Learning Linear Non-Gaussian Graphical Models with Multidirected Edges

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Abstract

In this paper we propose a new method to learn the underlying acyclic mixed graph of a linear non-Gaussian structural equation model given observational data. We build on an algorithm proposed by Wang and Drton [14], and we show that one can augment the hidden variable structure of the recovered model by learning multidirected edges rather than only directed and bidirected ones. Multidirected edges appear when more than two of the observed variables have a hidden common cause. We detect the presence of such hidden causes by looking at higher order cumulants and exploiting the multi-trek rule [9]. Our method recovers the correct structure when the underlying graph is a bow-free acyclic mixed graph with potential multi-directed edges.

1 Introduction

Building on the theory of causal discovery from observational data, we propose a method to learn linear non-Gaussian structural equation models with hidden variables. Importantly, we allow each hidden variable to be a parent of multiple of the observed variables, and we represent this graphically via multi-directed edges. Therefore, given observational data, we seek to find an acyclic mixed graph whose vertices correspond to the observed variables, and which has directed and multi-directed edges.

Figure 1: The graph in Figure 1a is directed acyclic. After marginalization of vertices 1 and 5, the resulting mixed graph with directed and bidirected edges only is that in Figure 1c. If we allow multidirected edges, we can capture the hidden variable structure better via the graph in Figure 1b, which also has a 3-directed edge.

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Consider an acyclic mixed graph \( G = (V, D, H) \), where \( V = \{1, \ldots, p\} \) is the set of vertices, \( D \) is the set of directed edges, and \( H \) is the set of multi-directed edges, i.e., \( H \) consists of tuples of vertices such that the vertices in each tuple have a hidden common cause. The graph in Figure 1c has only directed and bidirected edges, while the one in Figure 1b also has a 3-directed edge. Both of these mixed graphs represent the directed acyclic graph in Figure 1a with the variables 1 and 5 unobserved. Representing hidden variables via such edges is quite commonly used for causal discovery [7].

We restrict our attention to the class of Linear Structural Equation Models (LSEMs). A mixed graph \( G \) gives rise to a linear structural equation model, which is the set of all joint distributions of a random vector \( X = (X_1, \ldots, X_p) \) such that the variable \( X_i \) associated to vertex \( i \) is a linear function of a noise term \( \epsilon_i \) and the variables \( X_j \), as \( j \) varies over the set of parents of \( i \), denoted \( \text{pa}(i) \), (i.e., the set of all vertices \( j \) such that \( j \to i \in E \)). Thus,

\[
X_i = \sum_{j \in \text{pa}(i)} b_{ij} X_j + \epsilon_i, \quad i \in V.
\]

When the variables \( X_1, \ldots, X_p \) are Gaussian, we are only able to recover the mixed graph up to Markov equivalence from observational data [7, 6]. When the variables are non-Gaussian, however, it is possible to recover the full graph from observational data. This line of work originated with the paper [10] by Shimizu et al. in which a linear non-Gaussian structural equation model corresponding to a directed acyclic graph (DAG), i.e., a graph without confounders, can be identified from observational data using independent component analysis (ICA). Instead of ICA, the subsequent DirectLiNGAM [11] and Pairwise LiNGAM [5] methods use an iterative procedure to estimate a causal ordering; Wang and Drton [15] give a modified method that is also consistent in high-dimensional settings in which the number of variables \( p \) exceeds the sample size \( n \).

Hoyer et al. [4] consider the setting where the data is generated by a linear non-Gaussian acyclic model (LiNGAM), but some variables are unobserved. Their method, like ours, recovers an acyclic mixed graph with multidirected edges. However, it uses overcomplete ICA and requires the number of latent variables in the model to be known in advance. Furthermore, current implementations of overcomplete ICA algorithms often suffer from local optima and can’t guarantee convergence to a global one. To avoid using overcomplete ICA while still identifying unobserved confounders, Tashiro et al. [13] propose a procedure, called ParcelLiNGAM, which tests subsets of observed variables. Wang and Drton [14], however, show that this procedure works whenever the graph is ancestral, and propose a new procedure, called BANG, which uses patterns in higher-order moment data, and can identify bow-free acyclic mixed graphs, a set of mixed graphs much larger than the set of ancestral graphs. The BANG algorithm, however, recovers a mixed graph which only contains directed and bidirected edges.

