Identifiability of AMP chain graph models

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Abstract
We study identifiability of Andersson-Madigan-Perlman (AMP) chain graph models, which are a common generalization of linear structural equation models and Gaussian graphical models. AMP models are described by DAGs on chain components which themselves are undirected graphs.

For a known chain component decomposition, we show that the DAG on the chain components is identifiable if the determinants of the residual covariance matrices of the chain components are monotone non-decreasing in topological order. This condition extends the equal variance identifiability criterion for Bayes nets, and it can be generalized from determinants to any super-additive function on positive semidefinite matrices. When the component decomposition is unknown, we describe conditions that allow recovery of the full structure using a polynomial time algorithm based on submodular function minimization. We also conduct experiments comparing our algorithm’s performance against existing baselines∗.

1 Introduction

Probabilistic graphical models offer architectures for modeling and representing uncertainties in decision making. From a computational standpoint, graphical representations enable efficient algorithms for inference, e.g., message passing, loopy belief propagation, and other variational inference methods [Kschischang et al., 2001]. They have found applications in a wide range of domains, e.g., image processing, natural language processing and computational biology; see [Lauritzen, 1996, Koller and Friedman, 2009, Wainwright and Jordan, 2008] and references therein for examples.

A typical application of graphical models is to encode causal information. An influential article by Pearl [1995] elucidated how Bayesian networks can be used to represent causal processes and allow identification of causal effects. Bayesian networks are directed acyclic graphs (DAGs) in which the nodes represent variables of interest. Each node has a functional dependency on its parents, as determined by the graph. A popular way to substantiate Bayesian networks is as a linear structural equation model (SEM) where variables that correspond to nodes in the graph are a linear function of their parents’ values plus additive independent noise (often Gaussian) [Bollen, 1989, Spirtes et al., 2000b]. Hoyer et al. [2008] defined the more general additive noise model where each node is an arbitrary function of its parents with an additive independent noise.

While Bayesian networks offer a clear conceptual way to model the causal structure of a system, they are in practice very hard to infer from data, as they require knowledge of how every single variable is generated. In applications involving hundreds of variables (e.g., in computational biology), this requirement is unreasonable, particularly because at the end, we may only be interested in causal effects on a few target variables. Furthermore, in SEMs modeled by Bayesian networks, the noise terms of different variables must be independent whereas in real-world systems, correlations can arise for various reasons (e.g., latent confounders). An interesting middle ground is the notion of chain graphs [Lauritzen and Wermuth, 1989a]. Here, the variable set is partitioned into chain components, and there is a DAG on these chain components. The variables inside each chain component, however, are connected by undirected edges, not directed ones. See Figure 1 for an illustration. Thus, chain graph models interpolate between directed (causal) models and undirected (probabilistic) models.

There are several prevalent interpretations of chain graph models, namely the Lauritzen-Wermuth-Frydenberg (LWF) [Lauritzen and Wermuth, 1989a, Frydenberg, 1990], Alternative Markov Property or
Figure 1: Chain graphs. Each shaded region is a maximal chain component.

Andersson-Madigan-Perlman (AMP) [Andersson et al., 2001], and Multivariate Regression (MVR) [Cox and Wermuth, 1993]. They differ in the conditional independence relations implied by the graphical structure. In this work, we restrict ourselves to the AMP interpretation, which is the most natural one from a generative viewpoint. Let $C$ be an AMP chain graph on $n$ nodes. Suppose the nodes are partitioned into chain components $\{\tau\}$. Then, we say that a random variable $X \in \mathbb{R}^n$ is generated by $C$ if for every chain component $\tau$:

$$X_\tau = M_\tau X_{\text{Pa}(\tau)} + Z_\tau$$

(1.1)

where $X_\tau$ is $X$ restricted to $\tau$, $\text{Pa}(\tau) = \{v : \exists u \in \tau, v \rightarrow_C u\}$, $M_\tau$ is a matrix satisfying:

$$(M_\tau)_{uv} \neq 0 \implies v \rightarrow_C u,$$

and $Z_\tau$ is an independent multivariate Gaussian drawn from $N(0, \Sigma_\tau)$ where $\Sigma_\tau$ satisfies:

$$(\Sigma_\tau^{-1})_{uv} \neq 0 \implies u \not\rightarrow_C v$$

The last condition ensures that $N(0, \Sigma_\tau)$ is Markovian with respect to the undirected induced subgraph $C_\tau$ on $\tau$. One may also consider the additive noise AMP formulation where each

$$X_\tau = f_\tau(X_{\text{Pa}(\tau)}) + Z_\tau,$$

(1.2)

the noise $Z_\tau$ is as above, and the function $f_\tau$ is arbitrary, provided it satisfies the directed graph structure:

$$\frac{\partial f_\tau}{\partial X_v} \neq 0 \implies v \rightarrow_C u.$$
(a) Additive noise AMP with known chain component decomposition: We give a general class of identifiability conditions (generalizing the equal variance condition for linear SEMs) that imply identifiability of the DAG on a known collection of chain components. For instance, the DAG is identifiable if the determinant of the conditional covariance of a chain component $\tau$ given $\tau$’s parents is the same for all $\tau$. More generally, it is sufficient for this determinant to be monotonically non-decreasing with respect to a topological order on the chain components. The same is true if the trace or the permanent satisfies the monotonicity condition.

