus quantifier elimination [2, Chapter 4]. One such project would be to classify smoothness of double Markovian models on small vertex sets. Exploiting Theorem 3.23, this reduces to multiple smoothness queries for smaller models. It seems like a worthwhile computational challenge to compile a table of the pairs of small connected graphs which have a smooth model. We determined that for \( n = 3, 4, 5 \) there are \( 4 + 55 + 2644 \) pairs of connected graphs which induce pairwise inequivalent CI structures modulo isomorphy and duality. For more information on computations see [https://gaussoids.de/doublemarkov.html](https://gaussoids.de/doublemarkov.html).

### 4. Examples, counterexamples, and conjectures

**Example 4.1.** Consider the double Markovian CI structure arising from \( G = H = \overline{X} \), namely \( \{(14), (14|23), (23), (23|14)\} \). A computation in Macaulay2 shows that (the Zariski closure of) the model \( M(G, H) \) has three irreducible components while it was determined in [14, Example 4.1] that the correlation model \( M_1(G, H) = M(G, H) \cap \text{PD}_{4,1} \) has four. Thus there are algebraic differences between \( M_1(G, H) \) and \( M(G, H) \).
Example 4.2. Continuing Example 2.17, suppose that $G = H$ is the complete graph on $N = 12 \cdots n$ minus the edge 12. These double Markovian models are singular at the identity matrix but the models of all proper minors of $\langle G, G \rangle$ are smooth. According to [14, Proposition 4.2] with $C_1 = \emptyset$ and $C_2 = N \setminus 12$, the singular locus of this model is again a Gaussian CI model and it is described as a submodel of $\mathcal{M}(G, G)$ by the CI statements

\begin{align*}
(12) & \text{ and } (12|C_2), \\
(1|j) & \text{ and } (2|j) \text{ for all } j \in C_2.
\end{align*}

All but one of them are simple zero constraints on the covariance matrix. By Schur complement, the remaining almost-principal minor equals

$$
\det \Sigma_{12|C_2} = (\sigma_{12} - \Sigma_{1,C_2} \Sigma_{C_2}^{-1} \Sigma_{C_2,2}) \det \Sigma_{C_2}.
$$

By all the marginal independence statements in (*), the vectors $\Sigma_{1,C_2}$ and $\Sigma_{C_2,2}$ as well as the entry $\sigma_{12}$ are zero, so the right-hand side of this equality vanishes, and $(12|C_2)$ is implied by the marginal statements. Thus, the singular locus is in fact a linear subspace of $\text{Sym}^2(\mathbb{R}^n)$ of codimension $2n - 3$, intersected with PD$_n$. This shows that double Markovian models can have singular loci of arbitrarily large dimension.

It is instructive to compute the concrete case of $n = 4$. The maximal possible dimension of the correlation model in this case is $|E_G| = 5$. However, $\mathcal{M}_1(G, G)$ is of dimension $4 < 5$. Indeed, the only conditions on a positive definite matrix $\Sigma \in \mathcal{M}_1(G, G)$ are $\sigma_{12} = 0$ and $(\Sigma^{-1})_{12} = 0$, which, using $\sigma_{12} = 0$, writes as

$$
f := \sigma_{13}(\sigma_{24}\sigma_{34} - \sigma_{23}) + \sigma_{14}(\sigma_{23}\sigma_{34} - \sigma_{24}) = 0.
$$

This is an irreducible polynomial, so the Zariski closure of $\mathcal{M}_1(G, G)$, which can be viewed as the vanishing set of the above polynomial inside the affine space where we forget the variable $\sigma_{12}$, is irreducible. In this case, the ideal $\text{SCI}_G,G$ is prime even without saturation, and it coincides with $\mathcal{I}(\mathcal{M}_1(G, G)) = \langle \sigma_{12}, f \rangle$. Moreover, we can see again that $\mathcal{M}_1(G, G)$ is connected: for every positive definite matrix $\Sigma$ satisfying $\sigma_{12} = 0$ and $f = 0$, scale all variables except for $\sigma_{34}$ by some $\varepsilon$ tending to 0. This preserves the two equations and establishes a path inside $\mathcal{M}_1(G, G)$ connecting $\Sigma$ to a matrix with only the entry $\sigma_{34} \in (-1, 1)$ possibly non-zero. The set of these matrices is clearly connected. As computed above, in the singular locus all variables but $\sigma_{34}$ are forced to zero, showing that it is a line inside PD$_4$. In particular, failure of smoothness is not always due to reducibility for double Markovian models.

In Example 4.2, we have $G = H = \emptyset$ an almost complete graph, where only one edge is missing. This model is singular at the identity matrix and therefore shows that the sufficient condition for smoothness in Theorem 3.8, namely that $G \cup H = K_N$, cannot be weakened. The singular locus in this example is a submodel described by the occurrence of additional CI statements. However, this is not always the case, as [14, Example 4.3] discovered.

Example 4.3. Let $G = \overline{\begin{array}{ccc} & & \\
& X & \\
& \end{array}}$ and $H = \overline{\begin{array}{cccc}
& & & \\
& & X & \\
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& & & \\n\end{array}}$ The model $\mathcal{M}_1(G, H)$ agrees with its inverse model up to permutation of $N$. Moreover, $G \cup H = K_4$ is the complete graph, so this model is smooth of the expected dimension $|E_G \cap E_H| = 4$. However, neither $\mathcal{M}_1(G, H)$ nor its inverse lie in the graphical model $\mathcal{M}(G \cap H)$. Indeed, for every $\Sigma \in \mathcal{M}_1(G, H)$ the condition $(\Sigma^{-1})_{12} = 0$ translates into $\sigma_{12} = 13\sigma_{23} + \sigma_{14}\sigma_{24}$, in particular $\sigma_{12}, \sigma_{13}, \sigma_{14}, \sigma_{23}, \sigma_{24}$ can all be non-zero.
at the same time. The same is true for the inverse model, as it arises from the permutation exchanging 1 with 4 and 2 with 3.

Example 4.4. Consider the disjoint graphs $G = \bigotimes$ and $H = \square$. The semi-definite model with ones on the diagonal consists of the five points

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & \pm 1 & 0 & 0 \\ \pm 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & \mp 1 \\ 0 & 0 & \mp 1 & 1 \end{pmatrix},$$

where the signs of the first two rows and last two rows agree, respectively, but are independent of each other. Thus semi-definite models can be disconnected even in dimension zero.

We have no analogue of Example 4.4 with positive definite matrices, and semi-definite models with no restriction on the diagonal are connected as they are star-shaped with respect to the zero matrix. The question if double Markovian models are connected in general is open.

Conjecture 4.5. For any $G, H$, the models $\mathcal{M}(G, H)$ and $\mathcal{M}_1(G, H)$ are connected.

The two statements in Conjecture 4.5 are equivalent. Moreover, $\mathcal{M}_1(G, H) \setminus \{I_n\}$ can be disconnected as the 1-dimensional smooth case shows. Connectedness of $\mathcal{M}_1(G, H)$ implies:

Conjecture 4.6. The model $\mathcal{M}_1(G, H)$ is smooth if it has the maximal dimension $|E_G \cap E_H|$. Moreover, if $\mathcal{M}_1(G, H)$ is smooth, its Zariski closure is irreducible.

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