POSITIVITY IN LINEAR GAUSSIAN STRUCTURAL EQUATION MODELS

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ABSTRACT. We study a notion of positivity of Gaussian directed acyclic graphical models corresponding to a non-negativity constraint on the coefficients of the associated structural equation model. We prove that this constraint is equivalent to the distribution being conditionally increasing in sequence (CIS), a well-known subclass of positively associated random variables. These distributions require knowledge of a permutation, a CIS ordering, of the nodes for which the constraint of non-negativity holds. We provide an algorithm and prove in the noise-less setting that a CIS ordering can be recovered when it exists. We extend this result to the noisy setting and provide assumptions for recovering the CIS orderings. In addition, we provide a characterization of Markov equivalence for CIS DAG models. Further, we show that when a CIS ordering is known, the corresponding class of Gaussians lies in a family of distributions in which maximum likelihood estimation is a convex problem.

1. Introduction

Many random systems exhibit some form of positive dependence. Examples in statistical physics include the ferromagnetic Ising Model [9] as well as general classes of lattice gas models and percolation models [8]. In fields such as finance [2], psychometrics [25, 29, 21] and biology (see [18] and further discussion in [17, Section 1.1]), positive dependence naturally arises [3]. In recent years, there has been an increased interest in exploiting this and related notions of positive dependence in statistical modelling and in machine learning.

This research direction has been particularly fruitful in the context of Gaussian and related distributions. Well studied examples of positive dependence in Gaussian models include: positive association defined by nonnegativity of all correlations [23], totally positive distributions (also known as MTP₂ distributions) defined by nonnegativity of all partial correlations [27, 16], and mixtures of these two scenarios as discussed in [17]. Various methods have been developed for covariance matrix estimation in the Gaussian setting [5, 2, 28, 33]. In applications, where the assumption of positive dependence is appropriate, these methods perform extremely well with no need for explicit regularization [2, 24].

An important problem, which motivates our work, is that none of these notions of positive dependence are suitable in the context of directed acyclic graphical models, also known as Bayesian networks¹. For a simple example, consider a Gaussian vector

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¹For background on Bayesian networks and associated graphical models, see e.g. [14].

 $X=(X_1,X_2,X_3)$ such that all partial correlations are non-negative. In other words, expressing partial correlations in terms of marginal correlation coefficients $\rho_{ij}=\operatorname{corr}(X_i,X_j)$, we require that

$$\rho_{12} - \rho_{13}\rho_{23} \ge 0, \quad \rho_{13} - \rho_{12}\rho_{23} \ge 0, \quad \rho_{23} - \rho_{12}\rho_{13} \ge 0.$$

If X is Markov to the DAG $2 \to 1 \leftarrow 3$, or equivalently, if $\rho_{23} = 0$, then, from the last inequality, we necessarily have that $\rho_{12}\rho_{13} = 0$. In other words, a Bayesian network with a v-structure cannot have all partial correlations non-negative. Given that two DAGs are Markov equivalent if and only if they have the same skeleton and v-structures (see Theorem 4.1), adding the MTP₂ constraint would severely restrict the class of Bayesian networks.

In this paper, we study a natural form of directional positive dependence that is suitable for Gaussian models on directed acyclic graphs (DAGs). We introduce the model through its representation via linear structural equations [22]. If G is a DAG with m nodes representing the Gaussian vector $X = (X_1, \ldots, X_m)$, then the distribution of X lies in the associated DAG model if it admits the stochastic representation

$$X_i = \sum_{j \in \text{Pa}(i)} \Lambda_{ij} X_j + \varepsilon_i \quad \text{for all } i = 1, \dots, m,$$
(1.1)

where Pa(i) denotes the set of parents of the node i in the DAG G, $\Lambda_{ij} \in \mathbb{R}$, and $\varepsilon_i \sim N(0, \sigma_i^2)$ are mutually independent. In matrix form, this can be written as $X = \Lambda X + \varepsilon$, where $\Lambda_{ij} = 0$ unless $j \to i$ in G.

Remark 1.1. Let D be a diagonal matrix representing the covariance matrix of ε . Denoting the covariance matrix of X by Σ (we assume throughout that it is full rank), then (1.1) implies

$$\Sigma = (I - \Lambda)^{-1} D(I - \Lambda)^{-\top},$$

which is equivalent to the following equality for the precision matrix $K = \Sigma^{-1}$:

$$K = (I - \Lambda)^{\top} D^{-1} (I - \Lambda).$$

The following natural notion of positivity in Gaussian DAG models is the central theme of our paper.

Definition 1.2. A Gaussian vector X is positively DAG dependent with respect to a DAG G if X admits the stochastic representation (1.1) with all Λ_{ij} nonnegative. We denote the subset of Gaussian DAG models $\mathbb{M}(G)$ over G that satisfy this property by $\mathbb{M}_+(G)$.

Other approaches have been proposed to define positive dependence on DAGs; see, for example, [30, 32] and references therein. To explain the relationship between these different notions, we note that positive DAG dependence is closely related to the following classical notion of positive dependence.

Definition 1.3. A random vector $X = (X_1, ..., X_m)$ is conditionally increasing in sequence (CIS) if for every $i \in [m]$ and every fixed $x_i \in \mathbb{R}$, it holds that

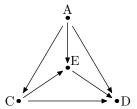
$$\mathbb{P}\big(\{X_i \ge x_i\}\big| (X_j = x_j)_{j < i}\big)$$

is a non-decreasing function in (x_1, \ldots, x_{i-1}) , when equipped with the coordinate-wise partial order.

In the context of DAGs, the papers [30, 32] investigated a similar notion which they called a "weak monotonic effect" or "positive influence". If a parent $k \in \text{Pa}(i)$ of a particular vertex i has the property that

$$\mathbb{P}\Big(\{X_i \ge x_i\} \Big| \bigcap_{j \in \text{Pa}(i)} (X_j = x_j)\Big)$$

is a non-decreasing (non-increasing) function in x_k then k is said to have a weak monotonic positive effect on i. Notably, this condition can be used to infer the presence/absence of certain edges in the graph. To provide a specific example, consider the DAG from [30, Example 5] with variables A denoting air pollution levels, E denoting antihistamine treatment, D denoting asthma incidence, and C denoting bronchial reactivity in the following figure.



From context, it is reasonable to assume that the directed edges (A, D), (A, E) and (A, C) are weak positive monotonic effects, and similarly the edges (C, E) and (C, D) are weak positive monotonic effects. The following argument can be used to test the causal relationship $E \to D$: From [30, Theorem 4] it follows that the covariance of E and D must be non-negative due to the weak positive monotonic effects of the other edges. Thus if the observed covariance of E and D was negative (which is the desired medical objective), we would conclude the presence of the edge $E \to D$ even without measuring the variables A and C.

We will show that the notion of positive dependence of a DAG considered in this work (stated in Definition 2.6) is the same as assuming a weak positive monotonic effect of *every* parent on its child. This example showing how positive dependence can be used to derive causal relationships motivates our study of Markov equivalence of these models.

In this work, we link the class of CIS models (which a priori make no reference to any DAG structure) to positive DAG dependence. In particular, we will discuss the problem of ordering the variables in such a way that it is CIS and identifying when there exists such an ordering. The resulting DAG could be used for causal inference.

In Theorem 2.1 below, we show that a Gaussian vector X is CIS if and only if it is positively DAG dependent with respect to the full DAG with arrows $i \to j$ for all i < j. It follows that the Gaussian CIS condition has a simple algebraic formulation. Let $K = UU^T$ be the Cholesky decomposition (U is upper triangular with positive diagonal entries) and $K = \Sigma^{-1}$ is the inverse covariance matrix of X. Then our notion of positive dependence restricts the signs of the off-diagonal entries of U to be non-positive. This constraint is convex, which makes computing the maximum likelihood estimator (MLE) particularly tractable.

In practice, K may admit such a signed Cholesky factorization only after permuting its rows and columns. Thus, part of the problem is to recover a permutation

matrix P that makes such a signed factorization possible. Maximizing the likelihood over all m! permutation matrices is infeasible. Instead, we propose a simple algorithm for learning such a permutation, and we provide statistical guarantees for the proposed algorithm.

We will often contrast the class of CIS Gaussian vectors X with the well-known and well-studied class of multivariate totally positive distributions of order 2 (MTP₂), which requires that its density p on \mathbb{R}^m satisfies

$$p(x)p(y) \le p(x \lor y)p(x \land y)$$
 for all $x, y \in \mathbb{R}^m$,

where \vee is the componentwise maximum and \wedge is the componentwise minimum. This inequality appeared in [8], where it was shown to imply positive association for general distributions. In the Gaussian case MTP₂ was shown to be equivalent to the precision matrix (inverse covariance matrix) being an M-matrix [12].

