Constraints in Gaussian Graphical Models

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In this paper, we consider the problem of finding the constraints in bow-free acyclic directed mixed graphs (ADMGs). ADMGs are a generalisation of directed acyclic graphs (DAGs) that allow for certain latent variables. We first show that minimal generators for the ideal $I(G)$ containing all the constraints of a Gaussian ADMG $G$ corresponds precisely to the pairs of non-adjacent vertices in $G$. The proof of this theorem naturally leads to an efficient algorithm that fits a bow-free Gaussian ADMG by maximum likelihood. In particular, we can test for the goodness of fit of a given data set to a bow-free ADMG.

Keywords: Graphical model, ADMG, BAP, SEM, model selection, fitting.

1. Introduction

Graphical models provide a powerful formalism for dealing with uncertainty for probabilistic modelling and inference, by encoding independence constraints into graphical representations. One popular graphical model representing the joint probability distribution is a directed acyclic graph (DAG), where each vertex corresponds to a random variable and each arrow represents a 'direct effect'. The use of DAGs as a language for describing casual models has a long history in statistics, beginning with the seminal works by Wright [24, 25] with an emphasis on genetics. These models were later applied to econometrics [12] and the social sciences [3]. Today, DAGs are widely used in machine learning, bioinformatics and many other applications [14].

An important parametric subclass of DAG models are the linear structural equation models (SEMs). In fact, Wright’s work was originally within the SEM class. For the Gaussian case, given a DAG $G = (V, E)$, the linear SEM is given as

$$X_i = \sum_{j \in \text{pa}(i)} \lambda_{ij} X_j + \epsilon_i, \quad i \in V,$$

where $\text{pa}(i)$ represents the set of parents of the vertex $i$, each $\lambda_{ij}$ is the regression coefficient obtained from regressing $X_i$ on $X_j$ (this coefficient is an unknown) and each $\epsilon_i$ is an independent and centered Gaussian random variable with mean zero. The random vector $X$ that solves the above SEM will follow a Gaussian distribution with mean zero and a structured covariance matrix. Each SEM naturally corresponds to a set of covariance matrices that can exist in this model, which we denote $\mathcal{M}(G)$. In particular, for a DAG $G$, the set of conditional independences yields an implicit description of $\mathcal{M}(G)$ [10, 13]. The conditional independences can be found graphically using the concept of $d$-separation [16]. We will provide a more rigorous definition of $\mathcal{M}(G)$ in Section 2.

The popularity of DAGs stems from their well-understood theory, and several structural learning algorithms use observed conditional independences to find all compatible DAGs [20]. Often, however, we might not be able to observe all relevant variables. The resulting marginal distribution over the observed variables might satisfy additional constraints resulting from the marginalisation, as we
will show in Example 1.1. Models defined by these constraints can be obtained from the DAG via a latent projection operation \[ \text{[23]} \]. This will produce an acyclic directed mixed graph (ADMG), with the structural equation model

\[
X_i = \sum_{j \in \text{pa}(i)} \lambda_{ji} X_j + \epsilon_i
\]

on the observed variables \( X_i \), each \( \lambda_{ij} \) as before and each \( \epsilon_i \) a (not necessarily independent) centered Gaussian random variable.

**Example 1.1.** Consider the Verma graph in Figure 1 where vertex 5 is a latent variable. The graph on the right, \( G \), represents the latent projection of the Verma graph. In both graphs, there are no conditional independences involving only the observed variables \( X_1, X_2, X_3 \) and \( X_4 \). However, we do have a constraint on the corresponding covariance matrix \( \Sigma \), in the sense that \( \Sigma \in \mathcal{M}(G) \) only if

\[
f_{\text{Verma}}(\Sigma) = \sigma_{11}\sigma_{13}\sigma_{22}\sigma_{34} - \sigma_{12}\sigma_{13}\sigma_{34} - \sigma_{11}\sigma_{14}\sigma_{22}\sigma_{33} + \sigma_{12}\sigma_{14}\sigma_{33} - \sigma_{11}\sigma_{13}\sigma_{23}\sigma_{24} + \sigma_{11}\sigma_{14}\sigma_{23}\sigma_{24} - \sigma_{12}\sigma_{13}\sigma_{14}\sigma_{23} = 0.
\]

While the latent projection operator does not change the equality constraints \[ \text{[18]} \], one should note that the SEMs with correlated errors is in fact a larger model than the actual marginal model. In particular, some inequality constraints in the actual model are not captured in the SEM \[ \text{[7]} \].

On non-parametric models, the graph decomposition result \[ \text{[21]} \] leading to Tian’s algorithm \[ \text{[18, 22]} \] provides a way for finding constraints in non-parametric graphs. For instance, the constraint in Example 1.1 can be seen as the independence between \( X_3 \) and \( X_4 \) after fixing \( X_2 \) and \( X_3 \) (i.e. after removing all edges pointing into vertices 2 and 3). Tian’s algorithm, though non-parametrically complete, will fail to find the Gaussian constraint on the ‘gadget’ graph in Figure 2:

\[
\sigma_{11}\sigma_{22}\sigma_{34} - \sigma_{13}\sigma_{14}\sigma_{22} + \sigma_{13}\sigma_{12}\sigma_{24} - \sigma_{23}\sigma_{11}\sigma_{24} = 0.
\]
Let $\mathcal{I}(G)$ denote the ideal of polynomials such that $f \in \mathcal{I}(G)$ if and only if $f(\Sigma) = 0$ for all $\Sigma \in \mathcal{M}(G)$. Recent attempts by Drton et al. [8] on restricted set separations only manages to provide sufficient conditions for a polynomial to be a member of $\mathcal{I}(G)$. In particular, there are some constraints (e.g. [8, Examples 6.1, 6.2]) which fail to satisfy the conditions of their theorem.

In this paper, we will first prove that the constraints are in one-to-one correspondence with non-adjacent vertices in a bow-free ADMG. This proof provides us with a natural algorithm to compute the matrix of all the regression coefficients $\Lambda$, and the covariance matrix of the error terms $\Omega$, in addition to finding the generators for $\mathcal{I}(G)$ symbolically in a given bow-free ADMG, $G$. We will then provide an application for $\mathcal{I}(G)$ to test if $\Sigma \in \mathcal{M}(G)$ for a given dataset $X \sim N(0, \Sigma)$ and a graphical model $G$. We then show that computing $\mathcal{I}(G)$ symbolically is generally intractable; while this can be remedied by bootstrapping (Example 4.6), we will develop a more practical approach. In particular, this method allows us to output the MLEs $\hat{\Lambda}$, $\hat{\Omega}$ and $\hat{\Sigma}$. While other algorithms for fitting SEMs exist and are widely used [6], these have a similar computational complexity to ours.

This paper is organised as follows: In Section 2, we will give a rigorous definition of the models we study, and provide a background on the current knowledge on this problem. In Section 3, we will study the properties of the constraints, where we prove our main result. In Section 4, we will provide an algorithm to compute $\Lambda$, $\Omega$ and $\mathcal{I}(G)$ given the true value of $\Sigma$ and a particular graphical model $G$. We also explore the complexity of this algorithm in this section. In Section 5, we will provide a practical approach using maximum likelihood to fit a Gaussian ADMG. In particular, this will allow us to test whether a particular dataset came from a given graphical model, as well as finding the MLEs $\hat{\Lambda}$, $\hat{\Omega}$ and $\hat{\Sigma}$. Finally, in Section 6, we will apply our algorithm to a real data example.

2. Preliminaries

2.1. Acyclic Directed Mixed Graphs

A directed mixed graph is a triple $G = (V, D, B)$ where $V$ is a set of vertices, $D$ is the set of directed edges ($\rightarrow$) and $B$ is the set of bidirected edges ($\leftrightarrow$). Two vertices, $i, j \in V$, are adjacent if they are connected by an edge. We denote adjacent vertices with $i \sim j$. Two edges are incident if they share a vertex. A directed walk of length $\ell$ is a sequence of $\ell + 1$ adjacent vertices $v_0, \ldots, v_n$, each connected by a directed edge $v_i \rightarrow v_{i+1}$. A path is a walk where all vertices are distinct. A directed path of length $\ell$ is a path of the form $v_0 \rightarrow v_1 \rightarrow \cdots \rightarrow v_\ell$. Similarly, a bidirected path of length $\ell$ is a path of the form $v_0 \leftrightarrow v_1 \leftrightarrow \cdots \leftrightarrow v_\ell$. A directed walk of length $\ell \geq 3$ is a directed cycle if $v_0 = v_\ell$ and all other vertices $v_j$ are distinct (for $0 < j < \ell$). An acyclic directed mixed graph (ADMG) is a directed mixed graph without any directed cycles. A directed acyclic graph (DAG) is an ADMG without any bidirected edges.

Suppose $i, j \in V$ and the edge $i \rightarrow j$ is present. We say $i$ is a parent of $j$ and $j$ is a child of $i$. The sets of all parents and children of $x$ are denoted $\text{pa}(x)$ and $\text{ch}(x)$ respectively. A topological ordering of the vertices in a graph is an ordering $1 < 2 < \cdots < k$ such that $i \in \text{pa}(j)$ implies that $i < j$. In an ADMG, a topological ordering always exists.