(ii) AMP with unknown chain component decomposition: We give an identifiability condition for recovering the chain components as well as the DAG for the standard AMP chain graph model. Informally, the requirement is quite natural: the variables in each chain component should be tightly correlated, while as a whole, each chain component should have large variance conditioned on its parents. More formally, the conditions are that:

(a) If $S$ is a proper subset of a chain component $\tau$:
\[
\det(\text{Cov}(X_S | X_{S \setminus \tau}, X_{Pa(\tau)})) < 1
\]

(b) $\det(\text{Cov}(X_\tau | X_{Pa(\tau)}))$ is greater than 1 and monotonically non-decreasing with a topological order on the chain components $\tau$.

In our conditions, the determinant of the covariance matrix of Gaussians plays a central role, and this is for good reason. If $X \sim N(0, \Sigma)$ is an $n$-dimensional Gaussian, then $\det(\Sigma)$ is the generalized variance of $X$ and is related to its differential entropy. Namely, the differential entropy of $X$ is $\frac{1}{2}(\log \det(\Sigma) + n \log(2\pi e))$; see, e.g., Krause et al. [2008], Yu [2015]. So, one can interpret condition (a) above as: If $S$ is a proper subset of $\tau$, its differential entropy conditioned on $\tau$ and $\tau$’s parents is smaller than a threshold. Similarly, the first part of condition (b) can be restated as: If $S$ equals $\tau$, the differential entropy of $S$ conditioned on its parents is larger than a threshold.

These identifiability conditions come with polynomial time algorithms. Notably, our algorithm for recovering the chain components in (ii) above involves a non-trivial submodular function minimization, in contrast to the more straightforward algorithms known for identifying linear SEMs and Bayesian networks [Park, 2020, Gao et al., 2020] under analogous conditions.

1.1 Technical Overview

In this section, we describe some of the intuition behind our identifiability conditions.

Known chain components. Consider Figure 2 which shows two chain graphs $C_1$ and $C_2$; the question is to determine which of these graphs is generating a given joint distribution $(X_1, X_2, X_3)$. In $C_1$, let $\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim N(0, \Sigma_1)$, and $X_3 = \beta_1 X_1 + Z$, where $\beta_1 \neq 0$ and $Z \sim N(0, \sigma^2)$. In $C_2$, let $\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} \beta_2 \\ 0 \end{pmatrix} X_3 + Z$ where $\beta_2 \neq 0$, $Z \sim N(0, \Sigma_2)$ and $X_3 \sim N(0, \sigma^2)$. Assume $\text{Det}(\Sigma_1) = \text{Det}(\Sigma_2) = \sigma^2$, so that in both models, the determinant of the covariance of each chain component conditioned on its parents is $\sigma^2$.

We claim that in this case, one can distinguish between $C_1$ and $C_2$ based on the generated distribution. Our algorithm first finds the chain component $\tau$ minimizing $\det(\text{Cov}(X_\tau))$. Note that for $C_1$, using the
independence of $Z$:  
\[
\text{Cov}(X_3) = \text{Cov}(\beta X_1 + Z) = \beta^2 \text{Cov}(X_1) + \text{Cov}(Z) > \text{Cov}(Z),
\]
assuming\footnote{In this work, we make the assumption everywhere that all covariance matrices are strictly positive definite.} that $\text{Cov}(X_1) > 0$. Hence, $\det(\text{Cov}(X_3)) > \det(\text{Cov}(X_2))$. On the other hand for $C_2$, $\det(\text{Cov}(X_2)) > \sigma^2 = \det(\text{Cov}(X_1))$. Thus, the chain component with the smallest determinant of the covariance can be identified as the first in a topological ordering. This can be understood as the uncertainty level of the parents is less than its children. Once the first chain component is known, we can select the second by choosing the one that minimizes the determinant of its covariance conditioned on the first chain component, and so on. It suffices to find the topological order because as described in Appendix A of Gao et al. [2020], one can identify the directed edges by standard variable selection methods.

Note that the only property we used of the determinant is that $\det(A + B) > \det(A)$ if $B$ is strictly positive definite. This property holds not only for the determinant but for many natural matrix functions. For example for any $i$, the diagonal entries $(A + B)_{ii} > A_{ii}$ when $A$ and $B$ are positive definite. Carrying out the same logic as above but now using projection to diagonal entries instead of determinants implies that the chain component DAG is identifiable when all the individual variables have equal variance, extending the result of Peters and Bühlmann [2014] to chain graphs. In fact, there is a large class of functions called “generalized matrix functions” that satisfy the desired super-additivity condition and hence result in identifiability conditions for the DAG on chain components.

**Unknown chain components.** Consider again $C_1$ from Figure 2, but suppose now that we do not have the chain component partitioning. Let $(X_1, X_2, X_3)$ be generated as described above. In addition to imposing the condition that $\det(X_1) = \sigma^2$, we now also require that: (i) $\det(\text{Cov}(X_1 | X_2))$ and $\det(\text{Cov}(X_2 | X_1))$ are\footnote{\text{det}(\text{Cov}(X_2 | X_1)) is well defined, since $(X_1, X_2)$ are jointly Gaussian, and hence, for any choice of $x_1$, $\text{Cov}(X_2 | X_1 = x_1)$ is the same.} strictly less than 1, and (ii) $\sigma^2$ is strictly greater than 1.