Definition 1.4 (M-matrix). A positive definite $m \times m$ matrix $A = [a_{i,j}]_{1 \le i,j \le m}$ is an M-matrix if the entries satisfy $a_{i,j} \le 0$ for all $i \ne j$. The space of symmetric, positive definite M-matrices of dimension $m \times m$ is denoted $\mathcal{M}_m(\mathbb{R})$.

- 1.1. Outline. Section 2 expounds upon the relationship between CIS distributions and DAG models while also providing motivating examples both in the Gaussian and non-Gaussian settings. Section 3 provides examples that distinguish CIS distributions from MTP₂ and other positively associated distributions along with an illustration that CIS orderings may not provide sufficient information to recover the underlying Markov equivalence class. Section 4 dives deeper into Markov equivalence for CIS orderings. Section 5 shifts the focus to parameter estimation and fitting: Cholesky factor models are introduced for the purpose of characterizing the MLE of Λ and D of a CIS distributed vector assuming the underlying CIS ordering is known. Section 6 concerns recovering a CIS ordering, first in the population case and then proving consistency of a noisy version of our proposed algorithm under simple assumptions on Λ . In this section, we also prove results on what sorts of CIS orderings are possible for a distribution.
- 1.2. **Notation.** For a DAG G = (V, E), we denote the set of parent nodes of a vertex i by Pa(i) and the set of children nodes of a vertex i by Ch(i). If there are several DAGs over the same vertex set V under consideration, we write $Pa_G(i)$ and $Ch_G(i)$ to indicate the dependence on the particular DAG G. We will mostly use $V = [m] = \{1, \ldots, m\}$ or subsets of [m].

When we say a function $f: \mathbb{R}^k \to \mathbb{R}$ is increasing (non-decreasing) in \mathbb{R}^k , we mean that f is increasing (non-decreasing) in each variable. Moreover for a subset $A \subset [k]$, if we write $(x_j)_{j \in A}$, or equivalently, x_A , we mean the tuple formed by taking the entries of x that are indexed by A, keeping the original order.

We denote the set of $m \times m$ positive semidefinite matrices by $\mathcal{S}_m(\mathbb{R})$ and the subset of positive definite matrices by $\mathcal{S}_m^+(\mathbb{R})$. Further, I always denotes the identity matrix. When M is an $s \times t$ matrix with $A \subset [s]$ and $B \subset [t]$, then $M_{A,B}$ is the submatrix of size $|A| \times |B|$ with entries $M_{i,j}$ with $i \in A$ and $j \in B$. Following [14, Section 5.1.1], if a matrix operation appears with the subset indices, e.g., $M_{A,A}^{-1}$ the matrix operation is performed first — so $M_{A,A}^{-1}$ is the submatrix of M^{-1} indexed by A, whereas $(M_{A,A})^{-1}$ is the inverse of the submatrix of M indexed by A. We will use the shorthand $\backslash i$ for $[m]\backslash i$.

When we consider collections of permutations, we use one line notation and use parentheses around those elements that can be ordered in any way, so for instance (123)45 is the set of permutations for which $\sigma(4) = 4$ and $\sigma(5) = 5$ and 1,2,3 can be arbitrarily assigned to the values $\sigma(1)$, $\sigma(2)$ and $\sigma(3)$, that is, $(123)45 = \{12345, 13245, 21345, 23145, 31245, 32145\}$.

2. Structure of Positive Dependence on a DAG

2.1. Basic results and definitions. We start by stating the main result of this section, which links the classical concept of CIS dependence and positive DAG dependence.

Theorem 2.1. A Gaussian vector X is CIS if and only if it is positively DAG dependent with respect to the full DAG with $i \rightarrow j$ for all i < j.

The proof relies on a lemma that we prove first.

Lemma 2.2. Let $Z = (Z_1, ..., Z_m) \sim \mathcal{N}_m(\mu, \Sigma)$ be a Gaussian random vector on \mathbb{R}^m with mean $\mu \in \mathbb{R}^m$ and covariance $\Sigma \in \mathcal{S}_m^+(\mathbb{R})$, let $K = \Sigma^{-1}$ be the precision matrix. The function

$$\mathbb{P}\Big(\{Z_i \ge x_i\} \Big| \bigcap_{j \ne i} \{Z_j = x_j\}\Big) \tag{2.1}$$

is non-decreasing in $(x_j)_{j\neq i}$ if and only if $K_{i,j} \leq 0$ for all $j \neq i$. Moreover, this statement is equivalent to the following two statements:

- (a) $\mathbb{E}[Z_i|Z_{\setminus i}]$ is a non-decreasing function in $(Z_j)_{j\neq i}$.
- (b) $Z_i = \sum_{j \neq i} \Lambda_{ij} Z_j + \varepsilon_i$ with $\Lambda_{ij} \geq 0$ and ε_i Gaussian and independent of $(Z_j)_{j \neq i}$.

Proof. It is a classic result [19, Theorem 1.2.11 (b)] that

$$Z_i|Z_{\backslash i} \sim \mathcal{N}\Big(\mu_i + \Sigma_{i,\backslash i}(\Sigma_{\backslash i,\backslash i})^{-1}(Z_{\backslash i} - \mu_{\backslash i}), \Sigma_{i,i} - \Sigma_{i,\backslash i}(\Sigma_{\backslash i,\backslash i})^{-1}\Sigma_{i,\backslash i}^{\top}\Big),$$

but note that by the Schur complement formula,

$$K_{i,i} = \left(\Sigma_{i,i} - \Sigma_{i,\setminus i} (\Sigma_{\setminus i,\setminus i})^{-1} \Sigma_{i,\setminus i}^{\top}\right)^{-1},$$

$$K_{i,\setminus i} = -K_{i,i} \Sigma_{i,\setminus i} (\Sigma_{\setminus i,\setminus i})^{-1},$$

and $K_{i,i} > 0$ by positive definiteness. Hence we may rewrite the mean of $Z_i | Z_{i}$ as

$$\mu_i - \frac{K_{i,\backslash i}}{K_{i,i}} (Z_{\backslash i} - \mu_{\backslash i}).$$

It is then clear that the function in the statement of the lemma is non-decreasing in $x_{\setminus i}$ only if the entries of $K_{i,\setminus i}$ are all non-positive. Note that this is also the condition on the conditional mean in (a). Equivalence with (b) follows from the fact that

$$\varepsilon_i := Z_i - \mathbb{E}[Z_i|Z_{\setminus i}]$$

is a mean zero Gaussian variable. Since $\mathbb{E}[\varepsilon_i Z_j] = 0$ for all $j \neq i$, and all (ε, Z) are jointly Gaussian, it follows that ε_i is independent of $Z_{\setminus i}$ as claimed.

Proof of Theorem 2.1. Using Lemma 2.2(b) recursively starting with i = m we get that X is CIS if and only if

$$X_i = \sum_{j=1}^{i-1} \Lambda_{ij} X_j + \varepsilon_i$$
 for all $i = 1, \dots, m$

with $\Lambda_{ij} \geq 0$ and ε_i independent of X_1, \ldots, X_{i-1} . This is precisely (1.1) when applied to the full DAG with $j \to i$ for all j < i.

Theorem 2.1 together with Remark 1.1 gives the following important algebraic characterization of Gaussian CIS distributions.

Corollary 2.3. The vector $X \sim \mathcal{N}_m(\mu, \Sigma)$ is CIS if and only if $K = UU^{\top}$ with U upper triangular with positive diagonal and non-positive off-diagonal entries.

Note that the CIS property relies on the ordering of the variables in the vector X. The following definition is a natural extention of the CIS property; see also [20].

Definition 2.4. If there exists a permutation σ of [m] such that $(X_{\sigma(1)}, \ldots, X_{\sigma(m)})$ is CIS, then we say σ is a CIS ordering of X. If for every permutation σ of [m] we have that the vector $(X_{\sigma(1)}, \ldots, X_{\sigma(m)})$ is also CIS, then we say X is conditionally increasing (CI).

Interestingly, in the Gaussian case CI equals MTP₂ (see Section 3). Next, let G = (V, E) be a DAG. A permutation σ of V is a topological ordering if $a \to b$ implies $\sigma(a) < \sigma(b)$. It is well-known that if G is a DAG, there exists a permutation of V that is a topological ordering. In relation to the structural equation model, it is useful to recall that if a DAG is topologically ordered then Remark 1.1 takes on a particularly nice form with Λ lower triangular. Denote by CIS $_{\sigma}$ the set of all Gaussian distributions such that $(X_{\sigma(1)}, \ldots, X_{\sigma(m)})$ is CIS. The following result gives an important characterization of Gaussian positive DAG dependent distributions $\mathbb{M}_+(G)$.