Our method builds on the BANG procedure. We can identify a bow-free acyclic mixed graph, and, in addition, join bidirected edges together into a multi-directed edge whenever more than two of the observed variables have a hidden common cause.

The rest of the paper is organized as follows. In Section 2 we give the necessary background on mixed graphs, linear structural equation models, and multi-treks. In Section 3 we present our algorithm (MBANG) and we prove that it recovers the correct graph as long as the empirical moments are close enough the the population moments. In Section 4 we present numerical results, including simulations of different graphs and error distributions, and an application of our algorithm to a real dataset. We conclude with a short discussion in Section 5.
2 Background

In this section we introduce the key concepts that we use throughout the paper, including mixed graphs with multi-directed edges, linear structural equation models, multi-treks and cumulants.

2.1 Mixed graphs with multi-directed edges

The notion of a mixed graph is widely used in graphical modelling, where bidirected edges depict unobserved confounding. In this paper a mixed graph is also allowed to contain multi-directed edges to depict slightly more complicated unobserved confounding.

Definition 1. (a). We call $G = (V, D, H)$ a mixed graph, where $V = \{1, \ldots, p\}$ is the set of vertices, $D \subseteq V \times V$ is the set of directed edges, and $H$ is the set of multi-directed edges (all $k$-directed edges for $k \geq 2$). (see part (b)).

(b). For $k \geq 2$, a $k$-directed (or multi-directed) edge between distinct nodes $i_1, \ldots, i_k \in V$, denoted by $(i_1, \ldots, i_k)$, is the union of $k$ directed edges with the same hidden source and sinks $i_1, \ldots, i_k$ respectively. Multi-directed edges are unordered.

![Figure 2: Examples of multi-directed edges.](image)

Our method is able to recover bow-free acyclic mixed graphs. A mixed graph is bow-free if it does not contain a bow, and a bow consists of two vertices $i, j \in V$ such that there is both a directed and a multidirected edge between $i$ and $j$. In other words, $i \rightarrow j \in D$ and there exists $h \in H$ such that $i, j \in h$. A mixed graph is acyclic if it does not contain any directed cycles, where a directed cycle is a sequence of directed edges of the form $i_1 \rightarrow i_2, i_2 \rightarrow i_3, \ldots, i_\ell \rightarrow i_1$.

![Figure 3: Examples of a bow and a cycle.](image)

Acyclic mixed graphs with potential multidirected edges are all one can hope to recover from observational data. Suppose for a moment that we have data coming from a directed acyclic graph (DAG) where a subset of the variables is unobserved, e.g., consider the DAG in Figure 4a where we only observe variables 1, 4, and 5.

Hoyer et al. [4] show that any directed acyclic graphical model in which some of the variables are unobserved is observationally and causally equivalent to a unique canonical model, where a canonical model is a non-Gaussian Linear Structural Equation Model corresponding to an acyclic mixed graph $G = (V, D, H)$ such that none of the latent variables have any parents, and each latent variable has at least two children. This means, that the distribution of the
observed variables in the original model is identical to that in the canonical model, and causal relationships of observed variables in both models are identical. Therefore, we can focus our attention on the set of canonical models, which can be represented precisely by acyclic mixed graphs with multi-directed edges. The graph in Figure 4b is the canonical model corresponding to the one in Figure 4a.

![Figure 4: An example of two observationally and causally equivalent models from [4].](image)

2.2 Linear Structural Equation Models

Let \( G = (V, D, H) \) be an acyclic mixed graph as defined in the previous section. It induces a statistical model, called a linear structural equation model, or LSEM, for the joint distribution of a collection of random variables \( (X_i, i \in V) \), indexed by the graph’s vertices. The model hypothesizes that each variable is a linear function of its parent variables and a noise term \( \varepsilon_i \):

\[
X_i = b_{0i} + \sum_{j \in \text{pa}(i)} b_{ji} X_j + \varepsilon_i, \quad i \in V, \tag{1}
\]