Now, we can show that  
\[
\det(\text{Cov}(X_2)) = \min_{S \subseteq \{1,2,3\}} \det(\text{Cov}(X_S)).
\]
Observe that $\det(\text{Cov}(X_3)) > \det(\text{Cov}(X_2))$ already follows from the earlier discussion. We now compare $\det(\text{Cov}(X_2))$ to $\det(\text{Cov}(X_1))$ and $\det(\text{Cov}(X_3))$. We use the fact that:  
\[
\det(\text{Cov}(X_2)) = \det(\text{Cov}(X_1)) \cdot \det(\text{Cov}(X_2 | X_1)).
\]
This follows from standard facts about multivariate Gaussians. From our assumption $\det(\text{Cov}(X_2 | X_1)) < 1$, we get that $\det(\text{Cov}(X_1)) > \det(\text{Cov}(X_2))$. The same holds for $\det(\text{Cov}(X_3))$. Finally, we need to show that $\det(\text{Cov}(X_123)) > \det(\text{Cov}(X_2))$. Again, we can invoke the above fact:  
\[
\det(\text{Cov}(X_123)) = \det(\text{Cov}(X_2)) \cdot \det(\text{Cov}(X_3 | X_12)).
\]
Our conclusion follows from the assumption $\sigma^2 > 1$.

For a general chain graph, it similarly follows that the non-empty set $S$ minimizing $\det(\text{Cov}(X_S))$ is the topologically smallest. We can identify the next component by conditioning on the components already discovered, which results in a Gaussian on the rest, and then finding a non-empty subset with conditional covariance matrix of smallest determinant. This algorithm can be implemented efficiently. The reason is that for any positive definite $n \times n$-matrix $M$, the function $F(S) = \log \det(M[S, S])$, where $M[S, S]$ is the submatrix on rows and columns indexed by $S \subseteq [n]$, is submodular. $F$, as noted earlier, corresponds to the differential entropy of a Gaussian vector with covariance $M$, which is a submodular function, plus an additional modular term. The problem of submodular function minimization has a long and rich history, beginning with the seminal works of Grötschel et al. [1981, 2012] and continuing to the current day [Iwata et al., 2001, Schrijver, 2000, Lee et al., 2015, Dadush et al., 2018, Jiang, 2021]. Thus, we can invoke any of these known polynomial-time algorithms for submodular function minimization to recover the chain components in topological order.
1.2 Related Work

Chain graph models contain both directed and undirected edges and can be used to represent both association and causation in real-world applications [Sonntag, 2016]. The three following interpretations are the best known in the literature: LWF [Lauritzen and Wermuth, 1989b, Wermuth and Lauritzen, 1990, Frydenberg, 1990] which generalizes both Markov random fields and Bayesian networks; AMP [Andersson et al., 2001, 2006] which directly extends the DAG Markov property; and MVR [Cox and Wermuth, 1993, 2014] which originates from viewing undirected edges as representing hidden common causes.

The literature on learning pure DAG models is vast. One popular approach is to exploit the constraints imposed by Markov structure, e.g., the PC algorithm and its variants, like Fast Causal Inference (FCI), Really Fast Causal Inference (RFCI) and Cyclic Causal Discovery (CCD) [Spirtes et al., 2000a,b, Richardson, 2013, Colombo et al., 2011, Tom Claassen and Smyth, 2013, Harris and Drton, 2013, Colombo and Maathuis, 2014]. Another important class of algorithms aims to maximize a score function over the space of DAG’s, such as Greedy Equivalence Search (GES) [Chickering, 2002, Ramsey et al., 2017, Nandy et al., 2018] and a recent line of work that formulates score maximization as a continuous optimization problem (e.g., [Zheng et al., 2018, 2020, Wei et al., 2020]). This latest direction has resulted in algorithms that learn the DAG structure with deep learning methods (e.g., Yu et al. [2019], Lachapelle et al. [2020], Wang et al. [2020]).

A probability distribution may be Markov with respect to many Bayes networks; so for exact identifiability, one needs to impose more structural constraints on the DAG model. For Structural Equation Models (SEM’s), identifiability can be established by leveraging asymmetries between variable pairs Shimizu et al. [2006], Mooij et al. [2016], restricting SEMs to having additive noise, such as linear non-Gaussian acyclic model (LiNGAM) [Shimizu et al., 2006], general additive noise models [Peters et al., 2014], Post-nonlinear model (PNL) [Zhang et al., 2016], or equal and unknown error variance [Peters and Bühlmann, 2014, Ghoshal and Honorio, 2017, Eberhardt, 2017, Ghoshal and Honorio, 2018, Chen et al., 2019, Glymour et al., 2019, Park and Kim, 2020, Park, 2020, Guo et al., 2020].