Theorem 2.5. For a DAG G it holds that

$$\mathbb{M}_+(G) = \mathbb{M}(G) \cap \mathrm{CIS}_{\sigma},$$

where σ is any topological ordering of G.

Proof. We first show $\mathbb{M}_+(G) \subseteq \mathbb{M}(G) \cap \mathrm{CIS}_{\sigma}$. The inclusion $\mathbb{M}_+(G) \subseteq \mathbb{M}(G)$ follows by definition. To argue that $\mathbb{M}_+(G) \subseteq \mathrm{CIS}_{\sigma}$ let \widehat{G} be the complete DAG whose only topological ordering is σ . It is clear that $\mathbb{M}_+(G) \subseteq \mathbb{M}_+(\widehat{G})$ and $\mathbb{M}_+(\widehat{G}) = \mathrm{CIS}_{\sigma}$ by Theorem 2.1. Consequently, $\mathbb{M}_+(G) \subseteq \mathbb{M}(G) \cap \mathrm{CIS}_{\sigma}$.

To show the opposite inclusion, note that if X has distribution in $\mathbb{M}(G)$ then the representation (1.1) holds. Since X is CIS_{σ} and σ is a topological ordering, we get from Lemma 2.2(b) that the coefficients Λ_{ij} must be non-negative and so the distribution of X lies in $\mathbb{M}_+(G)$.

Although we focus in this paper on the Gaussian case, we note that Lemma 2.2 suggests a more general definition, which is in line with [30, 32]. Consider a random vector X with values in $\mathcal{X} = \prod_{i=1}^{m} \mathcal{X}_i$ where $\mathcal{X}_i \subseteq \mathbb{R}$. We always assume that X admits a density function with respect to some product measure on \mathcal{X} .

Definition 2.6. Suppose that X is a distribution that is Markov to a directed acyclic graph G. Then X is positively DAG dependent with respect to G if, for every i the condition survival function

$$\mathbb{P}\Big(\{X_i \ge x_i\} \Big| \bigcap_{j \in \text{Pa}(i)} \{X_j = x_j\}\Big)$$

is non-decreasing in $(x_j)_{j \in Pa(i)}$.

We will use this more general definition to motivate some non-Gaussian examples int he following discussion.

- 2.2. Motivating examples. Positive DAG dependence is often present in small, well-designed studies. Some examples of datasets that both are well modeled by DAGs and the variables in the system are positively correlated, can be found in educational research or medical psychology; see, e.g., [1, 13]. There are also two general popular datasets, where DAG positive dependence appears naturally. These are fictitious datasets that were constructed to mimic real processes. The first dataset was introduced in [15]. It consists of sequences of "yes" and "no" responses from patients with suspected lung disease to the following questions:
 - (D) Has shortness-of-breath
 - (A) Had a recent trip to Asia
 - (L) Has Lung Cancer
 - (T) Has Tuberculosis
 - (E) Either (T) or (L), or both, are true
 - (X) Has a chest X-ray with a positive test
 - (S) Is a smoker
 - (B) Has Bronchitis

In modeling the relationships of these variables, we take 1 to be the response "yes" and 0 to be "no" and use a binary-valued Bayesian network illustrated in Figure 1 below to encode the relationships between variables, following [15].

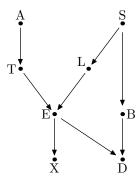


FIGURE 1. The node letters are the parenthetical letters in the list above. The variable E represents the logical statement "Tuberculosis (T) or Lung Cancer (L)".

In [15, Table 1], a ground truth joint distribution was defined for this example using the conditional probabilities

It is clear that the above model is positive dependent with respect to the given DAG by inspecting the probabilities directly and checking that the condition in Definition 2.6 holds.

Another dataset that is used in the context of Gaussian DAGs is the crop analysis dataset discussed in Section 2.1 in [26]. The underlying DAG and the node descriptions is given in Figure 2. The dataset assumes the following conditional node distributions:

$$\begin{split} E &\sim \mathcal{N}(50, 100) \\ G &\sim \mathcal{N}(50, 100) \\ V \mid G, E &\sim \mathcal{N}(-10.36 + 0.5G + 0.77E, 25) \\ N \mid V &\sim \mathcal{N}(45 + 0.1V, 99) \\ W \mid V &\sim \mathcal{N}(15 + 0.7V, 51) \\ C \mid N, W &\sim \mathcal{N}(0.3N + 0.3W, 39.06) \end{split}$$

Here, again, positive DAG dependence is part of the construction because all the conditional means depend positively on the conditioning variables.

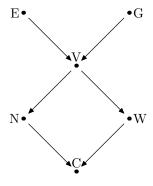


FIGURE 2. The DAG representing the crop dataset from [26]. The nodes are: E (environmental potential), G (genetic potential), V (vegetative organs), N (number of seeds), W (seeds mean weight), C (crop).

3. Illustrative theoretical examples

Denote MTP₂ to be the set of all MTP₂ Gaussians, and PA to be the set of all positively associated Gaussians; see [6] for a discussion of association. In [20] it is shown that for general distributions, the MTP₂ property implies CI which in turn implies CIS, and CI is equal to MTP₂ in the Gaussian case. Thus, in the Gaussian case, for every permutation σ we have:

$$\mathrm{MTP}_2 \quad = \quad \bigcap_{\tau} \mathrm{CIS}_{\tau} \quad \subset \quad \mathrm{CIS}_{\sigma} \quad \subset \quad \bigcup_{\tau} \mathrm{CIS}_{\tau} \quad \subset \quad \mathrm{PA}, \qquad (3.1)$$

where the intersection and the union are taken over all orderings. As we will see, even in the Gaussian case, all the inclusions are strict. We first give a simple example which is not MTP_2 but is CIS.

Example 3.1. Consider the upper triangular matrix

$$U = \begin{bmatrix} 1 & 0 & -a \\ 0 & 1 & -b \\ 0 & 0 & 1 \end{bmatrix}$$

with a, b > 0. If $K = UU^{\top}$ is the precision matrix of a Gaussian $X = (X_1, X_2, X_3)$, then X is CIS by Corollary 2.3. However,

$$K = \begin{bmatrix} 1 & 0 & -a \\ 0 & 1 & -b \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -a & -b & 1 \end{bmatrix} = \begin{bmatrix} 1+a^2 & ab & -a \\ ab & 1+b^2 & -b \\ -a & -b & 1 \end{bmatrix},$$

which is not an M-matrix, therefore X is not MTP₂. As a structural equation model, we may write X as

$$X_1 = \varepsilon_1$$

$$X_2 = \varepsilon_2$$

$$X_3 = aX_1 + bX_2 + \varepsilon_3,$$

where $(\varepsilon_1, \varepsilon_2, \varepsilon_3)$ is a standard $\mathcal{N}(0, I_3)$ Gaussian. This is a DAG with a v-structure, $1 \to 3 \leftarrow 2$. Note that $K_{12} > 0$ and so 123 and 213 are the only possible CIS orderings.

The above example is significant in that it shows that for Gaussian distributions, the class of CIS ordered graphical models is substantially larger than MTP₂ Gaussians. In particular it is known that v-structures cannot occur for MTP₂ graphical models in a very general setting [7]. From this standpoint, it is quite appealing to be able to extend from MTP₂ distributions to CIS distributions, since v-structures are significant in determining Markov equivalence classes, which we discuss in the next section.

Example 3.1 shows that a distribution that is CIS may not be CIS with respect to other orderings. In consequence, the inclusion $CIS_{\sigma} \subset \bigcup_{\tau} CIS_{\tau}$ is also strict (unless m=2). As a demonstration that the last inclusion in (3.1) is strict, we give the following example which is a positive associated Gaussian where *no reordering* of X is CIS.

Example 3.2. Let X be a centered Gaussian with covariance

$$\Sigma = \begin{bmatrix} 5 & 4 & 7 & 8 \\ 4 & 9 & 8 & 7 \\ 7 & 8 & 11 & 11 \\ 8 & 7 & 11 & 14 \end{bmatrix}.$$

Since all entries of Σ are positive, by [23], X is a positive associated Gaussian. However,

$$K = \begin{bmatrix} 94 & 25 & -55 & -23 \\ 25 & 7 & -15 & -6 \\ -55 & -15 & 33 & 13 \\ -23 & -6 & 13 & 6 \end{bmatrix},$$

since each row of the above matrix has a positive off-diagonal entry it follows that there is no $j \in [4]$ such that $\mathbb{E}[X_j|X_{\setminus j}]$ is a non-decreasing function in $X_{\setminus j}$, from which we conclude that there is no CIS ordering of X.