**Definition 2.1.** Let $i, j \in V$. If there is both a directed and a bidirected edge connecting $i$ and $j$, we say that $i$ and $j$ form a bow. If a directed mixed graph has no bows, we say that the graph is bow-free.
2.2. Structural Equation Models

An ADMG $G = (V, D, B)$ induces a statistical model for the joint distribution of a collection of random variables $X_i$, where $i \in V$. In this paper, we shall only consider the Gaussian case in which the functional relationships are linear. This gives us a structural equation model

$$X_i = \sum_{j \in \text{pa}(i)} \lambda_{ji} X_j + \epsilon_i,$$

where each $\lambda_{ji}$ is an unknown regression coefficient and each $\epsilon_i$ is a (not necessarily independent) centered Gaussian random variable. Let $\Lambda = (\lambda_{ij}) \in \mathbb{R}^{V \times V}$ be the matrix holding the unknown coefficients, and $\epsilon = (\epsilon_i)$ be the random error vector. We can rewrite the system of structural equations as

$$X = \Lambda^T X + \epsilon.$$

Let $\Omega = (\omega_{ij}) = \text{Cov}[\epsilon] \in \mathbb{R}^{V \times V}$ be a covariance matrix of $\epsilon$. Note that by construction of the structural equation model, $\lambda_{ij} = 0$ if the edge $i \rightarrow j \notin D$ and $\lambda_{ij}$ arbitrary otherwise. This gives us a natural definition for a set containing all possible such $\Lambda$,

$$\mathbb{R}^D := \{\Lambda \in \mathbb{R}^{V \times V} : \lambda_{ij} = 0 \text{ if } i \rightarrow j \notin D\}.$$

Since $G$ is acyclic, if $\Lambda \in \mathbb{R}^D$, there is a topological ordering of vertices such that $\Lambda$ is a strictly upper triangular matrix. In particular, $I - \Lambda$ is invertible with determinant one. Then $X = (I - \Lambda)^{-1} \epsilon$ is the unique solution to the structural equations. Hence, $X$ has the covariance matrix

$$\Sigma := \text{Cov}[X] = (I - \Lambda)^{-T} \Omega(I - \Lambda)^{-1}.$$

Suppose $\Omega$ is a positive definite matrix with $\omega_{ij} = 0$ if “$i \leftrightarrow j$” $\notin B$. Let $PD(V)$ be the cone of positive definite $V \times V$ matrices. Similar to $\Lambda$, we can define a set containing all possible such matrices $\Omega$,

$$PD(B) := \{\Omega \in PD(V) : \omega_{ij} = 0 \text{ if } i \neq j \text{ and } "i \leftrightarrow j" \notin B\}.$$

By Cramer’s rule [1], entries in the covariance matrix in (2) are rational functions of the entries in $\Lambda$ and $\Omega$. We define the linear structural equation model given by an ADMG $G = (V, D, B)$ to be the family of all multivariate normal distributions on $\mathbb{R}^V$ with covariance matrix in the set

$$\mathcal{M}(G) := \{(I - \Lambda)^{-T} \Omega(I - \Lambda)^{-1} : \Lambda \in \mathbb{R}^D, \Omega \in PD(B)\}.$$

The set $\mathbb{R}^D \times PD(B)$ is semialgebraic. Since $\mathcal{M}(G)$ is the image of this set under a rational map, by the Tarski-Seidenberg theorem, $\mathcal{M}(G)$ is also a semialgebraic set; hence, it admits a finite polynomial description. We are interested in the polynomial equations satisfied by the matrices in $\mathcal{M}(G)$. Let $\Sigma = (\sigma_{ij})$ and define $\mathbb{R}[\Sigma]$ to be the polynomial ring with indeterminates $\sigma_{ij}$ for $1 \leq i, j \leq V$. The polynomial relations we seek to understand form the vanishing ideal of $\mathcal{M}(G)$,

$$\mathcal{I}(G) := \{f \in \mathbb{R}[\Sigma] : f(\Sigma) = 0, \forall \Sigma \in \mathcal{M}(G)\},$$

which contains all the constraints of $G$.

**Definition 2.2.** Let $\phi : \Theta \rightarrow N$ be a rational map defined everywhere on the parameter space $\Theta$ into the natural parameter space $N$ of an exponential family. The model $\mathcal{M} = \text{im } \phi$ is said to be
• globally identifiable if $\phi$ is a one-to-one function.
• generically identifiable if $\phi^{-1}(\phi(\theta)) = \{\theta\}$ for almost all $\theta \in \Theta$.

Note that for all graphical models $\mathcal{M}(G)$ that are globally identifiable, $G$ is bow-free (the converse is not true in general) [19]. Hence, the graph class we are considering covers all globally identifiable graphs.

2.3. Latent Projections

Given a DAG with latent variables, we can associate an ADMG using the latent projection [18, 23]:

**Definition 2.3** (Latent projection). Let $G$ be a DAG with vertex set $V \cup L$, where vertices in $V$ are observed, vertices in $L$ are latent and $\cup$ denotes disjoint union. The latent projection $G'$ is a directed mixed graph with vertex set $V$, where for every pair of distinct vertices $i, j \in V$:

1. $G'$ contains an edge $i \to j$ if there exists a directed path $i \to \cdots \to j$ on which every non-endpoint vertex is in $L$.
2. $G'$ contains an edge $i \leftrightarrow j$ if there exists a path between $i$ and $j$ such that all the non-endpoint vertices are non-colliders in $L$ and the edges incident to both $i$ and $j$ are pointing towards those vertices (i.e. $i \leftarrow \cdots \to j$).

We have given an example of a latent projection in Figure 1. In particular, suppose $G$ is a DAG and $G'$ is its latent projection, then $G'$ is an ADMG and $\mathcal{I}(G) = \mathcal{I}(G')$ [18]. However, some inequality constraints on DAG models with latent variables are not captured by linear SEMs [9].

3. Properties of the Vanishing Ideal

In this section, we will show that there is a constraint corresponding to each pair of non-adjacent vertices in an ADMG $G$. Further algebraic properties of $\mathcal{I}(G)$ can be found in Appendix B.

First, we rearrange (2) to obtain

\[
(I - \Lambda)^T \Sigma (I - \Lambda) = \Omega.
\]

By equating each entry in $(I - \Lambda)^T \Sigma (I - \Lambda)$ that corresponds to a zero entry in $\Omega$ (i.e. missing bidirected edge), we obtain a system of equations in terms of the unknowns $\lambda_{ij}$ only. Since $\Sigma$ is a covariance matrix, it is symmetric. As any matrix congruent to a symmetric matrix is also symmetric, $(I - \Lambda)^T \Sigma (I - \Lambda)$ is also a symmetric matrix. By assumption, $\Omega$ is a covariance matrix, and is hence symmetric with non-zero diagonal entries. Therefore, it suffices to equate only the strictly upper or strictly lower triangular entries of both matrices.

Define the matrices $A = (a_{ij}) = (I - \Lambda)^T \Sigma$ and $B = (b_{ij}) = (I - \Lambda)^T \Sigma (I - \Lambda)$, where each entry is a polynomial in which the indeterminates are entries in $\Sigma$. Evaluating the matrix multiplication, we obtain

\[
a_{ij} = \sigma_{ij} - \sum_{\ell=1}^{i-1} \lambda_{\ell i} \sigma_{\ell j},
\]

\[
b_{ij} = a_{ij} - \sum_{\ell=1}^{i-1} \lambda_{ij} a_{\ell i}.
\]
Equating each entry of both matrices in (3), we obtain $b_{ij} = \omega_{ij}$. Before proceeding, we shall first provide a brief remark on notation.

**Notation:** Note that the $\lambda_{ij}$ might be zero either due to an absence of directed edges between the vertices $i$ and $j$, or because the regression coefficient $\lambda_{ij}$ in the linear equation (1) happens to evaluate to zero (after regressing $X_i$ on $X_j$). To differentiate these two cases, we write $\lambda_{ij} \equiv 0$ for the former case and $\lambda_{ij} = 0$ for the latter. Similarly we write $\omega_{ij} \equiv 0$ if there are no bidirected edges between vertices $i$ and $j$ and $\omega_{ij} = 0$ if $\omega_{ij}$ happens to evaluate to zero.

**Lemma 3.1.** Suppose $k$ is fixed and each regression coefficient $\lambda_{ij}$ is known for $1 \leq i < j \leq k-1$. Then the $b_{ki}$’s are linearly independent symbolically in $\lambda_{ik}$ for $1 \leq i \leq k-1$.

**Proof.** We have

$$b_{k1} = a_{k1},$$
$$b_{k2} = a_{k2} - \lambda_{12} a_{k1},$$
$$\vdots$$
$$b_{k,k-1} = a_{k,k-1} - \sum_{\ell=1}^{k-2} \lambda_{\ell,k-1} a_{k\ell},$$

where the coefficients of each $a_{ki}$ is known for $1 \leq i \leq k-1$. Hence, by row operations, the $b_{ki}$’s are linearly independent in $\lambda_{ik}$ if and only if the $a_{ki}$’s are linearly independent for $1 \leq i \leq k-1$. The equations for the $a_{ki}$’s are:

$$a_{k1} = \sigma_{1k} - \lambda_{1k} \sigma_{11} - \cdots - \lambda_{1,k-1} \sigma_{1,k-1},$$
$$a_{k2} = \sigma_{2k} - \lambda_{1k} \sigma_{12} - \cdots - \lambda_{1,k-1} \sigma_{2,k-1},$$
$$\vdots$$
$$a_{kj} = \sigma_{jk} - \lambda_{1k} \sigma_{1j} - \cdots - \lambda_{1,k-1} \sigma_{j,k-1},$$
$$\vdots$$

which we can rewrite into a matrix as

$$
\begin{pmatrix}
a_{k1} \\
a_{k2} \\
\vdots \\
a_{k,k-1}
\end{pmatrix} =
\begin{pmatrix}
\sigma_{11} & \sigma_{12} & \cdots & \sigma_{1,k-1} \\
\sigma_{12} & \sigma_{22} & \cdots & \sigma_{2,k-1} \\
\vdots & \vdots & \ddots & \vdots \\
\sigma_{1,k-1} & \sigma_{2,k-1} & \cdots & \sigma_{k-1,k-1}
\end{pmatrix}
+ \begin{pmatrix}
\sigma_{1k} \\
\sigma_{2k} \\
\vdots \\
\sigma_{k-1,k}
\end{pmatrix} + \begin{pmatrix}
-\lambda_{1k} \\
-\lambda_{2k} \\
\vdots \\
-\lambda_{k-1,k}
\end{pmatrix}.
$$

Now the matrix in the middle is a submatrix of $\Sigma$ with the first $k-1$ rows and columns, and is positive definite and hence non-singular by assumption. Therefore, the $a_{ki}$’s are linearly independent.

Note that in a bow-free ADMG, if we have a bidirected edge between vertices $i$ and $j$, then there are no directed edges between $i$ and $j$ by definition. Hence, $\omega_{ij} \neq 0 \implies \lambda_{ij} \equiv 0$ for all $0 \leq i < j \leq V$. Similarly, $\lambda_{ij} \neq 0 \implies \omega_{ij} \equiv 0$ for all $0 \leq i < j \leq V$. 
Theorem 3.2. Let $G$ be a bow-free ADMG. Then, there exists a generating set $Z$ for $\mathcal{I}(G)$ such that each pair of non-adjacent vertices $i \neq j$ in $G$ is in bijection with an element in $Z$. Furthermore, we can express each directed edge $\lambda_{ij}$ or bidirected edge $\omega_{ij}$ as a rational with the entries in $\Sigma$ as indeterminates. Hence, $G$ is generically identifiable.