AMP chain graphs, our focus in this work, have been less widely studied than pure DAG models and more in the statistics literature than computer science. Informally speaking, Peña [2015] showed that any AMP model can be viewed as arising from a DAG causal model subject to selection bias. Levitz et al. [2001] introduced a pathwise separation criterion to characterize conditional independence relations in AMP chain graphs. Roverato [2005], Studený et al. [2009], Peña [2017a] studied the equivalence classes of chain graph models, and [Peña, 2018] provided a factorization for positive distributions that are Markov with respect to an AMP chain graph. Drton et al. [2009] showed that the AMP conditional independence relations may lead to non-smooth models for discrete variables. Peña [2014b, 2016] investigated extensions to the AMP model, e.g., the marginal AMP model (MAMP) that is a common generalization of AMP and MVR. When the chain graph structure is known, Drton and Eichler [2006] proposed an algorithm for maximum likelihood estimation of the model parameters. Peña [2012, 2014a], Peña and Gomez-Olmedo [2016] proposed PC-LIKE, a constraint based algorithm under faithfulness assumptions for learning the structure of AMP and MAMP models. Peña also designed a score-based algorithm for AMP model structure learning similar to the work on additive noise models [Peña, 2017b] and an algorithm based on answer set programming [Peña, 2016]. Recently, Javidian et al. [2020] solved the problem of efficiently finding minimal separating sets in AMP chain graphs and obtained a new decomposition-based structure learning algorithm called Lcd-AMP.

2 Notations and Preliminaries

**Probability.** We need the following useful fact about conditional covariance. The proof is a simple generalization of the standard proof for law of total variance.

**Fact 2.1** (Law of Conditional Covariance). If $X, Y, Z$ are random variables with strictly positive distributions with each component having finite second moment, then:

$$
\text{Cov}(X | Y) = \mathbb{E}[\text{Cov}(X | Y, Z) | Y] + \text{Cov}(\mathbb{E}[X | Y, Z] | Y).
$$

The following result yields a very useful decomposition for covariance of normal distributions.
Fact 2.2. If \( X = (X_A, X_B) \) is distributed jointly as a Gaussian \( N(0, \Sigma) \), then:

\[
\text{det}(\text{Cov}(X)) = \text{det}(\text{Cov}(X_A)) \cdot \text{det}(\text{Cov}(X_B | X_A))
\]

where \( \text{Cov}(X_B | X_A) = \text{Cov}(X_B | X_A = x_A) \) is independent of \( x_A \).

Proof. It is well-known that if \( \text{Cov}(X) = \begin{pmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{pmatrix} \):

\[
\text{Cov}(X_A) = \Sigma_{AA} \quad \text{Cov}(X_B | X_A) = \Sigma_{BB} - \Sigma_{BA} \Sigma_{AA}^{-1} \Sigma_{AB}
\]

On the other hand, it follows from the properties of Schur complement that: \( \text{det}(\Sigma) = \text{det}(\Sigma_{AA}) \cdot \text{det}(\Sigma_{BB} - \Sigma_{BA} \Sigma_{AA}^{-1} \Sigma_{AB}) \). The result follows. \( \square \)

Chain Graphs. Following conventions in the field, a variable is denoted by an uppercase letter, e.g., \( X \), and its value is denoted by the corresponding lowercase letter, \( x \). The state space of \( X \) is \( \mathbb{Z} \). Graphs in this paper contain both directed (‘\( \to \)’) and undirected (‘\( \to \)’) edges. Below we will further invoke the most central definitions and notations used in this paper. For a general account, we refer the reader to Lauritzen [1996] and Edwards [2012].

A chain graph \( C \) consists of a vertex set \( V \) and an edge set \( E \in V \times V \). A path in \( C \) is a sequence of distinct vertices \( < v_0, \ldots, v_n > \) such that \( v_{i-1} \) and \( v_i \) are adjacent for all \( 1 \leq i \leq k \), and is called a cycle if \( v_n = v_0 \). Moreover, a semi-directed cycle exists if \( v_1 \to v_2 \) is in \( C \) and \( v_i \to v_{i+1}, v_i \leftarrow v_{i+1} \) or \( v_i \to v_{i+1} \) is in \( C \) for all \( 1 \leq i < n \). Chain graph \( C \) is a graph has no semi-directed cycles. Two vertices joined by an edge are called adjacent. For vertices \( u, v \in E \) but \( (v, u) \not\in E \), we write \( u \to v \), where vertex \( u \) is a parent of \( v \). If both \( (u, v) \in E \) and \( (v, u) \in E \), we denote it by \( u \sim v \), which means \( u \) is a neighbor of \( v \). The vertex set of a chain graph can be partitioned into chain components \( \tau \mid \tau \in \mathcal{T}, (V = \cup_{\tau \in \mathcal{T}} \tau) \). Edges within chain components are undirected whereas edges between two chain components are directed. For any subset \( S \), the set of parents of \( v \) is denoted as \( \text{Pa}(v) := \{ v \in V \mid S \mid v \to s \in \mathcal{C} \text{ for some } s \in S \} \), the set of children of \( v \) is denoted as \( \text{Ch}(v) := \{ v \in V \mid S \mid s \to v \in \mathcal{C} \text{ for some } s \in S \} \), the set of neighbors is denoted as \( \text{Ne}(v) := \{ v \in V \mid S \mid v \sim s \in \mathcal{C} \text{ for some } s \in S \} \). A chain graph with no directed edges is an undirected graph (UG), while a chain graph with no undirected edges is a DAG. If there exists a directed path between chain components \( k \to \cdots \to j \), then \( k \) is an ancestor of its descendant \( j \). The set of ancestors and descendants are denoted as \( \text{An}(j) \) and \( \text{De}(k) \). A source node is any node \( X_r \) such that \( \text{Pa}(X_r) = \emptyset \). A sink node is any node \( X_s \) such that \( \text{Ch}(X_s) = \emptyset \). Ancestral set is any set \( A \in V \) such that \( X_r \in A \Rightarrow \text{Pa}(r) \in A \). The chain components \( \tau \) of a chain graph are the connected components of the undirected graph obtained by removing all directed edges from the chain graph. In a DAG, all chain components are singletons. For \( S \subseteq V \), \( C_S \) denotes the induced subgraph on \( S \).