The next result studies the relation between CIS_{σ} models.

Proposition 3.3. Suppose $X = (X_1, ..., X_m)$ has a Gaussian distribution. If m = 2 then (X_1, X_2) is CIS if and only if (X_2, X_1) is CIS. If $m \ge 3$ then $\text{CIS}_{\sigma} = \text{CIS}_{\sigma'}$ if and only if $\sigma(k) = \sigma'(k)$ for k = 3, ..., m.

Proof. The bivariate case follows because (X_1, X_2) is CIS if and only if $\operatorname{Cov}(X_1, X_2) \geq 0$, which is symmetric in (X_1, X_2) . Suppose $m \geq 3$. The "if" implication follows directly from the definition and from the m=2 case. For the "only if" implication assume with no loss in generality that $\sigma'=\operatorname{id}$. We construct a distribution that lies in $\operatorname{CIS}_{\operatorname{id}}$ and show that it lies in $\operatorname{CIS}_{\sigma}$ if and only if $\sigma=\operatorname{id}$ or $\sigma=(2,1,3,\ldots,m)$. Let U be an upper triangular matrix of the form

$$U = \begin{bmatrix} 1 & 0 & -1 & -2 & \cdots & -(m-3) & -(m-2) \\ 0 & 1 & -1 & -1 & \cdots & -1 & -1 \\ 0 & 0 & 1 & -1 & \cdots & -1 & -1 \\ \vdots & \vdots & \ddots & \ddots & & & \\ 0 & 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \end{bmatrix}.$$

The distribution we construct has covariance Σ such that $K = \Sigma^{-1} = UU^{\top}$. Since all the upper off-diagonal entries are non-positive, this distribution is CIS_{id} . Denote the rows of U by U_1, \ldots, U_m . Note that

$$U_1^\top U_2 \ > \ \cdots \ > \ U_1^\top U_{m-1} \ = \ 1 \ > \ 0,$$

and so $K_{1i}>0$ for all $i=2,\ldots,m-1$. This shows that every CIS ordering of this random vector must have m as the last index. If m=3, then we are done. If $m\geq 4$, consider the marginal distribution over $A=\{1,\ldots,m-1\}$. Because U is upper triangular, we get that $(\Sigma_{A,A})^{-1}=U_{A,A}U_{A,A}^{\top}$. Note that $U_{A,A}$ has the same form as U but with m-1 replacing m. Thus, by the same argument as above,

$$(\Sigma_{A,A})_{1i}^{-1} > 0$$
 for all $i = 2, \dots, m-2$.

This shows that every CIS ordering of our constructed distribution must have m-1 as the penultimate index. If m=4, we are done. If $m\geq 5$, take $A\setminus\{m-1\}$ as the new A and proceed as above. In this way we show that for this distribution σ is a CIS ordering only if $\sigma(k)=k$ for $k=3,\ldots,m$.

There are qualitative properties of CIS distributions that contrast with MTP_2 distributions. It is known ([11, Proposition 3.2]) that if X is MTP_2 distributed then any marginal distribution of X also satisfies the MTP_2 property. The next example shows that a Gaussian CIS random variable does not satisfy this property.

Example 3.4. Let $X = (X_1, X_2, X_3, X_4)$ be a centered Gaussian with covariance

$$\Sigma = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{3}{4} & \frac{29}{16} \\ \frac{1}{4} & \frac{5}{4} & \frac{7}{4} & \frac{77}{16} \\ \frac{3}{4} & \frac{7}{4} & \frac{17}{4} & \frac{167}{16} \\ \frac{29}{16} & \frac{77}{16} & \frac{167}{16} & \frac{1737}{64} \end{bmatrix}.$$

It can be checked directly that (X_1, X_2, X_3, X_4) is CIS. However, the inverse of Σ_{134} is

$$\begin{bmatrix} \frac{205}{24} & -\frac{23}{12} & \frac{1}{6} \\ -\frac{23}{12} & \frac{14}{3} & -\frac{5}{3} \\ \frac{1}{6} & -\frac{5}{3} & \frac{2}{3} \end{bmatrix}.$$

Since the last row of this matrix has a positive off-diagonal entry, we conclude that (X_1, X_3, X_4) is not CIS.

However, the following result, which follows immediately from the definition, shows that certain conditionals and marginals preserve the CIS property. result .

Proposition 3.5. Let X be a CIS distributed centered Gaussian. Then the following distributional properties hold:

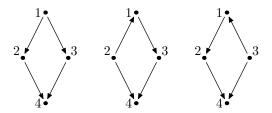
- (1) The conditional distribution of (X_{k+1}, \ldots, X_m) given (X_1, \ldots, X_k) is CIS.
- (2) The vector (X_1, \ldots, X_k) is CIS for every $1 \le k \le m$.

Theorem 2.5 shows a relation between CIS orderings and positive DAG dependence. The following example describes a complication that can arise. Namely, we consider a DAG whose possible topological orderings are 1(23)4, the union of all CIS orderings for all Markov equivalent DAGs is (123)4, but for special distributions in the model it is possible that 4321 is a valid CIS ordering.

Example 3.6. Consider the DAG model defined by the upper triangular matrix

$$U = \begin{bmatrix} 1 & -a & -b & 0 \\ 0 & 1 & 0 & -c \\ 0 & 0 & 1 & -d \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

with a,b,c,d>0. The Markov equivalence class of this DAG consists of the following three DAGs.



The corresponding precision matrix is given by

$$K = UU^{\top} = \begin{bmatrix} 1 + a^2 + b^2 & -a & -b & 0 \\ -a & 1 + c^2 & cd & -c \\ -b & cd & 1 + d^2 & -d \\ 0 & -c & -d & 1 \end{bmatrix}$$

Since $K_{23} = cd > 0$, it is clear that any CIS ordering has 1 or 4 as the last element and 1 is actually possible. Since (X_1, X_2, X_3) is always CI, we conclude that all orderings (123)4 are CIS². By direct computation we see that for $\Sigma = K^{-1}$,

$$(\Sigma_{234})^{-1} = \begin{bmatrix} \frac{(a^2+1)c^2+b^2(c^2+1)+1}{1+a^2+b^2} & \frac{a^2cd-ab+(b^2+1)cd}{1+a^2+b^2} & -c\\ \frac{a^2cd-ab+(b^2+1)cd}{1+a^2+b^2} & \frac{a^2(d^2+1)+(b^2+1)d^2+1}{1+a^2+b^2} & -d\\ -c & -d & 1 \end{bmatrix}.$$

In particular, if a, b are sufficiently large and c, d are sufficiently small such that $a^2cd - ab + (b^2 + 1)cd \le 0$, we also have that (X_2, X_3, X_4) is CI. In this case, each ordering (234)1 is also a CIS ordering. Thus the CIS orderings are of the form 1(23)4, 4(23)1 and (23)(14). Note that only the DAG with topological ordering 1(23)4 is in the Markov equivalence class, while the DAGs with topological ordering 4(23)1 and (23)(14) are not. This shows that the set of all CIS orderings contains only limited information about the underlying DAG.

The situation is not always that complicated. In Proposition 4.5 we will show that there is a large class of interesting hierarchical networks for which the possible CIS orderings are exactly the topological orderings.

Another property worth noting is that the space of MTP₂ Gaussian distributions amounts to the M-matrix constraint on K, which is convex in K. We can show that the space of K for which X is a CIS Gaussian is not convex in K.

Example 3.7. Let K_1 and K_2 be the precision matrices

$$K_{1} = \begin{bmatrix} 1 & -1 & -1 & -4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & -3 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & -1 & -1 & -4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & -3 \\ 0 & 0 & 0 & 1 \end{bmatrix}^{\top} = \begin{bmatrix} 19 & -1 & 11 & -4 \\ -1 & 1 & 0 & 0 \\ 11 & 0 & 10 & -3 \\ -4 & 0 & -3 & 1 \end{bmatrix},$$

$$K_{2} = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 \end{bmatrix}^{\top} = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}.$$

Clearly, by Corollary 2.3, we must have that Gaussians with precision matrices K_1 or K_2 are CIS ordered. However consider the sum

$$K = K_1 + K_2 = \begin{bmatrix} 21 & -2 & 11 & -4 \\ -2 & 3 & -1 & 0 \\ 11 & -1 & 12 & -4 \\ -4 & 0 & -4 & 2 \end{bmatrix}.$$

²The notation (123) stands for any permutation of these three.