Proof. We shall start by equating each entry in $B$ to each entry in $\Omega$. Since both $B$ and $\Omega$ are symmetric matrices, and the diagonal entries of $\Omega$ are non-zero, it suffices to consider only the strictly lower triangular entries. We will proceed by a row induction.

In the first row, we have no equations since we are only considering strictly lower triangular entries. In the second row, we have only one equation from equating the strictly lower triangular entries in (3):

$$b_{12} = \sigma_{12} - \lambda_{12}\sigma_{11} = \omega_{12}. \quad (4)$$

Now, we will consider the following three cases:

1. If $\lambda_{12} \neq 0$, then $\omega_{12} \equiv 0$ (since the graph is bow-free). Hence, we can solve (4) to obtain $\lambda_{12} = \frac{\sigma_{12}}{\sigma_{11}}$. In particular, we have no new constraints on $\Sigma$ since $\lambda_{12}$ was arbitrary.

2. If $\omega_{12} \neq 0$, then $\lambda_{12} \equiv 0$ and (4) gives us $\sigma_{12} = \omega_{12}$. Hence, we also have no new constraints on $\Sigma$ since $\omega_{12}$ was arbitrary.

3. If both $\lambda_{12} \equiv 0$ and $\omega_{12} \equiv 0$, equation (4) gives us $\sigma_{12} = 0$ which is a new constraint on $\Sigma$.

In particular, for any of these cases, either $\lambda_{12} \equiv 0$ (the directed edge is not present) or we can find an expression for $\lambda_{12}$ as a rational with the entries of $\Sigma$ as indeterminates. Furthermore, if both $\lambda_{12} \equiv 0$ and $\omega_{12} \equiv 0$ (vertices 1 and 2 are not adjacent), we have a corresponding constraint.

Now suppose that for the $k-1$th row, each of the regression coefficients $\lambda_{1,j}, \ldots, \lambda_{j-1,j}$ (for all $2 \leq j \leq k-1$) where the corresponding directed edge is present can be expressed as a rational with indeterminates in $\Sigma$. We want to show that each of the new regression coefficients, $\lambda_{i,k}, \ldots, \lambda_{k-1,k}$, can also be expressed as a rational with indeterminates in $\Sigma$ if the corresponding directed edge exists. Furthermore, we will show that for each $1 \leq i \leq k-1$, if the vertices $i$ and $k$ are not adjacent, we will obtain a new constraint on $\Sigma$.

In the $k$th row, equating entries in (3) we have the following $k-1$ equations:

$$b_{k1} = a_{k1} = \omega_{k1},$$
$$b_{k2} = a_{k2} - \lambda_{12}a_{k1} = \omega_{k2},$$
$$\vdots$$
$$b_{k,k-1} = a_{k,k-1} - \sum_{\ell=1}^{k-2} \lambda_{\ell,k-1} a_{k\ell} = \omega_{k,k-1},$$

where each $a_{kj} = \sigma_{jk} - \sum_{\ell=1}^{k-1} \lambda_{jk}\sigma_{\ell}$. Note that the coefficient of each $a_{kj}$ is either 1 or $-\lambda_{ij}$ for some $1 \leq i < j \leq k-1$. By the induction hypothesis, each $\lambda_{ij}$, for $1 \leq i < j \leq k-1$, can be expressed as a rational with indeterminates in $\Sigma$. Hence, the only unknowns in our equations are the $\lambda_{ik}$’s (from expanding $a_{kj}$) and the $\omega_{ki}$’s for $1 \leq i \leq k-1$.

Now, if $\omega_{ik} \equiv 0$ and $\lambda_{ik} \neq 0$ for all $1 \leq i \leq k-1$, we have $k-1$ equations with $k-1$ unknowns. On the other hand, if $\omega_{jk} \neq 0$ for some $j$, we must have $\lambda_{jk} \equiv 0$ and we still have the same number...
of equations as there are unknowns. However, if both \( \omega_{jk} \equiv 0 \) and \( \lambda_{jk} \equiv 0 \) for some \( j \) (i.e. there is missing edge between \( j \) and \( k \)), then we have one more equation than the number of unknowns. By induction hypothesis, the conditions of Lemma 3.1 are satisfied. Hence, the \( b_{ik} \)'s are linearly independent. Any subset of linearly independent equations is also linearly independent. Therefore, if we have the same number of equations as there are unknowns and each \( \lambda_{ik} \) can be expressed uniquely as a rational with indeterminates in \( \Sigma \). If we have more equations than unknowns, after solving for \( \lambda_{ik} \), we can substitute the rational back into the extra equations to obtain the constraints for the set \( Z \) we want to construct.

We have shown that each \( \lambda_{ij} \) can be expressed as a rational with entries in \( \Sigma \) as indeterminates, and that we can find a constraint in \( Z \) for each pair of non-adjacent vertices. Plugging \( \Lambda = (\lambda_{ij}) \) into (3), we can also express each \( \omega_{ij} \) as a rational with indeterminates in \( \Sigma \). Finally, we want to show that \( Z \) generates \( \mathcal{I}(G) \). Indeed, \( \mathcal{I}(G) \) is defined by all the functions \( f \) where \( f(\Sigma) = 0 \) for \( \Sigma \in \mathcal{M}(G) \). Hence, all the constraints must be obtained from the equation (2). By the previous paragraph, \( Z \) must generate the ideal containing all the constraints, \( \mathcal{I}(G) \).

In fact, we will show in Appendix B that the constraints we found in Theorem 3.2 are the minimal generators of \( \mathcal{I}(G) \) (i.e. if we remove one of those constraints, the remaining constraints will no longer generate \( \mathcal{I}(G) \)).

**Corollary 3.3.** Suppose we have a topological ordering on the vertices of an ADMG \( G \) and \( i, j \) are two non-adjacent vertices \( G \) such that \( i < j \) in the topological ordering. We can find the constraint corresponding to the missing edge between \( i \) and \( j \) by first assuming the edge is present, expressing \( \lambda_{ij} \) as a rational with indeterminates as the entries of \( \Sigma \) and finally equating \( \lambda_{ij} = 0 \).

**Proof.** We are simply solving the linearly independent system of equations in two different ways. In the proof of Theorem 3.2, we first substitute in \( \lambda_{ij} \equiv 0 \) before solving. Since we have more equations than unknowns, we obtain a constraint. Instead, now we solve for \( \lambda_{ij} \) symbolically, and substitute \( \lambda_{ij} \equiv 0 \) afterwards. Hence, we will obtain the same constraint which lies in \( Z \) (defined in Theorem 3.2).

Corollary 3.3 provides an alternate approach to finding constraints which is less computationally intensive in dense graphs with only a few missing edges.

**Example 3.4.** Consider the DAG where there is a missing edge (dotted) between vertices 1 and 3.

\[
\begin{array}{c}
1 \\
\rightarrow \\
2 \\
\rightarrow \\
3
\end{array}
\]

If we solve \( \Lambda \) with the directed edge \( \lambda_{13} \) present, we obtain \( \lambda_{13} = \frac{\sigma_{13-2}}{\sigma_{11-2}} \). Recall that the conditional covariance in a multivariate Gaussian is \( \Sigma_{A,B} = \Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA} \). Now, we can obtain the constraint by equating \( \lambda_{13} = 0 \) and clearing denominators:

\[
\lambda_{13} = \frac{\sigma_{13-2}}{\sigma_{11-2}} = 0 \implies \sigma_{13}\sigma_{22} - \sigma_{12}\sigma_{23} = 0,
\]

which is precisely the constraint that \( X_1 \) is independent of \( X_3 \) given \( X_2 \).
4. An Algorithm for Computing the Vanishing Ideal

The proof of Theorem 3.2 provides us with a natural algorithm for finding \( \mathcal{I}(G) \) given \( G \). Indeed, suppose \( G \) has \( v \) vertices. For rows \( j = 2 \) to \( j = v \), we consider a subset of the equations

\[
\begin{align*}
  b_{j1} &= a_{j1} = \omega_{j1} , \\
  b_{j2} &= a_{j2} - \lambda_{12}a_{j1} = \omega_{j2} , \\
  &\vdots \\
  b_{j,j-1} &= a_{j,j-1} - \sum_{\ell=1}^{j-2} \lambda_{\ell,j-1}a_{j\ell} = \omega_{j,j-1} ,
\end{align*}
\]

where \( \omega_{ji} \equiv 0 \). Using this system of equations, we can solve for each \( \lambda_{ij} \), obtained by expanding the \( a_{ji} \)'s, noting that each \( \lambda_{k\ell} \) for \( 1 \leq \ell \leq j-1 \) is solved in the previous iterations. If there are more equations than unknowns, we substitute the \( \lambda_{ij} \)'s into the remaining equations to obtain the required constraints.

In this section, we will provide a formal algorithm to compute for \( \mathcal{I}(G) \), \( \Lambda \) and \( \Omega \) both symbolically and numerically in terms of the true value of \( \Sigma \). We shall also discuss the complexity and provide some applications for this algorithm.