By taking into account the directed connections of chain components, AMP-chain graphs admits a topological ordering of its chain components. For statistical identifiability of chain graph \( C \), we will consider it sufficient to learn the partition into chain components \( \tau_1, \ldots, \tau_i \), and a topological ordering \( < \) such that \( \tau_j \to \tau_k \implies \tau_j < \tau_k \). One can learn the directed and undirected edges using standard parameter estimation algorithms.

Matrix Algebra. Our identifiability condition in the case of known chain components is in terms of positive and super-additive families, which we define next.

Definition 2.3. Let \( \mathbb{C}_n \) denote the cone of \( n \times n \) positive semidefinite matrices. We say that a real-valued function \( d_n : \mathbb{C}_n \to \mathbb{R} \) is positive and super-additive if: (i) \( d_n(A) > 0 \) for all positive definite matrices \( A \), and (ii) for all positive semidefinite matrices \( A, B \):

\[
d_n(A + B) \geq d_n(A) + d_n(B).
\]

A positive and super-additive family is a collection of functions \( f_n : \mathbb{C}_n \to \mathbb{R} \), each of which is positive and super-additive.

We have several examples of families of positive and super-additive functions:
Clearly, the projection on any diagonal element and the matrix trace function are positive and super-additive.

By Minkowski’s determinant theorem (see, e.g., Marcus and Minc [1992]), it is known that for all \( A, B \in \mathbb{C}^n \):
\[
(\det(A + B))^{1/n} \geq (\det(A))^{1/n} + (\det(B))^{1/n}.
\]
Hence, \( \{\det^{1/n} : \mathbb{C}_n \to \mathbb{R}\} \) is positive and super-additive.

For \( \chi \) an irreducible character on a subgroup \( H \) of \( S_n \) (the permutation group on \( n \) elements), define the generalized matrix function with respect to \( H \) and \( \chi \) as:
\[
d_H^\chi(A) = \sum_{\sigma \in H} \chi(\sigma) \prod_{i=1}^n a_{i,\sigma(i)}
\]
where \( A = (a_{i,j}) \). Schur [1918] showed that \( d_H^\chi(A) > 0 \) for all positive definite \( A \). It is also known (e.g., Merris [1997], p. 228) that they satisfy the super-additivity condition. Hence, the determinant, permanent, and the Hadamard matrix function (product of diagonal entries) all form positive and super-additive families.

### 3 Identifiability with known chain component decomposition

In this section, we give a general class of conditions which are sufficient to ensure that the DAG structure of the chain graph is identifiable from data generated by it. Here, the chain component decomposition \( \mathcal{D} \) is already known to the algorithm. \( \mathcal{D} \) consists of \( t \) disjoint maximal chain components that partition the variable set.

We formulate our results for general AMP chain graph models. They will immediately imply the conditions for additive noise AMP models mentioned in the Introduction.

**Algorithm 1:** Our algorithm for learning the topological order of a chain graph with chain component decomposition \( \mathcal{D} \) of size \( t \).

1. \( A, P \leftarrow \emptyset \);
2. \( i \leftarrow 0 \);
3. while \( |A| \neq t \) do
   4. \( \tau_i \leftarrow \arg \min_{\tau \in \mathcal{D}\setminus A} d_{\chi}(\text{Cov}(X_{\tau} | X_P)) \);
   5. \( A \leftarrow A \cup \{\tau_i\} \);
   6. \( P \leftarrow P \cup \tau_i \);
   7. \( i \leftarrow i + 1 \);
4. Return the ordering \((\tau_1, \ldots, \tau_t)\)

**Theorem 3.1.** Suppose the random variable \( X \) is generated by an AMP-CG \( \mathcal{C} \) with known chain component decomposition \( \mathcal{D} \). Then, \( \mathcal{C} \) is identifiable from \( P \) if there exists a topological ordering \( \pi \) of \( \mathcal{C} \) and a positive and super-additive family \( \{d_n : \mathbb{C}_n \to \mathbb{R}\} \) such that:
\[
d_{|\tau|} \left( \mathbb{E}_{X_{\text{Pa}(\tau)}} \text{Cov}(X_{\tau} | X_{\text{Pa}(\tau)}) \right) \leq d_{|\tau'|} \left( \mathbb{E}_{X_{\text{Pa}(\tau')}} \text{Cov}(X_{\tau'} | X_{\text{Pa}(\tau')}) \right)
\]
for any two chain components \( \tau, \tau' \) where \( \tau \prec_\pi \tau' \).

**Proof.** We show that Algorithm 1 recovers the chain graph under the assumptions of the Theorem 3.1. This follows immediately from the following lemma, as it shows that at every step \( i \), the algorithm chooses as \( \tau_i \) a chain component whose parents are contained in the current \( A \).