Then if $\Sigma = K^{-1}$, by the Schur Complement formula

$$\left(\Sigma_{[3],[3]}\right)^{-1} = K_{[3],[3]} - \frac{K_{[3],4}K_{4,[3]}}{K_{4,4}} = \begin{bmatrix} 13 & -2 & 3\\ -2 & 3 & -1\\ 3 & -1 & 4 \end{bmatrix}$$

which means that if X has covariance Σ , then $\mathbb{E}[X_3|X_1,X_2]$ is not a non-decreasing function of X_1 and X_2 due to the third row of the above matrix having an off-diagonal that is positive — the same will be true if we were to replace K by $\frac{K}{2}$, which implies that the convex combination of K_1 and K_2 does not stay in the class of precision matrices of CIS Gaussians.

The above example shows that even if we assume that a Gaussian is CIS ordered under a known permutation σ , we do not have convexity in the space of precision matrices K that parameterize this model. In Section 5, we show that there is a broad class of models, under which Gaussians that are CIS for a known permutation σ are included, for which computing the MLE is a convex optimization problem. While the results of Section 5 may be familiar to many practitioners, we did not find a direct reference and thought it worthwhile to specify these models explicitly. Most importantly for us however, is that computationally, once a CIS ordering is known, calculating the MLE for a CIS Gaussian can be done with similar efficiency as restricting to the MTP₂ class.

4. Markov equivalence for CIS models

One of the most fundamental limitations of Bayesian networks is that two different DAGs may represent the same conditional independence model, in which case we say that they are Markov equivalent. We recall the following classical result [31] that uses the concept of a skeleton, which for a DAG G is the undirected graph obtained from G by forgetting the directions of all arrows.

Theorem 4.1. Two DAGs G and H are Markov equivalent if and only if they have the same skeleton and v-structures. For a Gaussian X, we have $\mathbb{M}(G) = \mathbb{M}(H)$ if and only if G and H are Markov equivalent.

If G is a DAG then by [G] we denote the set of all DAGs Markov equivalent to G. There is another useful characterization of Markov equivalence proposed in [4], which describes elementary operations on DAGs that transform a DAG into a Markov equivalent DAG in such a way that G can be transformed to any graph in [G] by a sequence of these elementary operations. This elementary operation is given by flipping the arrow $i \to j$ whenever the pair i, j satisfies $\{i\} \cup \operatorname{Pa}(i) = \operatorname{Pa}(j)$. More specifically, given a DAG G over V, we say that an arrow $i \to j$ in G is covered if the graph H obtained from G by replacing $i \to j$ with $j \to i$ is also acyclic, and also $\operatorname{Pa}(i) = \operatorname{Pa}(j) \setminus \{i\}$. result of [4] states:

Theorem 4.2. We have $H \in [G]$ if and only if H can be obtained from G by a sequence of flips of covered arrows.

We say that H is CIS-Markov equivalent to G if $\mathbb{M}_+(G) = \mathbb{M}_+(H)$. We offer a similar characterization of CIS-Markov equivalence. An edge $i \to j$ is trivially covered if $\operatorname{Pa}(i) \cup \{i\} = \operatorname{Pa}(j) = \{i\}$.

Theorem 4.3. For a Gaussian X, we have $\mathbb{M}_+(G) = \mathbb{M}_+(H)$ if and only if H can be obtained from G by a sequence of flips of trivially covered arrows.

Note that when G is a complete DAG (with all possible $\binom{m}{2}$ edges), then $\mathbb{M}_+(G) = \mathrm{CIS}_{\sigma}$, where σ is the unique topological ordering of this DAG. This shows that Theorem 4.3 generalizes Proposition 3.3.

Proof. For the "if" part, it is enough to consider the case when H is obtained from G by a single flip of a trivially covered pair $i \to j$. By Theorem 4.2, $\mathbb{M}(G) = \mathbb{M}(H)$. Since i has no parents and it is the only parent of j, there is a permutation σ with $\sigma(1) = i$, $\sigma(2) = j$ that forms a topological ordering of G. Moreover, the permutation σ' obtained from σ by swapping i and j is a topological ordering of H. By Proposition 3.3, $\mathrm{CIS}_{\sigma} = \mathrm{CIS}_{\sigma'}$. By Theorem 2.5, $\mathbb{M}_+(G) = \mathbb{M}_+(H)$.

To show the "only if" part, first note that if $\mathbb{M}_+(G) = \mathbb{M}_+(H)$ then necessarily $\mathbb{M}(G) = \mathbb{M}(H)$. Via a contrapositive argument, suppose G and H are Markov equivalent but H is not obtained from G by a sequence of trivially covered edge flips. This means that there exists an arrow $i \to j$ in G and k with $k \in \operatorname{Pa}_G(i) \cap \operatorname{Pa}_G(j)$ such that $i \leftarrow j$ in H. To get a contradiction, it is enough to construct a distribution in $\mathbb{M}_+(G)$ such that in every CIS ordering j must come after i.

Let σ be a topological ordering of G. Without loss of generality assume $\sigma=\mathrm{id}$ and let i,j,k be as above. In particular, $1\leq k< i< j\leq m$. Let U be upper triangular such that $U_{ll}=1$ for all $l=1,\ldots,m,$ $U_{ij}=-1,$ $U_{kj}=-1$ and U is zero otherwise. Note that by the above, this U corresponds to a distribution in $\mathbb{M}_+(G)$ where some of the edges in G have zero coefficients. We will show that for any A containing $\{i,j,k\}$, neither i nor k can be the last one in a CIS ordering. To show this, note that $U_{A,A^c}=0,$ $U_{A^c,A}=0,$ and $U_{A^c,A^c}=I$. It follows that

$$(\Sigma_{A,A})^{-1} = U_{A,A} U_{A,A}^{\top}$$

and so $(\Sigma_{A,A})_{ik}^{-1} = 1 > 0$ showing that neither i nor k can be the last element in any CIS ordering of X_A . Using this recursively, starting from $A = \{1, \ldots, m\}$, we conclude that j must appear after i, k in every CIS ordering.

In Gaussian Bayesian networks the crucial observation is that if the Markov equivalence classes [G] and [H] are not equal then the Gaussian models $\mathbb{M}(G)$ and $\mathbb{M}(H)$ intersect at a measure zero set (we think about the geometry of these models as embedded in the space of covariance matrices). This means that for almost all ground-truth models we can learn the equivalence classes from the data. The analogous statement is unfortunately not true for CIS-Markov equivalence classes. For example, if m=3, the following two graphs lie in the same Markov equivalence class and different CIS-Markov equivalence classes



The intersection of $\mathbb{M}_+(G)$ and $\mathbb{M}_+(H)$ for these two graphs has full dimension and it contains the set of all inverse M-matrices.

Lemma 4.4. Suppose the distribution of X lies in $\mathbb{M}_+(G)$. Suppose that there exists k such that $i \to k \leftarrow j$ is a v-structure in G and suppose that $K_{ij} \neq 0$ (this holds generically). Then no CIS ordering of X finishes with i or j.

Proof. Without loss of generality assume that the trivial ordering $1 < 2 < \ldots < m$ is a topological ordering of G. In this case the matrix Λ in (1.1) is lower triangular. Then let $K = UU^{\top}$, with U upper triangular, be the precision matrix of X. By Remark 1.1 we have $U = (I - \Lambda)^{\top} D^{-1/2}$ and so for $i \neq j$ have $U_{uv} \leq 0$ if $u \to v$ in G and $U_{uv} = 0$ otherwise. We have

$$K_{ij} = \sum_{l} U_{il} U_{jl} = \sum_{l \in \operatorname{Ch}(i) \cap \operatorname{Ch}(j)} U_{il} U_{jl}.$$

This expresses K_{ij} as a sum of non-negative terms. Since this sum is non-zero by assumption, it must be strictly positive and so, neither i nor j can be the last ones in a CIS ordering.

As a corollary we get the following result.

Proposition 4.5. Consider a DAG G consising of k layers V_1, \ldots, V_k such that:

- (1) $V = V_1 \sqcup \cdots \sqcup V_k$,
- (2) only arrows from V_i to V_{i+1} are allowed in G,
- (3) $|V_i| \ge 2$ for all i = 1, ..., k-1 (only the last layer may contain one node),
- (4) every $v \in V_i$ for i = 1, ..., k-1 is contained in a v-structure (as a parent).