4.1. Matrix Equations

Suppose \( i < j \) in the topological ordering. Further suppose that \( \lambda_{k\ell} \) is known for all \( k < \ell < j \) as they were computed earlier in the algorithm. Recall that if we have \( \omega_{ij} = \omega_{ji} = 0 \), equating the entries of the symmetric matrix \( B \) with \( \Omega \), we obtain

\[
b_{ji} = b_{ij} = a_{ij} - \sum_{\ell=1}^{j-1} \lambda_{ij\ell}a_{i\ell} = 0 ,
\]

which can be rearranged into the matrix form:

\[
\begin{bmatrix}
  a_{i1} & \cdots & a_{i,j-1}
\end{bmatrix}
\begin{bmatrix}
  \lambda_{1j} \\
  \vdots \\
  \lambda_{j-1,j}
\end{bmatrix}
= [a_{ij}] .
\]

Furthermore, recall that in a bow-free graph, if \( \lambda_{ij} \neq 0 \), we must have \( \omega_{ij} = 0 \). Suppose \( i_1, \ldots, i_m \) are the parents of \( j \). Then \( \omega_{ipj} \equiv 0 \) for \( 1 \leq p \leq m \). The system of equations where \( b_{ipj} = 0 \) gives us the following matrix equation where we can solve for \( \lambda_{ipj} \):

\[
\begin{bmatrix}
  a_{i_1i_1} & \cdots & a_{i_1i_m} \\
  \vdots & \ddots & \vdots \\
  a_{i_mi_1} & \cdots & a_{i_mi_m}
\end{bmatrix}
\begin{bmatrix}
  \lambda_{i_1j} \\
  \vdots \\
  \lambda_{i_mj}
\end{bmatrix}
= \begin{bmatrix}
  a_{i_1j} \\
  \vdots \\
  a_{i_mj}
\end{bmatrix} .
\] (5)

Each \( a_{ipk} \) is known since \( a_{ipk} = \sigma_{ipk} - \sum_{\ell=1}^{i_{p-1}} \lambda_{ip\ell}\sigma_{\ell k} \), where each \( \lambda_{ip\ell} \) is solved from previous iterations as \( i_p \) is a parent of \( j \). Hence, the matrix equation indeed solves for \( \lambda_{kj} \) for all \( 1 \leq k \leq j-1 \). This leads to an algorithm for computing each regression coefficients \( \lambda_{ij} \) symbolically.
Algorithm 1.

Input: ADMG $G$ and a topological ordering.
Output: Symbolic values of all regression coefficients as a matrix $\Lambda = (\lambda_{ij})$.
Initialise: $j = 2$;
while $j \leq v$ do
  for $i_1, \ldots, i_m$ parents of $j$ do
    Solve for $\lambda_{i_p,j}$ for all $1 \leq p \leq m$ using the equation:
    $\begin{bmatrix} \lambda_{i_1,j} \\ \vdots \\ \lambda_{i_m,j} \end{bmatrix} = \begin{bmatrix} a_{i_1 i_1} & \cdots & a_{i_1 i_m} \\ \vdots & \ddots & \vdots \\ a_{i_m i_1} & \cdots & a_{i_m i_m} \end{bmatrix}^{-1} \begin{bmatrix} a_{i_1 j} \\ \vdots \\ a_{i_m j} \end{bmatrix}$,
    where $a_{ij} = \sigma_{ij} - \sum_{\ell=1}^{i-1} \lambda_{\ell i} \sigma_{\ell j}$.
  end
  $j = j + 1$.
end
return $\Lambda = (\lambda_{ij})$.

If we were given the numerical values of $\Sigma$, Algorithm 1 could also be used to compute the values of $\Lambda$ numerically. Alternatively, Algorithm 1 could be used to estimate $\Lambda$ given a sample covariance matrix $S$ by replacing the values of $\Sigma$ with $S$. We will see more of this in Example 4.6 and Section 5. After obtaining either the numeric or the symbolic values of $\Lambda$, we can compute the numeric or symbolic values for $\Omega$ respectively using the equation

$$\Omega = (I - \Lambda)^T \Sigma (I - \Lambda).$$

If both $\Lambda$ and $\Omega$ were computed symbolically, we could proceed to find the minimal generators for $\mathcal{I}(G)$.

Algorithm 2.

Input: Symbolic values of the $v \times v$ matrices $\Lambda$ and $\Omega$.
Output: A set of minimal generators for $\mathcal{I}(G)$.
Initialise: $\mathcal{I}(G) = \emptyset$;
for $j$ in $[2, v]$ do
  for $i$ in $[1, j]$ do
    if $\lambda_{ij} \equiv 0$ and $\omega_{ij} \equiv 0$; # i.e. vertices $i$ and $j$ are not adjacent
      then
        $b_{ij} = \sigma_{ij} - \sum_{k=1}^{j-1} \lambda_{kj} a_{ik}$; # where $\lambda$'s and $a$'s are in terms of $\sigma$'s.
        $\mathcal{I}(G) = \mathcal{I}(G) \cup \{b_{ij}\}$
      end
  end
end
return $\mathcal{I}(G)$.
The fact that the generators found are minimal follows from Corollary B.4. Note that while $\Lambda$ and $\Omega$ can be computed numerically, $I(G)$ must be computed symbolically.

**Warning:** If $\mathcal{M}(G)$ is not globally identifiable, there may be certain specific numerical values of $\Sigma$ such that at least one matrix in Algorithm 1 is singular. However, this would only affect the numerical computation for $\Lambda$. Furthermore, we can almost surely estimate $\Lambda$ from the sample covariance $S$ using Algorithm 1 numerically, as the set of troublesome points has zero measure within the model and hence should not occur empirically. We will provide an example of this later in Example 5.7.

### 4.2. Time Complexity

In this section, we show that while our algorithms can compute $\Lambda$ and $\Omega$ numerically in polynomial time, this is not the case for symbolic computations.

#### 4.2.1. Numerical Computations

We first introduce a naive bound for the numerical complexity of the above algorithm based on the number of vertices of $G$. We shall also assume that our numeric values of $\Sigma$ do not result in any singular matrices in Algorithm 1.

**Proposition 4.1.** Suppose $G$ is a bow-free ADMG with $v$ vertices. Then the complexity of finding $\Lambda$ and $\Omega$ numerically is at most $O(v^4)$.

**Proof.** The complexity of solving $k$ equations with $k$ unknowns using naive Gauss-Jordan elimination is $O(k^3)$. In our algorithm for finding the values of $\lambda_{ij}$’s, we first solve a linear equation with at most one unknown, then two linear equations with at most two unknowns and so on until we solved $v - 1$ linear equations with at most $v - 1$ unknowns. Since we have repeated this process $v - 1$ times, the complexity of finding the values of $\lambda_{ij}$’s is at most $O(v^4)$. Finally, since the complexity of matrix multiplication is $O(v^3)$, we can compute both $\Lambda$ and $\Omega$ in $O(v^4)$.

One might notice that each unknown $\lambda_{ij}$ corresponds precisely to a directed edge in $G$. Let $d$ be the number of directed edges in $G$. In a sparse graph where $d$ is small, it might be beneficial to express the complexity in terms of $d$ instead.

**Proposition 4.2.** Suppose $G$ is a bow-free ADMG with $d$ directed edges. The complexity of finding $\Lambda$ numerically is at most $O(d^3)$.

**Proof.** This follows from the fact that we have at least $d$ equations with exactly $d$ unknowns. Observe that each time when we apply the Gauss-Jordan elimination, we can solve for any subset of the $d$ unknowns. Therefore, we obtain the following optimization problem:

$$\begin{align*}
\text{maximise} & \quad O(k_1^3 + \cdots + k_d^3) \\
\text{subject to} & \quad k_1 + \cdots + k_d = d \\
\text{where} & \quad k_1, \ldots, k_d \in \mathbb{Z}_{\geq 0}.
\end{align*}$$

since the cubic term grows faster than the linear term, the maximum is obtained when $k_i = d$ for some $i$ and $k_j = 0$ for all $j \neq i$. \qed
Corollary 4.3. Suppose $G$ is a bow-free ADMG with $v$ vertices. Furthermore, suppose each vertex in $G$ has at most $p$ parents. Then the complexity of finding $\Lambda$ numerically is at most $O(vp^3)$.

**Proof.** We use the Gauss-Jordan elimination at most $v$ times, solving for at most $p$ unknowns each time. \qed

### 4.2.2. Symbolic Complications

Now, we will show that our algorithm does not run symbolic calculations in polynomial time by providing a simple counter-example. Since finding the generators of $\mathcal{I}(G)$ requires symbolic computation, we cannot compute $\mathcal{I}(G)$ in polynomial time in general.

Consider a complete DAG such as the graph shown below.

![Graph](image_url)

Using our algorithm, solving for $\Lambda$ symbolically, we obtain

$$
\lambda_{14} = \sigma_{14}/\sigma_{11}, \lambda_{24} = \sigma_{24}/\sigma_{22}, \lambda_{34} = \sigma_{34}/\sigma_{33}.
$$

In particular, the regression coefficient $\lambda_{ij}$ is precisely $\sigma_{ij} \cdot \text{pa}(i)/\sigma_{ii} \cdot \text{pa}(i)$ in a DAG \cite{17}. Recall that the conditional covariance matrix of a multivariate normal distribution is given by

$$
\Sigma_{AA-B} = \Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA}.
$$

Now, there are $|B|!$ different terms in $\det(\Sigma_{BB})$. Since $\sigma_{ij} \propto \det(\Sigma_{iV,jV})$ which has $(|V| + 1)!$ terms, the number of terms in $\lambda_{ij}$ increases factorially with respect to $|\text{pa}(i)|$. As Algorithm 1 requires us to invert matrices with entries as functions of $\lambda$, we could not solve for $\Lambda$ symbolically in polynomial time.

### 4.3. Applications and Examples

In this section, we shall first start with an example in which we compute $\Lambda$ and $\mathcal{I}(G)$ symbolically. We will then explore some applications of our algorithm such as using it for model verification.

#### 4.3.1. Finding minimal generators of $\mathcal{I}(G)$

We shall start with a simple symbolic example where we find the minimal generators for $\mathcal{I}(G)$.