\(^1\)The super-additivity of the determinant is also directly implied by the super-additivity of \( \det^{1/n} \).
Lemma 3.2. Let \( A \) be an ancestral set of chain components, and let \( P = \{ v : v \in \tau \in A \} \). Assume the condition (3.1) above. Suppose \( \tau_1 \) and \( \tau_2 \) are chain components in \( D \setminus A \) such that \( Pa(\tau_1) \subseteq A \) but \( Pa(\tau_2) \not\subseteq A \). Then:

\[
d_{|\tau_1|} \left( \mathbb{E} \frac{\text{Cov}(X_{\tau_1} | X_P)}{X_P X_{\tau_1}} \right) > d_{|\tau_2|} \left( \mathbb{E} \frac{\text{Cov}(X_{\tau_2} | X_P)}{X_P X_{\tau_2}} \right)
\]

Proof. Note that \( \tau_1 \) must precede \( \tau_2 \) in the topological ordering \( \pi \), and hence (3.1) holds with \( \tau = \tau_1 \) and \( \tau' = \tau_2 \). We invoke the law of conditional covariances (Fact 2.1).

\[
\mathbb{E} \frac{\text{Cov}(X_{\tau'} | X_P)}{X_P X_{\tau'}} = \mathbb{E} \frac{\text{Cov}(X_{\tau'} | X_P, X_{Pa(\tau')}) | X_P} + \mathbb{E} \frac{\text{Cov}(X_{\tau'} | X_P, X_{Pa(\tau')}) | X_P} \]

\[
= \mathbb{E} \frac{\text{Cov}(X_{\tau'} | X_P, X_{Pa(\tau')}) | X_P} + \mathbb{E} \frac{\text{Cov}(X_{\tau'} | X_P, X_{Pa(\tau')}) | X_P} \]

The second equality follows from the fact that \( X_{\tau'} \) is independent of \( X_P \), conditioned on \( X_{Pa(\tau')} \). Now, note that the second term in the last line above is positive definite if \( P \) does not contain \( Pa(\tau') \). Therefore, using the fact that \( d_{|\tau|} \) is positive and super-additive:

\[
d_{|\tau|} \left( \mathbb{E} \frac{\text{Cov}(X_{\tau'} | X_P)}{X_P X_{\tau'}} \right)
\]

\[
\geq d_{|\tau|} \left( \mathbb{E} \frac{\text{Cov}(X_{\tau'} | X_P, X_{Pa(\tau')}) | X_P} + d_{|\tau|} \left( \mathbb{E} \frac{\text{Cov}(X_{\tau'} | X_P, X_{Pa(\tau')}) | X_P} \right) \right) \]

\[
> d_{|\tau|} \left( \mathbb{E} \frac{\text{Cov}(X_{\tau'} | X_P, X_{Pa(\tau')}) | X_P} \right) \]

\[
\geq d_{|\tau|} \left( \mathbb{E} \frac{\text{Cov}(X_{\tau'} | X_P, X_{Pa(\tau)}) | X_P} \right) = d_{|\tau|} \left( \mathbb{E} \frac{\text{Cov}(X_{\tau'} | X_P, X_{Pa(\tau)}) | X_P} \right) \]

The third inequality is due to (3.1). The last equality holds since \( Pa(\tau) \subseteq P \), and hence, \( X_{\tau} \) is independent of \( X_P \setminus Pa(\tau) \) conditioned on \( X_{Pa(\tau)} \).

The following corollary is immediate.

Corollary 3.3. Suppose \( X \) corresponds to an additive noise model generated by a chain graph \( C \), i.e.:

\[
X_\tau = f_\tau(X_{Pa(\tau)}) + Z_\tau,
\]

where the noise term \( Z_\tau \) is independent of \( X_{Pa(\tau)} \), for all chain components \( \tau \) of \( D \).

Then, given the chain component decomposition, a topological ordering of \( D \) is identifiable from \( X \) if there exists a topological ordering \( \pi \) of \( D \) such that

\[
\det(\text{Cov}(Z_\tau)) \leq \det(\text{Cov}(Z_{\tau'}))
\]

for all chain components \( \tau \prec_\pi \tau' \).

4 General Identifiability

In this section, we establish identifiability conditions for recovering both the chain components as well as the DAG structure of chain graphs from the generated probability distribution. Here, by identifiability, we mean that the partitioning into chain components and the topological order on the chain components are uniquely specified. The exact set of directed and undirected edges can then be recovered using standard variable selection methods (as described in Appendix A of Gao et al. [2020]).
Algorithm 2: Infinite sample algorithm for learning the topological order of a chain graph with unknown chain components.