If the distribution of X lies in $\mathbb{M}_+(G)$ and $K_{ij} \neq 0$ unless $i, j \in V_k$ (this holds generically), then the only possible CIS orderings of X are $(V_1) \cdots (V_k)$, where the notation (V_i) means that the vertices in V_i can be ordered in an arbitrary way. In particular, any possible CIS ordering of X is a topological ordering of G.

5. Maximum likelihood estimation in $\mathbb{M}_+(G)$

In this section we show that maximum likelihood estimation in the model $\mathbb{M}_+(G)$ for a given G is straightforward and amounts to solving a convex optimization problem. Consider a Gaussian vector $X \sim \mathcal{N}_m(0, \Sigma)$ and let $K = \Sigma^{-1}$. Since K is positive definite, by [10, Corollary 3.5.6] we have that there exists a unique upper triangular matrix U whose diagonals are all 1, and a diagonal matrix D with strictly positive diagonals such that $K = UDU^{\top}$. Moreover, the relation between K and the pair (D, U) is one-to-one. Equivalently, we obtain the stochastic representation

$$X = \Lambda X + \varepsilon, \tag{5.1}$$

where $\Lambda = (I_m - U)^{\top}$ is lower triangular with zero diagonals, and $\varepsilon \sim \mathcal{N}_m(0, D^{-1})$.

Definition 5.1. Let $\mathcal{L}_i \subseteq \mathbb{R}^i$ be sets for each i = 1, ..., m-1. A Cholesky factor model consists of all Gaussian distributions such that the inverse-covariance matrix satisfies $K = UDU^{\top}$ with D a diagonal matrix and $U = (I_m - \Lambda)^{\top}$ with

$$\Lambda_i := (\Lambda_{i,1}, \dots, \Lambda_{i,i-1}) \in \mathcal{L}_{i-1}$$
 for $i = 2, \dots, m$.

Remark 5.2. In the case that $\mathcal{L}_i = [0, \infty)^i$, we recover the CIS model on X. If $\mathcal{L}_i = \mathbb{R}^i$ we simply have the space of all covariance matrices.

Remark 5.3. If the DAG G is known, we can always assume without loss of generality that the id permutation is a topological ordering of G. In other words, the matrix Λ in Remark 1.1 is lower triangular. Thus $\mathbb{M}(G)$ is a Cholesky factor model with the support of Λ_i equal to the parent set $\mathrm{Pa}(i)$. The model $\mathbb{M}_+(G)$ is obtained by additional non-negativity constraints.

If we want to make the constraints on Λ explicit we denote the model by $F(\mathcal{L}_1,\ldots,\mathcal{L}_{m-1})$. Maximum likelihood estimation for such models links to the problem of least squares estimation in linear regression as follows. Given n independent observations of X from this model, we stack them in the matrix $\mathbf{X} \in \mathbb{R}^{n \times m}$. We denote by $\mathbf{x}_1,\ldots,\mathbf{x}_m$ the columns of \mathbf{X} and by $\mathbf{Z}_i := \mathbf{X}_{[n],[i-1]}$ the $\mathbb{R}^{n \times (i-1)}$ matrix obtained from the first i-1 columns of \mathbf{X} .

Theorem 5.4. If $(\hat{D}, \hat{\Lambda})$ is the maximum likelihood estimator for a Cholesky factor model $F(\mathcal{L}_1, \ldots, \mathcal{L}_{m-1})$, then each $\hat{\Lambda}_i$ for $i = 2, \ldots, m-1$ is given as a minimizer of the quadratic problem

minimize
$$\frac{1}{n} \|\mathbf{x}_i - \mathbf{Z}_i \Lambda_i^\top\|^2$$
 subject to $\Lambda_i \in \mathcal{L}_{i-1} \subseteq \mathbb{R}^{i-1}$.

Moreover,

$$\hat{D}_{ii} = n \|\mathbf{x}_i - \mathbf{Z}_i \hat{\Lambda}_i^{\top}\|^{-2}$$

for all $i = 1, \ldots, m$.

Proof. We have $K = (I_m - \Lambda)^{\top} D(I_m - \Lambda)$, where Λ is strictly lower triangular with $\Lambda_i \in \mathcal{L}_{i-1}$ for i = 2, ..., m. As before, set $U = (I_m - \Lambda)^{\top}$. Since $\det(U) = 1$ and D is diagonal, the corresponding log-likelihood function $\log \det(K) - \frac{1}{n} \operatorname{tr}(\mathbf{X}^{\top} \mathbf{X} K)$ can be written as

$$\sum_{i=1}^{m} \log D_{ii} - \frac{1}{n} \sum_{i=1}^{m} D_{ii} ((\mathbf{X}U)^{\top} \mathbf{X}U)_{ii}.$$
 (5.2)

The expression $((\mathbf{X}U)^{\top}\mathbf{X}U)_{ii}$ is simply the squared-norm of the *i*-th column of $\mathbf{X}U$, which is equal to

$$\mathbf{x}_i - \sum_{j=1}^{i-1} \Lambda_{ij} \mathbf{x}_j = \mathbf{x}_i - \mathbf{Z}_i \Lambda_i^{\top}.$$

Thus, maximizing (5.2) is equivalent to minimizing

$$-\sum_{i=1}^{m} \log D_{ii} + \sum_{i=1}^{m} \frac{D_{ii}}{n} \|\mathbf{x}_{i} - \mathbf{Z}_{i} \Lambda_{i}^{\top}\|^{2}.$$
 (5.3)

The *i*-th squared term in (5.3) depends only on Λ_i . This means that minimizing (5.3) in a Cholesky factor model can be done term by term. Once the optimizer for Λ is found, D can be handled in a straightforward way.

Theorem 5.4 gives also a simple condition on the existence of the MLE.

Proposition 5.5. The MLE in Theorem 5.4 exists if and only if each set \mathcal{L}_i is closed and for every i = 1, ..., m-1,

$$\mathbf{x}_i \notin \{\mathbf{Z}_i \Lambda_i^\top : \Lambda_i \in \mathcal{L}_i\}.$$

In particular, if there are subsets $A_i \subseteq [i-1]$ such that $\mathcal{L}_i = \operatorname{span}\{\mathbf{x}_j : j \in A_i\}$, then the MLE exists with probability 1 as long as $n \geq \max_i |A_i|$.

It is now straightforward to compute the optimal value for the log-likelihood.

Corollary 5.6. If the MLE exists, then the optimal value of the log-likelihood is

$$-\sum_{i=1}^{m} \log \left(\frac{1}{n} \|\mathbf{x}_i - \mathbf{Z}_i \hat{\Lambda}_i^{\top} \|^2 \right) - m.$$

Recall that in the linear regression problem, given a vector $\mathbf{x}_i \in \mathbb{R}^n$ and the matrix $\mathbf{Z}_i \in \mathbb{R}^{n \times (i-1)}$, the least squares estimator is given precisely as the minimizer of $\|\mathbf{x}_i - \mathbf{Z}_i \theta\|^2$ over $\theta \in \mathbb{R}^{i-1}$. If this minimizer is unique, it is given by the well-known formula

$$\hat{\theta} = (\mathbf{Z}_i^{\top} \mathbf{Z}_i)^{-1} \mathbf{Z}_i^{\top} \mathbf{x}_i. \tag{5.4}$$

If \mathbf{Z}_i does not have full column rank, the optimum is obtained over an affine space. Replacing the inverse above with the pseudo-inverse gives the solution with the smallest norm. The following result follows almost immediately.

Proposition 5.7. If the constraints $\mathcal{L}_1, \ldots, \mathcal{L}_{m-1}$ are all linear, then the MLE $(\hat{D}, \hat{\Lambda})$ in the Cholesky factor model $F(\mathcal{L}_1, \ldots, \mathcal{L}_{m-1})$ can be given in closed form.

6. Finding a CIS ordering

Having established that the MLE can be easily computed in $\mathbb{M}_+(G)$ for any fixed G, we now explore the harder problem of estimating Σ knowing that the distribution of \mathbf{X} lies in $\mathbb{M}_+(G)$ for some G. By Theorem 2.5, $\mathbb{M}_+(G) = \mathbb{M}(G) \cap \mathrm{CIS}_{\sigma}$ for any topological ordering σ of G. Thus, if we know a topological ordering of G the problem can be solved by running regressions in the order given by σ and adding a LASSO penalty to learn a sparse representation. Using the fact that $\mathbb{M}_+(G) = \mathbb{M}(G) \cap \mathrm{CIS}_{\sigma}$ for any topological ordering σ of G, we do not need to search over all orderings but can restrict ourselves to CIS orderings for the underlying distribution. In this section, we show that these can be efficiently recovered.