**Example 4.4.** Let $G$ be the Verma graph in Figure 1; we have

$$
\Lambda = \begin{bmatrix}
0 & \lambda_{12} & \lambda_{31} & 0 \\
0 & 0 & \lambda_{23} & 0 \\
0 & 0 & 0 & \lambda_{34} \\
0 & 0 & 0 & 0
\end{bmatrix}, \quad \Omega = \begin{bmatrix}
\omega_{11} & 0 & 0 & 0 \\
0 & \omega_{22} & \omega_{24} & 0 \\
0 & 0 & \omega_{33} & 0 \\
0 & \omega_{24} & 0 & \omega_{44}
\end{bmatrix}.
$$
In particular, the entries \( \lambda_{14} = \lambda_{24} = 0 \) and the only non-zero off-diagonal entry of \( \Omega \) is \( \omega_{24} \). In the first iteration of our algorithm, we obtain \( \lambda_{12} = \sigma_{11}^{-1} \sigma_{12} \). In the second iteration, we have

\[
\begin{bmatrix}
\lambda_{13} \\
\lambda_{23}
\end{bmatrix} = \begin{bmatrix}
a_{11} & a_{12} \\
a_{21} & a_{22}
\end{bmatrix}^{-1}
\begin{bmatrix}
a_{13} \\
a_{23}
\end{bmatrix},
\]

where \( a_{ij} = \sigma_{ij} - \sum_{k=1}^{i-1} \lambda_{ki} \sigma_{kj} \). Solving this matrix equation, we obtain

\[
\lambda_{13} = \frac{\sigma_{13} - \sigma_{12}}{\sigma_{11}} \quad \text{and} \quad \lambda_{23} = \frac{\sigma_{23} - \sigma_{22}}{\sigma_{21}}.
\]

In the last iteration, we have \( \lambda_{34} = a_{33}^{-1} a_{34} = \sigma_{34} / \sigma_{33} \). Note that we could have computed \( \Omega \) symbolically by equation (3). Finally, since the only pair of non-adjacent vertices are 1 and 4, we have

\[
\mathcal{I}(G) = \langle b_{41} \rangle = \langle \sigma_{14} - \sum_{k=1}^{3} \lambda_{k4} \sigma_{1k} \rangle = \langle \sigma_{14} - \lambda_{34} \sigma_{13} \rangle
\]

\[
= \langle \sigma_{11} \sigma_{13} \sigma_{22} \sigma_{34} - \sigma_{12}^2 \sigma_{13} \sigma_{34} - \sigma_{11} \sigma_{14} \sigma_{22} \sigma_{33} + \sigma_{12} \sigma_{14} \sigma_{33} \rangle
\]

\[
- \sigma_{11} \sigma_{13} \sigma_{23} \sigma_{24} + \sigma_{11} \sigma_{14} \sigma_{23}^2 + \sigma_{12} \sigma_{13}^2 \sigma_{24} - \sigma_{12} \sigma_{13} \sigma_{14} \sigma_{23},
\]

which is exactly what we have in Example 1.1. Note that the second to last equality comes from the fact that both \( \lambda_{14} \equiv 0 \) and \( \lambda_{24} \equiv 0 \).

Note that in this specific example, we are able to express each \( \lambda_{ij} \) as a rational with a strictly positive denominator (of the form \( \sigma_{aa,b} \)). However, this might not be the case if the graph is not globally identifiable.

### 4.3.2. Model Selection

Now, suppose we have a dataset \( X \) generated from \( N(0, \Sigma) \). Given such a data set \( X \) and a graphical model \( G \), we want to test \( H_0 : \Sigma \in \mathcal{M}(G) \) against \( H_1 : \Sigma \notin \mathcal{M}(G) \). In the first example, we shall test for \( H_0 \) given that we know a generating set of \( \mathcal{I}(G) \). We denote this generating set as \( Z \).

**Example 4.5 (Model selection using \( Z \)).** Suppose we have four variables. We shall first fix \( \Sigma \) by picking the following values for \( \Lambda \) and \( \Omega \):

\[
\Lambda = \begin{bmatrix}
0 & 0.5 & 0.25 & 0 \\
0 & 0 & 0.5 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0
\end{bmatrix} \quad \text{and} \quad \Omega = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0.25 \\
0 & 0 & 1 & 0 \\
0 & 0.25 & 0 & 1
\end{bmatrix}.
\]

Now, we generate a dataset \( X \) where we sample 1000 data points from \( N(0, \Sigma) \). Now, suppose that we only observe \( X \) (and not \( \Sigma \)) and want to test if \( \Sigma \) fits our Verma model \( \mathcal{M}(G) \).

For each \( f \in Z \), we can use bootstrap to generate multiple sample covariance matrices and test whether \( f = 0 \) is in the 95% confidence interval. In the Verma model, we only have one such polynomial \( f \in Z \). In our case, the 95% confidence interval is \((-0.125, 0.0675)\). Hence, we do not have sufficient evidence to reject \( H_0 \).

Repeating the above simulation 1000 times where we generate a different dataset \( X \) each iteration, we found that in 940 of the cases, 0 is contained in the 95% confidence interval.
On the other hand, we can also provide a non-example. For instance, if we generate some $\Sigma \notin \mathcal{M}(G)$, where $G$ is still the Verma graph, by changing the numerical values of $\Lambda$ to be

$$
\Lambda = \begin{bmatrix}
0 & 0.5 & 0.25 & 0.2 \\
0 & 0 & 0.5 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0
\end{bmatrix}.
$$

Clearly, $\Sigma \notin \mathcal{M}(G)$ since there is a missing edge between 1 and 4 but $\lambda_{14} \neq 0$.

Repeating the simulation in Example 4.5 with this new value of $\Sigma$, we obtain that the 95% confidence interval is $(-0.409, -0.179)$. In particular, 0 is no longer in the confidence interval. This is expected since our dataset $X$ is now generated from $N(0, \Sigma)$ for some $\Sigma \notin \mathcal{M}(G)$. Hence, we have strong evidence to reject $H_0$. In fact, repeating this simulation 1000 times as before, we see that 0 is not contained in the 95% confidence interval for any of those cases.

While the previous example did provide us with a method to test for verification, we have previously seen that the algorithm for computing $Z$ does not run in polynomial time. In fact, there is an efficient way of testing $H_0 : \Sigma \in \mathcal{M}(G)$ against $H_1 : \Sigma \notin \mathcal{M}(G)$ without finding $Z$ explicitly.

Using Corollary 3.3, instead of testing $f = 0$ for each $f \in Z$, we could test for $\lambda_{ij} = 0$ for each pair of non-adjacent vertices $i$ and $j$, with the assumption that $\lambda_{ij} \neq 0$. This is done by first adding a directed edge between vertices $i$ and $j$ and running a bootstrap on the sample to produce a covariance matrix, which is then used as an input in Algorithm 1. We have already seen in Proposition 4.1 that this can be done in $O(n^4)$ time.

**Example 4.6 (Model Selection without $\mathcal{I}(G)$).** Let $G$ be the Verma graph and $\Sigma$ be the same covariance matrix as in Example 4.5. Let $e$ be the directed edge pointing from vertex 1 to 4. Once again, we shall first generate a dataset $X$ by sampling 1000 data points from $N(0, \Sigma)$. Next, we use a bootstrap to generate multiple sample covariance matrices. For each sample covariance matrix, we apply Algorithm 1 to the graph $G \cup \{e\}$, where we assume there is a directed edge between vertex 1 and 4 (so $\lambda_{14} \neq 0$). In our case, the 95% confidence interval for $\lambda_{14}$ is $(-0.0530, 0.0917)$ which contains 0. Hence, we do not have sufficient evidence to reject $H_0$.

Once again, generating 1000 different samples of $X$ and re-running this simulation, we found that in 940 of the cases, 0 is in the 95% confidence interval.

## 5. Fitting bow-free ADMGs

While the bootstrap in Example 4.6 does allow us to test for $\Sigma \in \mathcal{M}(G)$ in polynomial time, we have to run the bootstrap once for each missing edge. For sparse graphs, we might have to run several bootstraps which is inefficient. In this section, we shall first fit a dataset $X$ to a given graphical model $G$ by the maximum likelihood. We shall first use Algorithm 1 and equation (3) to find starting points for $\Lambda$ and $\Omega$, then we will use hill-climbing to find the MLEs $\hat{\Lambda}$, $\hat{\Omega}$ and $\hat{\Sigma}$. We can then use the likelihood ratio test to test $H_0 : \Sigma \in \mathcal{M}(G)$ against $H_1 : \Sigma \notin \mathcal{M}(G)$.

### 5.1. Convexity of the Log-Likelihood Function

The strict concavity of the log-likelihood function for an unconstrained Gaussian model is well known [26]. We shall adapt the proof to show that this function is also strictly concave in $\mathcal{M}(G)$. 
We know that the log-likelihood function for the covariance matrix $\Sigma$ is given by
\[
\ell(\Sigma) = -\frac{n}{2} \log \det \Sigma - \frac{n}{2} \text{tr}(S\Sigma^{-1}).
\]

Now, suppose that we want to maximise $\ell(\Sigma)$ such that we still have $\Sigma \in \mathcal{M}(G)$. We can substitute $\Sigma = (I - \Lambda)^{-T} \Omega (I - \Lambda)^{-1}$ into the log-likelihood function to ensure that $\Sigma \in \mathcal{M}(G)$. The objective function hence becomes
\[
\ell(\Lambda, \Omega) = \frac{n}{2} \log \det K - \frac{n}{2} \text{tr}(SK),
\]
where $K = \Sigma^{-1} = (I - \Lambda)\Omega^{-1}(I - \Lambda)^T$. Now, let $A \in \mathbb{R}^D$ and $B$ be a symmetric matrix. We have
\[
\nabla \ell(\Lambda, \Omega) = \frac{n}{2} \text{tr}(K^{-1} \nabla K) - \frac{n}{2} \text{tr}(S \nabla K),
\]
\[
\nabla^2 \ell(\Lambda, \Omega) = -\frac{n}{2} \text{tr}(K^{-1} \nabla K K^{-1} \nabla K - K^{-1} \nabla^2 K)) - \frac{n}{2} \text{tr}(S \nabla^2 K),
\]
where we shorten $\nabla_{A \times B} \ell$ to $\nabla$ for the sake of cleanliness, and
\[
\nabla K = -A \Omega^{-1}(I - \Lambda)^T - (I - \Lambda)\Omega^{-1}B \Omega^{-1}(I - \Lambda)^T - (I - \Lambda)\Omega^{-1}A^T,
\]
\[
\nabla^2 K = 2A \Omega^{-1}B \Omega^{-1}(I - \Lambda)^T + 2A \Omega^{-1}A^T + 2(I - \Lambda)\Omega^{-1}B \Omega^{-1}B \Omega^{-1}(I - \Lambda)^T + 2(I - \Lambda)\Omega^{-1}B \Omega^{-1}A^T.
\]

Lemma 5.1. Both $\nabla K$ and $\nabla^2 K$ are symmetric matrices.