1. $P \leftarrow \emptyset$;
2. $i \leftarrow 1$;
3. $\tau_1 = \arg\min_{S \subseteq V, S \neq \emptyset} \det(\text{Cov}(X_S))$;
4. $P \leftarrow P \cup \tau_1$;
5. while $V \setminus P \neq \emptyset$ do
6. $\tau_i \leftarrow \arg\min_{S \subseteq V \setminus P, S \neq \emptyset} \det(\text{Cov}(X_S \mid X_P))$;
7. $P \leftarrow P \cup \tau_i$;
8. $i \leftarrow i + 1$;
9. Return the topological sort $\left(\tau_1, \ldots, \tau_i\right)$

Theorem 4.1. Suppose the random variable $X$ is generated by an AMP-CG $C$ with unknown structure. Then, $C$ is identifiable from $X$ if the following three conditions hold:

(i) For all chain components $\tau$ and all non-empty proper subsets $S \subset \tau$:
\[ \det(\text{Cov}(X_S \mid X_{\tau \setminus S}, X_{\text{Pa}(\tau)})) < 1. \]

(ii) For all chain components $\tau$:
\[ \det(\text{Cov}(X_\tau \mid X_{\text{Pa}(\tau)})) > 1. \]

(iii) There is a topological order $\pi$ on the chain components such that for all $\tau \preceq_\pi \tau'$:
\[ \det(\text{Cov}(X_\tau \mid X_{\text{Pa}(\tau)})) \leq \det(\text{Cov}(X_{\tau'} \mid X_{\text{Pa}(\tau')})). \]

Proof. For simplicity, suppose that there is a unique topological order $\tau_1 \preceq \tau_2 \preceq \cdots \preceq \tau_m$ for the components outside $P$. The proof easily extends to the general case. Let $\tau_{<i} = \tau_1 \cup \cdots \cup \tau_{i-1}$.

Consider any non-empty subset $S$ that is disjoint from $P$. We claim:
\[
\det(\text{Cov}(X_S \mid X_P)) = \prod_{i=1}^{m} \det(\text{Cov}(X_{S \cap \tau_i} \mid X_{S \cap \tau_{<i}}, X_P)) \geq \prod_{i=1}^{m} \det(\text{Cov}(X_\tau \mid X_{\text{Pa}(\tau_i)})) \geq \det(\text{Cov}(X_{\tau_1} \mid X_{\text{Pa}(\tau_1)})).
\]

(4.1) is a consequence of Fact 2.2. To prove (4.2), we invoke the law of conditional covariance (Fact 2.1):
\[
\det(\text{Cov}(X_{S \cap \tau_i} \mid X_{S \cap \tau_1}, X_P)) = \det(\text{Cov}(X_{S \cap \tau_i} \mid X_{\text{Pa}(\tau_i)}, X_{S \cap \tau_1}, X_P)) + \det(\text{Cov}(X_{S \cap \tau_1} \mid X_{\text{Pa}(\tau_1)}) \mid X_{S \cap \tau_1}, X_P)
\geq \det(\text{Cov}(X_{S \cap \tau_i} \mid X_{\text{Pa}(\tau_i)}))
\]

The last inequality uses the positive semi-definiteness of covariance matrices and super-additivity of the determinant. The proof of (4.3) uses Fact 2.2 as follows:
\[
\det(\text{Cov}(X_{\tau_i} \mid X_{\text{Pa}(\tau_i)})) = \det(\text{Cov}(X_{S \cap \tau_i} \mid X_{\text{Pa}(\tau_i)})) \cdot \det(\text{Cov}(X_{S \setminus \tau_i} \mid X_{S \cap \tau_i}, X_{\text{Pa}(\tau_i)})) \leq \det(\text{Cov}(X_{S \cap \tau_i} \mid X_{\text{Pa}(\tau_i)}))
\]
using condition (iii) of Theorem 4.1. (The last inequality is non-strict because \( \tau_i \setminus S \) may be empty.) The inequality (4.4) follows from conditions (i) and (ii) of Theorem 4.1.

For (4.4) to be an equality, \( S \) must be contained in exactly one component \( \tau \). For (4.3) to be an equality, \( S \) must equal \( \tau \). For (4.2) to be an equality, the parents of \( S \cap \tau = S \) must be contained in \( P \), and hence \( S = \tau = \tau_1 \).

Informally speaking, for any subset \( S \), given its complementary set and parents union of \( \tau \) in \( C \), we require the variables in each chain component to be tightly correlated. Besides, given the union of the parents of chain components \( \tau \), we require the clustered variables in each chain component to have large generalized variance. The third condition is the same one imposed in Section 3.

There is a geometric way to view the conditions in Theorem 4.1, which substantiates the intuition that they require each chain component to cluster together while having large variance as a whole. Recall that for any matrix \( M \), \( \det(M) \) corresponds to the volume of the parallelepiped spanned by the rows of \( M \). Let the chain components be denoted \( \tau_1, \ldots, \tau_k \) in a topological order. For \( i = 1, \ldots, k \), let \( M_i \) denote the covariance matrix of \( X_{\tau_i} \mid X_{\tau_1 \cup \cdots \cup \tau_{i-1}} \), and let \( M \) denote the full covariance matrix, \( \text{Cov}(X_{\tau_1 \cup \cdots \cup \tau_k}) \). From Fact 2.2,

\[
\det(M) = \det(M_1) \cdots \det(M_k). \tag{4.5}
\]

Let \( V_i \) denote the set of row vectors of \( M_i \), and we identify \( V_i \) with the parallelepiped it spans. Due to Equation 4.5, we can view each \( V_i \) as residing in a subspace orthogonal to the spans of other \( V_j \)’s, so that their volumes just multiply with each other. (Alternatively, construct a block diagonal matrix \( M' \) where the \( i \)’th block on the diagonal is \( M_i \); clearly, \( \det(M) = \det(M') \).) In this language, Condition (ii) in Theorem 4.1 says that the volume of each \( V_i \) is more than 1, and condition (iii) says that the volumes are non-decreasing with \( i \). Condition (i) says that for any \( V_i \), the volume of any sub-parallelepiped is larger than the volume of the whole. Intuitively, this means that the vectors in \( V_i \) form very small angles with each other, so that the volumes keep decreasing as more vectors are added.