6.1. Recovering a CIS ordering in the population case. In the following, we provide an algorithm that, given K, recovers a CIS ordering given that such an ordering exists. The algorithm is based on the following lemma.

Lemma 6.1. Suppose X is a CIS m-variate Gaussian. Suppose there exists $k \in [m-1]$ such that $K_{k, \setminus k} \leq 0$. Then $(X_1, \ldots, X_{k-1}, X_{k+1}, \ldots, X_m, X_k)$ is CIS.

Proof. Recalling Lemma 2.2, we have that X being a centered CIS ordered Gaussian is equivalent to

$$\mathbb{E}[X_j|X_{[j-1]}] = -\frac{\left(\Sigma_{[j],[j]}\right)_{j,[j-1]}^{-1}}{\left(\Sigma_{[j],[j]}\right)_{j,j}^{-1}} X_{[j-1]}$$

being a non-decreasing function in (X_1, \ldots, X_{j-1}) for all $j \in [m]$. We only need to check that the functions

$$\mathbb{E}[X_j|X_{[j-1]\setminus\{k\}}] \qquad j=k+1,\ldots,m, \tag{6.1}$$

$$\mathbb{E}[X_k|X_{\setminus k}]\tag{6.2}$$

are non-decreasing in their arguments, which, at least for the second function, follows automatically by the assumption $K_{k, \backslash k} \leq 0$. We now proceed by an induction argument starting from j=m working downward, to prove that the functions (6.1) are all non-decreasing in their arguments. We have

$$\mathbb{E}\left[X_m|X_{[m-1]\setminus\{k\}}\right] = -\frac{\left(\Sigma_{\setminus k,\setminus k}\right)_{m,[m-1]\setminus\{k\}}^{-1}}{\left(\Sigma_{\setminus k,\setminus k}\right)_{m,m}^{-1}}X_{[m-1]\setminus\{k\}},$$

then the Schur complement formula gives the following two statements:

$$\begin{split} \left(\Sigma_{\backslash k,\backslash k}\right)^{-1} &= K_{\backslash k,\backslash k} - \frac{K_{\backslash k,k}K_{k,\backslash k}}{K_{k,k}}, \\ \left(\Sigma_{[m-1],[m-1]}\right)^{-1} &= K_{[m-1],[m-1]} - \frac{K_{[m-1],m}K_{m,[m-1]}}{K_{m,m}}. \end{split}$$

By our assumption $K_{k,\backslash k} \leq 0$, we have that $\frac{K_{\backslash k,k}K_{k,\backslash k}}{K_{k,k}}$ is a non-negative rank-one matrix. Similarly, since X_m is the last in a CIS ordering of X, we have $K_{m,\backslash m} \leq 0$ and $\frac{K_{[m-1],m}K_{m,[m-1]}}{K_{m,m}}$ is a non-negative matrix. It follows then that

$$(\Sigma_{k,k})_{m,[m-1]\setminus\{k\}}^{-1} \le 0,$$

$$(\Sigma_{[m-1],[m-1]})_{k,[m-1]\setminus\{k\}}^{-1} \le 0.$$
(6.3)

The first inequality in (6.3) implies that the function in equation (6.1) for j=m is non-decreasing in its arguments. Our induction hypothesis is that for some $j^* \geq k+1$ we have shown for every $j=j^*+1,\ldots,m$, that

$$\left(\Sigma_{[j]\setminus\{k\},[j]\setminus\{k\}} \right)_{j,[j-1]\setminus\{k\}}^{-1} \le 0,$$

$$\left(\Sigma_{[j-1],[j-1]} \right)_{k,[j-1]\setminus\{k\}}^{-1} \le 0.$$
(6.4)

We will now prove that both of these inequalities are true for $j = j^*$ as well. By the second inequality in (6.4) (setting $j = j^* + 1$), and the fact that X is CIS ordered, we have that

$$(\Sigma_{[j^*],[j^*]})_{k,[j^*]\setminus\{k\}}^{-1} \le 0,$$

$$(\Sigma_{[j^*],[j^*]})_{j^*,[j^*-1]}^{-1} \le 0.$$
(6.5)

The Schur complement formula implies the following two equalities

$$(\Sigma_{[j^*]\setminus\{k\},[j^*]\setminus\{k\}})^{-1} = (\Sigma_{[j^*],[j^*]})_{[j^*]\setminus\{k\},[j^*]\setminus\{k\}}^{-1} - \frac{(\Sigma_{[j^*],[j^*]})_{[j^*]\setminus\{k\},k}^{-1}(\Sigma_{[j^*],[j^*]})_{k,k}^{-1}}{(\Sigma_{[j^*],[j^*]})_{k,k}^{-1}},$$

and

$$\begin{split} \left(\Sigma_{[j^*-1],[j^*-1]}\right)^{-1} &= \\ \left(\Sigma_{[j^*],[j^*]}\right)_{[j^*-1],[j^*-1]}^{-1} &- \frac{\left(\Sigma_{[j^*],[j^*]}\right)_{[j^*-1],j^*}^{-1} \left(\Sigma_{[j^*],[j^*]}\right)_{j^*,[j^*-1]}^{-1}}{\left(\Sigma_{[j^*],[j^*]}\right)_{j^*,j^*}^{-1}}. \end{split}$$

By the inequality of equation (6.5), it follows that

$$\begin{split} &\frac{\left(\Sigma_{[j^*],[j^*]}\right)_{[j^*]\backslash\{k\},k}^{-1}\left(\Sigma_{[j^*],[j^*]}\right)_{k,[j^*]\backslash\{k\}}^{-1}}{\left(\Sigma_{[j^*],[j^*]}\right)_{k,k}^{-1}} \geq 0,\\ &\frac{\left(\Sigma_{[j^*],[j^*]}\right)_{[j^*-1],j^*}^{-1}\left(\Sigma_{[j^*],[j^*]}\right)_{j^*,[j^*-1]}^{-1}}{\left(\Sigma_{[j^*],[j^*]}\right)_{j^*,j^*}^{-1}} \geq 0, \end{split}$$

from which the inequalities in equation (6.4) are proven for $j = j^*$. Given that the first inequality in equation (6.4) is equivalent to the function in (6.1) being non-decreasing in its arguments, we have proven the required result.

Lemma 6.1 allows us to find a row of the precision matrix K whose off-diagonals are non-positive and assume it is the last element of a CIS ordering. This is the basis of our algorithm.

Theorem 6.2. Suppose X is a centered multivariate Gaussian for which there exists a CIS ordering. Then the following procedure produces a permutation σ such that X_{σ} is CIS.

- (1) Initialize $O^{(1)} = [m]$ as the "leftover" set, $K^{(1)} = K$ as the current precision matrix, and $C^{(1)} = \{j : K_{j, \backslash j} \leq 0\}$ as the current candidate set.
- (2) For i = 1, ..., m, take an element of $k \in C^{(i)}$ and set $\sigma(m i + 1) = k$. Compute

$$\begin{split} O^{(i+1)} &= O^{(i)} \backslash \{k\}, \\ K^{(i+1)} &= \left(\Sigma_{O^{(i+1)},O^{(i+1)}} \right)^{-1}, \\ C^{(i+1)} &= \{j: K_{j,\backslash j}^{(i+1)} \leq 0\}. \end{split}$$

Proof. We must simply show that at each step $C^{(i)}$ is not empty, since at each step, the condition $K_{j,\backslash j}^{(i)} \leq 0$ is sufficient for the variable X_j to be a non-decreasing function in the variables X_v with $v \in O^{(i)} \setminus \{j\}$ by Lemma 2.2. This follows by existence of a CIS ordering along with Theorem 6.1. Indeed if a CIS ordering exists, then $C^{(1)} \neq \emptyset$, in which case, an arbitrary element of $C^{(1)}$ can be taken to be $\sigma(m)$. A simple induction argument shows that this is true for each $C^{(i)}$.

We illustrate this algorithm with an example.