Proof. First, note that $B$ is a symmetric matrix. Next, notice that $(I - \Lambda)\Omega^{-1}B \Omega^{-1}(I - \Lambda)^T$ is the conjugate transpose of a symmetric matrix is hence also symmetric. Finally, the first and last terms of $\nabla K$ are transposes of each other. Since $C + C^T$ is a symmetric matrix for any matrix $C$, $\nabla K$ is a symmetric matrix. Using similar arguments, one can also deduce that $\nabla^2 K$ is symmetric.

Theorem 5.2. If $\nabla K \neq 0$, then there exists an $\alpha > 1$ such that the log-likelihood function $\ell(\Sigma)$ is strictly concave on the region $\{\Sigma \in \mathcal{M}(G) : 0 < \Sigma < \alpha S\}$.

Proof. Note that the second derivative can be rewritten as
\[
\nabla^2 \ell(\Lambda, \Omega) = -\frac{n}{2} \text{tr}((\nabla K)^{1/2} K^{-1} (\nabla K)^{1/2}) - \frac{n}{2} \text{tr}(S(\nabla^2 K)^{1/2}).
\]

Since both $K^{-1} = \Sigma$ and $S$ are positive definite matrices and both $\nabla K$ and $\nabla^2 K$ are symmetric, each of the matrices $(\nabla K)^{1/2} \Sigma (\nabla K)^{1/2}$, $(\nabla^2 K)^{1/2} \Sigma (\nabla^2 K)^{1/2}$ and $(\nabla^2 K)^{1/2} S (\nabla^2 K)^{1/2}$ are positive semi-definite. Therefore, we have both $\text{tr}(\Sigma \nabla^2 K) \geq 0$ and $\text{tr}(S \nabla^2 K) \geq 0$.

Furthermore, the matrix $U = (\nabla K)^{1/2} \Sigma (\nabla K)^{1/2}$ is positive semi-definite and hence has positive eigenvalues. Since $\nabla K \neq 0$ and $\Sigma$ is full-rank (as it is positive definite), there is at least one strictly positive eigenvalue. Pick $\varepsilon = \text{tr}(U^2) > 0$.

Now, pick $\alpha > 1$ to be the largest such that if $\Sigma \prec \alpha S$, we have $\text{tr}(\Sigma \nabla^2 K) - \text{tr}(\alpha S \nabla^2 K) < \varepsilon$. Note that such a choice of $\alpha$ exists since if $\alpha = 1$, $\Sigma \prec S$ and we have $\text{tr}(\Sigma \nabla^2 K) - \text{tr}(S \nabla^2 K) < 0$. Hence, $\nabla^2 \ell < 0$ and therefore, $\ell$ is concave on this region. \qed
Corollary 5.3. For a large enough sample size, we can find the supremum of $\ell(\Sigma)$ for $\Sigma \in \mathcal{M}(G)$ using a hill-climbing algorithm.

Proof. Fix $\alpha > 1$ to be the constant in Theorem 5.2. For a large enough sample, we have that $0 \prec \Sigma \prec \alpha S$. Furthermore, in each iteration of the hill climbing, $\nabla K \neq 0$ as we will be terminating otherwise. Hence $\ell(\Sigma)$ is concave by Theorem 5.2.

5.2. MLE and Hypothesis Testing

We shall start by finding the MLE of $\Sigma$, given $\Sigma \in \mathcal{M}(G)$, by the hill-climbing algorithm through maximising $\Lambda$ and $\Omega$. We will then use a likelihood ratio test to decide whether we should reject $H_0$.

First, to run the hill-climbing algorithm mentioned in Corollary 5.3, we need a starting point for $\Lambda$ and $\Omega$. Fortunately, we can obtain a starting point for $\Lambda$, denoted $\tilde{\Lambda}$, from applying the sample covariance matrix $S$ to Algorithm 1. In particular, $\tilde{\Lambda} \in \mathbb{R}^D$. Now, from $\tilde{\Lambda}$, we can also obtain a starting point for $\Omega$, denoted $\tilde{\Omega}$ using the equations from Section 3:

$$\tilde{\omega}_{ij} = b_{ij} = a_{ij} - \sum_{\ell=1}^{j-1} \tilde{\lambda}_{\ell j} a_{i\ell}, \quad \text{where} \quad a_{ij} = S_{ij} - \sum_{\ell=1}^{i-1} \tilde{\lambda}_{\ell i} S_{\ell j}. \quad (7)$$

We will see in Section 5.3 that while $\tilde{\Omega}$ might not be positive definite, it is positive definite for a large enough sample size.

Proposition 5.4. If $\Sigma \in \mathcal{M}(G)$ and both $\Lambda$ and $\Omega$ are defined, then $\tilde{\Lambda}$ and $\tilde{\Omega}$ are $\sqrt{n}$-consistent estimators of $\Lambda$ and $\Omega$ respectively.

Proof. Since $S$ is a consistent estimator of $\Sigma$, $S$ converges to $\Sigma$ in probability. The symbolic values of both $\tilde{\Lambda}$ and $\Lambda$ are obtained by applying Algorithm 1 to $S$ and to $\Sigma$ respectively. In the former application, $\tilde{\Lambda}$ is expressed symbolically as additions and multiplications of the random variables $S_{ij}$, each converging in probability to $\sigma_{ij}$. Since $\Lambda$ is defined (ie. no entry is divided by zero), $\tilde{\Lambda}$ converges to $\Lambda$ in probability. Similarly, $\tilde{\Omega}$ is also expressed symbolically as additions and multiplications of $\lambda_{ij}$ and $S_{ij}$ by (7), each converging in probability to $\lambda_{ij}$ and $\sigma_{ij}$ respectively. Hence, $\tilde{\Omega}$ converges to $\Omega$ in probability.

Now since $S$ is $\sqrt{n}$-consistent for $\Sigma$ and the map from $S$ to $\tilde{\Lambda}$ and $\tilde{\Omega}$ is differentiable and non-singular, we get that $\tilde{\Lambda}$ and $\tilde{\Omega}$ are also $\sqrt{n}$-consistent for $\Lambda$ and $\Omega$ respectively.

Corollary 5.5. If $\Sigma \in \mathcal{M}(G)$, then $\tilde{\Sigma} = (I - \tilde{\Lambda})^{-T} \tilde{\Omega}(I - \tilde{\Lambda})^{-1}$ is a $\sqrt{n}$-consistent estimator for $\Sigma$.

Now, for the iterative step, we want to find the derivative of $\ell$ with respect to the entries in $\Lambda$ and $\Omega$. Observe that $\det((I - \Lambda)^{-T} \Omega(I - \Lambda)^{-1}) = \det(\Omega)$, the objective function we want to maximise becomes

$$\ell(\Lambda, \Omega) = -\frac{n}{2} \log \det \Omega - \frac{n}{2} \tr(S(I - \Lambda)\Omega^{-1}(I - \Lambda)^T).$$
Differentiating, we obtain
\[\frac{\partial \ell}{\partial \Lambda} = 2S(I - \Lambda)\Omega^{-1},\]
where \(\langle , \rangle\) denotes the Frobenius inner product with \(\langle M_1, M_2 \rangle = \text{tr}(M_1^T M_2)\). Hence, our partial derivatives are
\[\frac{\partial \ell}{\partial \Lambda} = 2S(I - \Lambda)\Omega^{-1},\]
and the partial derivatives \(\frac{\partial \ell}{\partial \Omega} = \Omega^{-1}(I - \Lambda)^T S(I - \Lambda)\Omega^{-1} - \Omega^{-1}\),
\[\frac{\partial \ell}{\partial \Omega} = \Omega^{-1}(I - \Lambda)^T S(I - \Lambda)\Omega^{-1} - \Omega^{-1},\]

and the partial derivatives \(\frac{\partial \ell}{\partial \lambda_{ij}}\) and \(\frac{\partial \ell}{\partial \omega_{ij}}\) are the \(ij\)-entries of \(\frac{\partial \ell}{\partial \Lambda}\) and \(\frac{\partial \ell}{\partial \Omega}\) respectively.

Let \(\hat{\Lambda}\) and \(\hat{\Omega}\) be the matrices found after applying the hill-climbing algorithm above from the starting points \(\tilde{\Lambda}\) and \(\tilde{\Omega}\). Let \(\hat{\Sigma} = (I - \hat{\Lambda})^{-T} \hat{\Omega}(I - \hat{\Lambda})^{-1}\). From Corollary 5.3, if \(\Sigma \in \mathcal{M}(G)\), \(\hat{\Sigma}\) is the MLE for \(\Sigma\) for sufficiently large \(n\).

**Warning:** If \(\Sigma \notin \mathcal{M}(G)\), \(\hat{\Sigma}\) might not be the MLE. This is because we might not be working in the concave region \(\{0 \prec \Sigma \prec \alpha S\}\) where the MLE resides. However the local maximum it converges to is sufficiently far enough from \(S\) that we would reject \(H_0\), recalling that the likelihood ratio statistic is \(2(\ell(S) - \ell(\hat{\Sigma}))\). Note that the \(p\)-value found here might be nonsensical.

**Example 5.6.** Let \(G\) be the Verma graph and \(\Sigma\) be the same as in Example 4.5. We first generate a dataset \(X\) by drawing 1000 samples from \(N(0, \Sigma)\). We then compute the MLE \(\hat{\Sigma}\) for \(\Sigma \in \mathcal{M}(G)\) given the dataset \(X\) using the hill-climbing algorithm above. This allows us to compute the likelihood ratio statistic. Iterating this 1000 times, we obtain the empirical CDF of the likelihood ratio statistic. In particular, when comparing to the CDF of \(\chi^2_1\), the Kolmogorov-Smirnov test gives us a \(p\)-value of 0.193 which suggests that there is no evidence that this distribution does not come from \(\chi^2_1\).