**Computational Efficiency.** It is known that Algorithm 2 can be implemented in polynomial time. This is because the optimization problems in lines 3 and 5 of the pseudocode correspond to submodular function minimization, as explained in Section 1.1. Solving submodular function minimization is in polynomial time (see, e.g., Iwata [2008]).

## 5 Experiments

In this section, we compare the performance of Algorithm 1 and Algorithm 2 on synthetic datasets to state-of-the-art methods for AMP-chain graph structure learning. Recall that as we showed in Theorem 3.1, the DAG on the chain components of an AMP chain graph is identifiable if (3.1) is satisfied for a positive and super-additive family \( d_\tau \). Here, we let \( d_\tau \) be the determinant operator, and hence dub our algorithm as Determinant of Covariance (DCOV).

**Synthetic Data Generation:** To generate the chain graph \( G \), in our first step, an undirected graph \( \mathcal{G} \) with \( n \) nodes is generated by using the Erdős Rényi (ER) model with an expected neighbor size \( s = 2 \) and then symmetrizing. Given the number of chain components \( c \), we split the interval \([1, n]\) into \( c \) equal-length sub-intervals \([I_1, \ldots, I_c]\) so that variable sets for each sub-interval forms chain components \( \tau_1, \ldots, \tau_c \). Meanwhile, for any \((i, j)\) pair, we set \( c_{i,j} = 0 \) if \( \exists \ell \in [I_i, j \in [I_m, \ell > m] \). Given the binary adjacency matrix \( C \), we generate the matrix \( M \) of edge weights by \( M_{i,j} \sim U(-1.5, -0.5) \cup U(0.5, 1.5) \) if \( c_{i,j} \neq 0 \) and \( M_{i,j} = 0 \) otherwise.
The observational i.i.d. data $X_\tau = M_\tau X_{Pa(\tau)} + Z_\tau$ is generated with a sample size $n = 1000$ and a variable size $d \in \{10, 20, 30, 40, 50\}$. $Z_\tau$ is an independent multivariate Gaussian drawn from $N(0, \Sigma_\tau)$ where $\Sigma_\tau$ is generated randomly with $\det(\Sigma_\tau) = 1$, satisfying the assumption of Corollary 3.3. Figure 3 illustrates how the synthetic AMP chain graph data is generated.

**Baseline Algorithms:** We compare our DCOV method against the PC-LIKE (Peña [2012, 2014a], Peña and Gomez-Olmedo [2016]), LCD-LIKE (Learn Chain Graphs via Decomposition), and LDCG algorithm (learn the largest deflagged graph based on the results of LCD-LIKE algorithm) (Javidian et al. [2020]). We use default parameters among those baseline algorithms in order to avoid skewing the results in favour of any particular algorithm as a result of hyperparameter tuning**. All the baseline algorithms above are implemented using R-packages (licensed under GPL-2 or GPL-3) such as ggm (Marchetti et al. [2006]), pcalg (Kalisch et al. [2012]), mgcv (Wood and Wood [2015]), np (Racine and Hayfield [2020]), and lcd (Ma et al. [2009]). We use rpy2 [Gautier, 2012] to access R-packages from Python and ensure that all algorithms can be compared in the same environment. The experiments were conducted on an Intel Core i7-9750H 2.60GHz CPU.

**Implementation of DCOV:** We implement Algorithm 2 in polynomial time using the Matlab toolbox “Submodular Function Optimization” [Krause, 2010]. We use MATLAB Engine API for Python to access Matlab-packages from Python. Each iteration of Algorithm 1 and Algorithm 2 needs to estimate the conditional covariance of the remaining chain components given those found so far. Our estimator of the conditional covariance is very similar to that considered by Gao et al. [2020] for Bayes networks. In particular, like them, we run a gam regression to estimate conditional expectations. We set the p-value with significance level of 0.001 for determining the parents of the node.

**Quantitative Experiment Results:** In our experiment, we use Structural Hamming Distance (SHD) as the evaluation metric. Figure 4 reports SHD of our proposed DCOV and other algorithms. The results are averaged over 20 independent repetitions. As shown in Figure 4, DCOV, under known chain component conditions, shows superior performance compared with all other baselines by wide margins. Under unknown chain component conditions, DCOV outperforms LDCG and LCD, and is comparable to the PC-LIKE algorithm. One limitation of this work is the lack of real datasets that can be modeled by chain graphs.

6 Conclusion

In this work, we address the problem of recovering AMP chain graph in polynomial time from observational data, and we proposed two algorithms for both known and unknown chain components to handle the problem. In our experiments, we implement the DCOV algorithm over known chain components. As future work, we are also interested in exploring a score-based approach for chain graph structure learning from observational data.

**The implementation of baseline algorithms is available at https://github.com/majavid/AMPCG2019.**
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