Example 6.3. Consider the four dimensional Gaussian distribution with covariance and precision matrix

$$\Sigma = \begin{bmatrix} 1 & 0.75 & 0.50 & 0.14 \\ 0.75 & 1 & 0.81 & 0.50 \\ 0.50 & 0.81 & 1 & 0.75 \\ 0.14 & 0.50 & 0.75 & 1 \end{bmatrix}, \qquad K = \begin{bmatrix} 2.77 & -2.51 & 0 & 0.88 \\ -2.51 & 5.49 & -3.2 & 0 \\ 0 & -3.2 & 5.49 & -2.51 \\ 0.88 & 0 & -2.51 & 2.77 \end{bmatrix}.$$

The matrix K has two rows with only non-positive off-diagonal entries. We choose $i_1 = 2$ and consider the marginal distribution over $\{1, 3, 4\}$. The matrix

$$(\Sigma_{134})^{-1} = \begin{bmatrix} 1.61 & -1.47 & 0.88 \\ -1.47 & 3.62 & -2.51 \\ 0.88 & -2.51 & 2.77 \end{bmatrix}$$

has one row with nonpositive off-diagonal entries; so we take $i_2 = 3$. This shows that both (1,4,3,2) and (4,1,3,2) are CIS orderings. Beginning with $i_1 = 3$ shows that also (1,4,2,3) and (4,1,2,3) are CIS orderings and there are no other CIS orderings of X.

6.2. **Noisy CIS Recovery.** In the noisy setting, we are given a matrix of observations $\mathbf{X} \in \mathbb{R}^{n \times m}$ where the rows are i.i.d and distributed according to $\mathcal{N}_m(0, \Sigma)$, where Σ is such that the distribution admits a CIS ordering. As in Section 5, we let \mathbf{x}_t refer to the t-th column of \mathbf{X} . For any $i \in \{1, \ldots, m\}$ and any nonempty $A \subseteq \{1, \ldots, m\} \setminus \{i\}$, denote by $\beta^{(i,A)}$ the vector of coefficients of the linear regression of \mathbf{x}_i on $\mathbf{X}_{[n],A}$. Then we have that

$$\beta^{(i,A)} = \Sigma_{i,A} \Sigma_{A,A}^{-1}.$$

When $\beta^{(i,A)} \geq 0$, we say \mathbf{x}_i can be positively regressed on $\mathbf{X}_{[n],A}$. For $\alpha > 0$, an estimator $\hat{\beta}^{(i,A)}$ (we suppress *n*-dependence for ease) of $\beta^{(i,A)}$ is said to be n^{α} , consistent if

$$n^{\alpha}(\hat{\beta}^{(i,A)} - \beta^{(i,A)}) \to 0$$

in probability as $n \to \infty$. Our noisy CIS recovery algorithm presented in the Theorem below will mimic the method of the previous section by inspecting the entries of $\hat{\beta}^{(i,A)}$ at each step, assuming a bound on the entries of $\beta^{(i,A)}$.

Theorem 6.4. Assume that there exists a CIS ordering of the distribution $\mathcal{N}_m(0,\Sigma)$ and there exists an $\epsilon^* = \epsilon^*(\Sigma) > 0$ such that for any $i \in V$ and $A \subseteq V \setminus \{i\}$, either $\beta^{(i,A)}$ is a non-negative vector or $\min_j \beta_j^{(i,A)} < -2\epsilon^*$. For an $\alpha > 0$, let $\hat{\beta}^{(i,A)}$ be an n^{α} -consistent estimators of $\beta^{(i,A)}$ and let ϵ_n be a sequence such that $\epsilon_n \to 0$ while $n^{\alpha}\epsilon_n \to \infty$.

We define an estimator $\hat{\sigma}$ through the following algorithm:

- (1) Initialize $A_1 = [m]$ to be the set of active variables and set t = 1.
- (2) If $t \leq m-2$, for each $i \in \mathcal{A}_t$, we compute $\hat{\beta}^{(i,\mathcal{A}_t\setminus\{i\})}$. At the first instance³ of i^* such that all entries of $\hat{\beta}^{(i^*,\mathcal{A}_t\setminus\{i^*\})}$ are greater than $-\epsilon_n$ we define

$$\hat{\sigma}(m-t+1) = i^*.$$

Define $A_{t+1} = A_t \setminus \{i^*\}$ and increment t and repeat this step until t = m-1.

(3) When t = m - 1 it must be that $|A_t| = 2$, in which case, we take $\hat{\sigma}(1)$ and $\hat{\sigma}(2)$ to be arbitrary.

As $n \to \infty$, $\hat{\sigma}$ will be a valid CIS ordering of $\mathcal{N}_m(0,\Sigma)$ with probability going to 1.

Proof. Depending on the sample size n, consider the event

$$\mathcal{E}^{(n)} = \bigcap_{i,A} \mathcal{E}^{(n)}_{i,A}, \qquad \mathcal{E}^{(n)}_{i,A} := \{ \|\hat{\beta}^{(i,A)} - \beta^{(i,A)}\|_{\infty} < \epsilon_n \}.$$
 (6.6)

By n^{α} -consistency of the estimators and the fact that $n^{\alpha} \epsilon_n \to \infty$, $\mathbb{P}(\mathcal{E}^{(n)}) \to 1$ as $n \to \infty^4$. Note that, by the definition of ϵ^* and the fact that $\epsilon_n < \epsilon^*$ if n is sufficiently large, conditionally on $\mathcal{E}^{(n)}$, this is equivalent to the fact that \mathbf{x}_i can be positively regressed on $\mathbf{X}_{[n],A}$. More specifically, let R_t for $t = 1, \ldots, m-3$, be the event that says that at the t-th step of the algorithm:

- (a) $\mathbf{X}_{[n],\mathcal{A}_t}$ admits a CIS ordering,
- (b) the algorithm correctly finds an \mathbf{x}_i that can be positively regressed on $\mathbf{X}_{[n],\mathcal{A}_t\setminus\{i\}}$.

³In practice we could score different potential choices to further improve the power of the method.

⁴Indeed if A_n , B_n are sequences of events such that $\mathbb{P}(A_n) \to 1$ and $\mathbb{P}(B_n) \to 1$ then $\mathbb{P}(A_n \cap B_n) \to 1$ simply because $\mathbb{P}((A_n \cap B_n)^c) = \mathbb{P}(A_n^c \cup B_n^c) \leq \mathbb{P}(A_n^c) + \mathbb{P}(B_n^c) \to 0$.

Note that (a) is automatically satisfied if t=1. Similarly, for an arbitrary t, (a) holds automatically conditionally on $R_1 \cap \ldots \cap R_{t-1}$, by Theorem 6.1. The probability of recovering a CIS ordering is $\mathbb{P}(R_1 \cap \ldots \cap R_{m-3})$ and we have

$$\mathbb{P}(R_1 \cap \ldots \cap R_{m-3}) = \mathbb{P}(R_1)\mathbb{P}(R_2|R_1)\cdots\mathbb{P}(R_{m-3}|R_1 \cap \ldots \cap R_{m-4}).$$

Denote $\mathbb{P}^{(n)}(\cdot) = \mathbb{P}(\cdot|\mathcal{E}^{(n)})$. We also have

$$\mathbb{P}^{(n)}(R_1 \cap \ldots \cap R_{m-3}) = \mathbb{P}^{(n)}(R_1)\mathbb{P}^{(n)}(R_2|R_1)\cdots\mathbb{P}^{(n)}(R_{m-3}|R_1 \cap \ldots \cap R_{m-4}).$$

As we said earlier, after conditioning on $\mathcal{E}^{(n)}$, X_i can be positively regressed on X_A if and only if all coefficients of $\hat{\beta}^{(i,A)}$ are greater than $-\epsilon$. This means that

$$\mathbb{P}^{(n)}(R_1) = \mathbb{P}^{(n)}(R_2|R_1) = \cdots = \mathbb{P}^{(n)}(R_{m-3}|R_1 \cap \ldots \cap R_{m-4}) = 1$$

implying that $\mathbb{P}^{(n)}(R_1 \cap \ldots \cap R_{m-3}) = 1$. This implies that $\mathbb{P}(R_1 \cap \ldots \cap R_{m-3}) \to 1$ as $n \to \infty^5$, which completes the proof.

Remark 6.5. The event $\mathcal{E}^{(n)}$ in (6.6) may have small probability for finite sample sizes. However, for the proof it is not necessary to define $\mathcal{E}^{(n)}$ as an intersection over all pairs (i, A). For example, it is sufficient to include only the pairs (i, A) such that $\mathbf{X}_{[n], A \cup \{i\}}$ admits a CIS ordering but \mathbf{x}_i cannot be positively regressed on $\mathbf{X}_{[n], A}$ (if Σ is an inverse M-matrix then there are no such pairs).

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⁵Indeed, if A_n, B_n are sequences of events such that $\mathbb{P}(A_n|B_n) = 1$ and $\mathbb{P}(B_n) \to 1$ then $\mathbb{P}(A_n \cap B_n) = \mathbb{P}(B_n) \to 1$. Since $\mathbb{P}(A_n) \ge \mathbb{P}(A_n \cap B_n)$, then also $\mathbb{P}(A_n) \to 1$.

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