**Example 5.7 (Point of unidentifiability).** Consider a graph that is not globally identifiable in Figure 3. From Algorithm 1, we obtain
\[
\lambda_{12} = \frac{\sigma_{12}}{\sigma_{11}},
\lambda_{23} = \frac{\sigma_{23}\sigma_{11} - \sigma_{12}\sigma_{13}}{\sigma_{11}\sigma_{22} - \sigma_{12}^2} = \frac{\sigma_{23,1}}{\sigma_{22,1}},
\lambda_{34} = \frac{\sigma_{11}\sigma_{22}\sigma_{34} - \sigma_{12}\sigma_{34}^2 - \sigma_{11}\sigma_{23}\sigma_{24} + \sigma_{12}\sigma_{13}\sigma_{24}}{\sigma_{11}\sigma_{22}\sigma_{33} - \sigma_{12}\sigma_{33}^2 - \sigma_{11}\sigma_{23}^2 + \sigma_{12}\sigma_{13}\sigma_{23}}.
\]
Observe that while the denominator of $\lambda_{23}$ is strictly positive (as it is in the form of $\sigma_{aa} B$), this is not the case for $\lambda_{34}$. In particular, we can find a positive definite $\Sigma$ such that the denominator of $\lambda_{34}$ is zero. Let

$$
\Sigma = \begin{bmatrix}
1 & 0.8 & 0.4375 & 0.76 \\
0.8 & 1 & 0.8 & 0.5 \\
0.4375 & 0.8 & 1 & 0.1 \\
0.76 & 0.5 & 0.1 & 1
\end{bmatrix}.
$$

The minimum eigenvalue of $\Sigma$ is 0.0664, hence $\Sigma$ is positive definite. However, with this particular value of $\Sigma$, the denominator of $\lambda_{34}$ is zero. Hence, we are unable to run Algorithm 1 numerically using this particular value of $\Sigma$ as we will be attempting to invert a singular matrix.

On the other hand, if we were to observe some sample covariance matrix $S$, the denominator for $\lambda_{23}$ is almost surely non-zero as there is zero probability of obtaining specific values in a continuous distribution. Hence, we should, in theory, almost surely be able to use Algorithm 1 to compute $\Lambda$ numerically. Unfortunately, as the sample sizes increase, the denominator gets closer to zero, which might result in an error on most computational software.

For our choice of $\Sigma$ and graph $G$, we encountered 2 errors out of 1000 trial runs if we draw $n = 1000$ samples from $N(0, \Sigma)$. If we increase this sample size to $n = 1,000,000$, we encountered 104 errors out of the 1000 trial runs.

In practice, it is extremely unlikely that one would encounter points of unidentifiability as it requires a specific value for $\Sigma$.

### 5.3. Small Sample Size and Eigenvalues

By Corollary 5.3, in order for us to be able to find the MLE using the hill-climbing algorithm, we must have a large enough sample size. In this section, we will examine the complications of having a small sample size or if the true value of $\Sigma$ has a small eigenvalue.

We will start with exploring the complications that arise with a small sample size.

**Example 5.8.** In this example, we shall repeat the setup of Example 5.6 for smaller sample sizes of $n = 10$ and $n = 20$.

In the $n = 10$ case, comparing the empirical CDF to the CDF of $\chi^2_1$, the Kolmogorov-Smirnov test gives us a p-value below $2.2 \times 10^{-16}$ which suggests strong evidence that the empirical distribution does not come from $\chi^2_1$. In particular, the output of $\hat{\Sigma}$ from our algorithm is likely not the MLE. On the other hand, when $n = 20$, the Kolmogorov-Smirnov test has a p-value of 0.657 when comparing the empirical CDF to that of $\chi^2_1$.

The plots of the empirical CDF (black) against the CDF of $\chi^2_1$ for sample sizes $n = 10$ and $n = 20$ are shown in Figure 4 and Figure 5 respectively.

However, on even smaller sample sizes (e.g. $n = 5$), we might run into the additional problem that $\hat{\Omega}$ is not positive definite. In this case, our algorithm is unable even to run the hill-climbing algorithm since the log-likelihood will be undefined. In this case, our hill-climbing algorithm will start at $(\hat{\Lambda}, \hat{\Omega}' = \hat{\Omega} + cI)$ where $c = -(\hat{c} - 1)$, where $\hat{c}$ is the minimum eigenvalue for $\hat{\Omega}$. This ensures that $\hat{\Omega}'$ is positive definite. As with the $n = 10$ example above, the output of $\hat{\Sigma}$ from our algorithm is not the MLE and thus the resulting statistic will not converge to a $\chi^2$ distribution. Note that the same issue will arise when the minimum eigenvalue for the true value of $\Sigma$ approaches zero.
Example 5.9. Consider the ‘gadget’ graph in Figure 2. Suppose the true value of $\Omega$ is

$$
\Omega = \begin{bmatrix}
1 & \rho & 0 & \rho \\
\rho & 1 & \rho & 0 \\
0 & \rho & 1 & 0 \\
\rho & 0 & 0 & 1 \\
\end{bmatrix},
$$

where $\rho = \frac{2-2\epsilon}{1+\sqrt{3}}$ in which $\epsilon$ is very small. Then $\epsilon$ is the minimum eigenvalue of $\Omega$. Further suppose that the values of all entries in $\Lambda$ is at most one. Then the minimum eigenvalue of $\Sigma$ will be very small as well. In this example, we shall let $\lambda_{13} = \lambda_{24} = 0.25$.

Let $\epsilon = 0.1$. After simulating data with a sample size of $n = 1000$ and iterating 1000 times, the empirical CDF we obtained closely matches to that of $\chi_1^2$ (p-value 0.854 by KS test) as shown in Figure 6. However, for $\epsilon = 0.01$, simulated data with a sample size of $n = 100,000$ might produce an estimate $\tilde{\Omega}$ that is not positive definite. Even when we repeat the simulation a sample size of $n = 1,000,000$, the empirical CDF does not come from the $\chi_1^2$ distribution as seen in Figure 7.

Proposition 5.10. Let $\epsilon \ll 1$ be the minimum eigenvalue for $\Sigma$. Then for every $0 < \alpha < 1$, the
approximate sample size required for the estimate $\hat{\Omega}$ to be positive definite with probability $1 - \alpha$ is $O(1/\epsilon^2)$

**Proof.** First note that the eigenvalues of a matrix with continuous entries are themselves continuous functions [15]. Furthermore, the minimum of two continuous functions is continuous. Therefore, the minimum eigenvalue of a matrix with continuous entries is a continuous function. But $\hat{\Omega}$ is a $\sqrt{n}$-consistent estimator of $\Omega$ by Proposition 5.4; the empirical value of $\epsilon$ comes from either a Gaussian or sub-Gaussian distribution with mean $\epsilon$ and variance $O(1/n)$ which we denote $D(\epsilon, O(1/n))$. If $n = O(1/\epsilon^2)$, we can draw a positive number from $D(\epsilon, O(\epsilon^2))$ with probability $1 - \alpha$ for any $0 < \alpha < 1$. \qed

6. Real Data Example

In this section, we shall showcase an application of our algorithm to validating a graphical model given a real dataset. In the study of American occupational structure [4], the following covariates were measured with a sample size of $n = 20700$:

- $V$: Father’s educational attainment,
- $X$: Father’s occupational status,
- $U$: Son’s educational attainment,
- $W$: Son’s status of first job,
- $Y$: Son’s status of occupation in 1962.

The data can be summarised as the following correlation matrix of $(V, X, U, W, Y)$:

$$S = \begin{bmatrix}
1.000 & 0.516 & 0.453 & 0.332 & 0.322 \\
0.516 & 1.000 & 0.438 & 0.417 & 0.405 \\
0.453 & 0.438 & 1.000 & 0.538 & 0.596 \\
0.332 & 0.417 & 0.538 & 1.000 & 0.541 \\
0.322 & 0.405 & 0.596 & 0.541 & 1.000
\end{bmatrix}.$$ 

At the significance level of $\alpha = 0.01$, the FCI algorithm [20] removes the edge between $V$ and $Y$ based on the conditional independence $Y \perp V \mid U, X$. At significance level $\alpha = 0.0001$, the FCI algorithm removes an additional edge between $V$ and $W$ based on the $m$-separation $W \perp V \mid U, X$. The skeletons identified by the FCI algorithm are shown in Figure 8 where the $o$—edgemark can be either a tail or an arrowhead.

![Figure 8](image-url)  
*Figure 8.* Skeleton inferred using the FCI algorithm with $\alpha = 0.01$ (left) and $\alpha = 0.0001$ (right).
Next, we produced valid graphical models based on the skeletons in Figure 8, the first of which satisfies the conditional independence $Y \independent V \mid U, X$ with the second satisfying both conditional independence $Y \independent V \mid U, X$ and $W \independent V \mid U, X$. These models are shown in Figure 9. Notice that our second graphical model is identical to the first with the edge $V \rightarrow W$ removed.

[Figure 9. Valid graphical models based on the $m$-separations.]

Using our algorithm to fit the correlation matrix to the first model, we obtain a p-value of 0.308. This shows that there is no evidence that the data collected did not come from the first model. However, comparing the MLE of the first and second model and running a likelihood ratio test, we found a p-value of $3.58 \times 10^{-5}$, indicating strong evidence of causal effect by the variable $V$ on $W$ in the context of the model. The reader could refer to [11] and [20] for a different application of the sample data.

7. Discussion

We have proven that, given a bow-free ADMG $G$, there is a one-to-one correspondence between the minimal generators in the vanishing ideal $\mathcal{I}(G)$ and non-adjacent vertices in $G$. The proof of this theorem provides us with a natural algorithm (Algorithm 1) to find $\sqrt{n}$-consistent estimators, $\tilde{\Lambda}$ and $\tilde{\Omega}$, for $\Lambda$ and $\Omega$ respectively. It can also be expanded to compute for $\mathcal{I}(G)$ (Algorithm 2). We further proved that while the numeric solutions for $\tilde{\Lambda}$ and $\tilde{\Omega}$ can be found in polynomial time, symbolic calculations using this algorithm are not tractable in general. At the time of writing, there are no algorithms that can compute $\mathcal{I}(G)$ in polynomial time.

We have also provided an efficient algorithm to fit a Gaussian ADMG using maximum likelihood. Unlike the RICF algorithm [6], our algorithm uses the hill-climbing algorithm, which is objectively faster than iterating regressions.

Appendix A: Commutative Algebra

Here, we shall introduce the basics of commutative algebra and algebraic geometry required to understand the paper. We will mainly be referring to Atiyah-Macdonald [2] for commutative algebra and Cox et al. [5] for algebraic geometry.

**Definition A.1.** A ring $R$ is a set with two binary operations (addition and multiplication) such that:

1. $R$ is an abelian group with respect to addition, that is
(a) \((a + b) + c = a + (b + c)\) for every \(a, b, c \in R\) (i.e. addition is associative).

(b) \(a + b = b + a\) for every \(a, b \in R\) (i.e. addition is commutative).

(c) There is an additive identity \(0 \in R\) such that \(a + 0 = a\) for all \(a \in R\).

(d) For each \(a \in R\), there is an additive inverse \(-a \in R\) such that \(a + (-a) = 0\).

2. Multiplication is associative.

3. Multiplication is distributive over addition, that is \(a(b + c) = ab + ac\) and \((b + c)a = ba + ca\) for all \(a, b, c \in R\).

4. There is a multiplicative identity \(1 \in R\) such that \(a1 = 1a = a\) for all \(a \in R\).

A unit in a ring \(R\) is an element \(a\) which “divides 1” (i.e. there exists \(b \in R\) such that \(ab = 1\)).

A field is a ring \(R\) where \(1 \neq 0\) and every non-zero element is a unit.

**Definition A.2.** We say that \(I\) is an ideal of a ring \(R\), denoted \(I \triangleleft R\), if

1. for every \(x, y \in I\), \(x + y \in I\).
2. for every \(x \in I\) and \(a \in R\), \(ax \in I\).

Let \(<x_1, \ldots, x_n>\) denote the ideal generated by \(x_1, \ldots, x_n\). In particular, we have \(<1> = R\). An ideal \(p\) is prime if \(p \neq <1>\) and if \(xy \in p\), then either \(x \in p\) or \(y \in p\). An ideal \(m\) is maximal if \(m \neq <1>\) and there do not exist an ideal \(a\) such that \(m \subsetneq a \subsetneq <1>\). Note that all maximal ideals are prime, but the converse does not hold in general.

**Definition A.3.** We say that a ring \(R\) is Noetherian if every ideal \(I \triangleleft R\) is finitely generated (i.e. \(\exists f_1, \ldots, f_N\) such that \(I = \langle f_1, \ldots, f_N \rangle\)).

**Theorem A.4** (Hilbert Basis Theorem). If \(R\) is a Noetherian ring, then \(R[X]\) is also a Noetherian ring.

**Proof.** See Theorem 7.5 of \([2]\). \(\square\)

For any field \(k\), the only ideals are \(<0>\) and \(<1>\). Hence, every field is Noetherian. In particular, \(\mathbb{R}\) is Noetherian. By the Hilbert Basis Theorem, \(\mathbb{R}(\Sigma)\) is a Noetherian ring.

**Definition A.5.** We say that a chain of prime ideals has length \(m\) if there is a strict chain of inclusions \(p_0 \subsetneq p_1 \subsetneq \cdots \subsetneq p_m\) where each \(p_i\) is a prime ideal. The height \(\text{ht}(p)\) of a prime ideal \(p\) is the supremum of the lengths of all chains of prime ideals contained in \(p\).

\[
\text{ht}(p) = \sup \{m : p_0 \subsetneq p_1 \subsetneq \cdots \subsetneq p_m = p\}.
\]

**Theorem A.6** (Krull’s Height Theorem). For any Noetherian ring \(R\), let \(p \triangleleft R\) be a prime ideal. Then, the height \(p\) is at most the number of generators of \(p\). Conversely, if \(p\) has height \(m\), then \(p\) is a minimal prime ideal over an ideal \(I \subseteq p\) generated by \(m\) elements. In particular, \(p\) is generated by at least \(m\) elements.
Definition A.7. Let $k$ be a field and $I \triangleleft k[x_1, \ldots, x_n]$ be an ideal. The variety defined by $I$ is the set

$$V(I) = \{ a \in k^n : f(a) = 0 \text{ for all } f \in I \}.$$ 

On the other hand, given a set $X \subseteq k^n$, the vanishing ideal of $X$ is defined as

$$I(X) = \{ f \in k[x_1, \ldots, x_n] : f(a) = 0 \text{ for all } a \in X \}.$$ 

A variety $X$ is reducible if we can write $X = X_1 \cup X_2$ for proper subsets $X_i \subseteq X$. Otherwise, $X$ is irreducible.

Theorem A.8. The variety $X$ is irreducible if and only if the vanishing ideal $I(X)$ is prime.

Proof. See Proposition 3 in Section 4.5 of [5].

Proposition A.9. If $k$ is an infinite field and $V$ is a variety defined by the rational parametrization

$$x_1 = \frac{f_1(t_1, \ldots, t_m)}{g_1(t_1, \ldots, t_m)},$$

$$\vdots$$

$$x_n = \frac{f_n(t_1, \ldots, t_m)}{g_n(t_1, \ldots, t_m)},$$

where $f_1, \ldots, f_n, g_1, \ldots, g_n \in k[t_1, \ldots, t_m]$, then $V$ is irreducible.

Proof. See Proposition 6 in Section 4.5 of [5].

Appendix B: Algebraic Properties of the Vanishing Ideal

Now that we can find the generators of $I(G)$ for any bow-free ADMG $G$, it is natural to ask if the elements in the set $Z$ we found form the minimal generators for $I(G)$, in the following sense.

Definition B.1. We say that the polynomials $f_1, \ldots, f_n$ are minimal generators for $I$ if we have $\langle f_1, \ldots, f_n \rangle = I$ but $\langle f_1, \ldots, f_{i-1}, f_{i+1}, \ldots, f_n \rangle \neq I$ for any $1 \leq i \leq n$. In other words, the polynomials $f_1, \ldots, f_n$ generate $I$ but if we remove any of the $f_i$ for $1 \leq i \leq n$, the remaining polynomials no longer generate $I$.

In this section, we will explore some of the algebraic properties of $I(G)$. In particular, we will show that $I(G)$ is a prime ideal with height $m$, where $m$ is the number of non-adjacent vertex pairs, and that the constraints corresponding to the non-adjacent pairs form the minimal generators of $I(G)$.

Proposition B.2. Given a bow-free ADMG $G$, $I(G)$ is a prime ideal.
\textbf{Proof.} By definition, the variety $\mathcal{M}(G)$ is defined by
\[ \Sigma \in \mathcal{M}(G) \iff \Sigma = (I - \lambda)^{-T}\Omega(I - \Lambda)^{-1}. \]
In particular, $\mathcal{M}(G)$ is a variety where each $\sigma_{ij}$ can be defined by a rational parametrization in terms of entries in $\Lambda$ and $\Omega$. By Proposition A.9, $\mathcal{M}(G)$ is an irreducible variety. Hence, the vanishing ideal $I(\mathcal{M}(G)) = \mathcal{I}(G)$ is prime (Theorem A.8).

\textbf{Theorem B.3.} If a bow-free ADMG $G$ has $m$ pairs of non-adjacent vertices, then $\mathcal{I}(G)$ has height $m$.

\textbf{Proof.} We shall prove by induction. Starting with a complete graph, $G_0$, there are no constraints. Hence, $\mathcal{I}(G_0) = \langle 0 \rangle$. Suppose we remove a directed edge from vertices $v_0$ to $v_1$ in $G_0$ to obtain a new graph, $G_1$. By Theorem 3.2, we can express the entries of $\Lambda$ and $\Omega$ as rationals with indeterminates in $\Sigma$ for the graph $G_0$. Then, by Corollary 3.3, the constraint in $G_1$ corresponds to $\lambda_{v_0v_1} = 0$. Since $\mathbb{R}(\Sigma)$ is a Noetherian ring (see Appendix A) and $\mathcal{I}(G_1)$ has one generator (i.e. $\lambda_{v_0v_1}$), by Theorem A.6, $\mathcal{I}(G_1)$ has a height of at most one. But we can find a chain of length one, namely $\langle 0 \rangle = \mathcal{I}(G_0) \subset \mathcal{I}(G_1)$, Hence, $\mathcal{I}(G_1)$ has height one.

Now suppose that $\mathcal{I}(G_k)$ has $k$ generators and height $k$ with $\mathcal{I}(G_0) \subset \cdots \subset \mathcal{I}(G_k)$. Let $G_{k+1}$ be the graph obtained from $G_k$ by removing a directed edge from $v_k$ to $v_{k+1}$. By Theorem 3.2, we have a constraint present in $G_{k+1}$ but not in $G_k$; hence, $\mathcal{I}(G_{k+1}) \supset \mathcal{I}(G_k)$. Furthermore, we can express $\Lambda$ and $\Omega$ as rationals with indeterminates in $\Sigma$ for $G_k$. By Corollary 3.3, $\mathcal{I}(G_{k+1}) = \mathcal{I}(G_k) \cup \{\lambda_{v_kv_{k+1}}\}$. Hence, $\mathcal{I}(G_0) \subset \cdots \subset \mathcal{I}(G_k) \subset \mathcal{I}(G_{k+1})$ and $\mathcal{I}(G_{k+1})$ has at most $k+1$ generators. Since $\mathcal{I}(G_k)$ is prime by Proposition B.2, we have a chain of length $k+1$. Thus any longest chain has a length of at least $k+1$. On the other hand, by Theorem A.6, $\mathcal{I}(G_{k+1})$ has a height of at most $k+1$; that is, any longest chain has a length of at most $k+1$. Hence, $\mathcal{I}(G_{k+1})$ has height $k+1$ and $k+1$ generators.

Therefore, given a graph $G$, we can add directed edges (with orientation satisfying the topological ordering) until we obtain the complete graph $G_0$. Hence, we obtain a chain of length $m$, $\langle 0 \rangle = \mathcal{I}(G_0) \subset \cdots \subset \mathcal{I}(G_m) = \mathcal{I}(G)$. But $G$ has $m$ generators, and hence has height at most $m$ by Theorem A.6. Therefore, this chain must be the longest possible and $\mathcal{I}(G)$ has height $m$.

\textbf{Corollary B.4.} The constraints corresponding to pairs of non-adjacent vertices form a set of minimal generators for $\mathcal{I}(G)$.

\textbf{Proof.} Let $m$ be the number of pairs of non-adjacent vertices. We have $m$ such constraints. Since $\mathcal{I}(G)$ has height $m$, by Theorem A.6, $\mathcal{I}(G)$ must have at least $m$ generators. Therefore, removing any one of these will no longer generate $\mathcal{I}(G)$.

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