where \( \text{pa}(i) = \{ j \in V : j \rightarrow i \in D \} \) is the set of parents of vertex \( i \). The variables \( \varepsilon_i, i \in V \) are assumed to have mean 0, and the coefficients \( b_{0i} \) and \( b_{ji} \) are unknown real parameters. Since we can center the variables \( X_i, \) we assume that the coefficients \( b_{0i} \) are all equal to 0. In addition, the multi-directed edge structure of \( G \) defines dependencies between the noise terms \( \varepsilon_i \), that is, if \( i \) and \( j \) are not connected by a multi-directed edge, then \( \varepsilon_i \) and \( \varepsilon_j \) are independent variables. In particular, if \( G \) is a DAG (directed acyclic graph), i.e., it does not have any multi-directed edges, then all noise terms \( \varepsilon_i \) are mutually independent. Typically termed a system of structural equations, the system \( \text{(1)} \) specifies cause-effect relations whose straightforward interpretability explains the wide-spread use of the models [8, 12].

We can rewrite the system \( \text{(1)} \) as

\[
X = BX + \varepsilon,
\]

where \( X = (X_1, \ldots, X_p)^T \), \( B = (b_{ij}) \) is the coefficient matrix satisfying \( b_{ij} = 0 \) whenever \( i \rightarrow j \not\in D \), and \( \varepsilon \) is the noise vector. Note that since \( G \) is assumed to be acyclic, we can permute the coefficient matrix \( B \) so that it is a lower triangular matrix. Therefore, the matrix \( I - B \) is invertible, and the system \( \text{(1)} \) can further be rewritten as

\[
X = (I - B)^{-1}\varepsilon.
\]

2.3 Cumulants and the multi-trek rule

We recall the notion of a cumulant tensor for a random vector [2].
Definition 2. Let $Z = (Z_1, \ldots, Z_p)$ be a random vector of length $p$. The $k$-th cumulant tensor of $Z$ is defined to be a $p \times \cdots \times p$ ($k$ times) table, $C^{(k)}$, whose entry at position $(i_1, \ldots, i_k)$ is

$$C^{(k)}_{i_1, \ldots, i_k} = \sum_{(A_1, \ldots, A_L)} (-1)^{k-1}(L-1)! \left[ \prod_{j \in A_i} Z_j \right] \cdots \left[ \prod_{j \in A_L} Z_j \right],$$

where the sum is taken over all partitions $(A_1, \ldots, A_L)$ of the set $\{i_1, \ldots, i_k\}$.

Note that if each of the variables $Z_i$ has zero mean, then we can restrict the summing over partitions for which each $A_i$ has size at least two. For example:

$$C^{(4)}_{i_1, i_2, i_3, i_4} = \mathbb{E}(Z_{i_1}Z_{i_2}Z_{i_3}Z_{i_4}) - \mathbb{E}(Z_{i_1}Z_{i_2})\mathbb{E}(Z_{i_3}Z_{i_4}) - \mathbb{E}(Z_{i_1}Z_{i_3})\mathbb{E}(Z_{i_2}Z_{i_4}) + \mathbb{E}(Z_{i_1}Z_{i_4})\mathbb{E}(Z_{i_2}Z_{i_3}).$$

We now recall the notion of a multi-trek from [9].

Definition 3. A $k$-trek in a mixed graph $G = (V, D, H)$ between $k$ nodes $i_1, i_2, \ldots, i_k$ is an ordered collection of $k$ directed paths $(P_1, \ldots, P_k)$ where $P_j$ has sink $i_j$ and either $P_1, \ldots, P_k$ have the same source of vertex, or there exists a multi-directed edge $h \in H$ such that the sources of $P_1, \ldots, P_k$ all lie in $h$.

Figure 5: Examples of multi-treks.

The following consequence of the multi-trek rule [9] connects cumulants of LSEMs to multi-treks.

Theorem 1 ([9]). Let $G = (V, D, H)$ be an acyclic mixed graph, and let $i_1, \ldots, i_k \in V$. Then,

$$C^{(k)}_{i_1, \ldots, i_k} = 0$$

for the $k$-th cumulant tensor $C^{(k)}$ of any random vector whose distribution lies in the LSEM corresponding to $G$ if and only if there is no $k$-trek between $i_1, \ldots, i_k$ in $G$.

3 Main Result

In this section we present our algorithm and we show that it recovers the correct graph given enough samples. In the chart below we illustrate how the algorithm works when applied to observational data coming from the graph in Figure 1a.
The BANG procedure produces a bow-free acyclic mixed graph with directed and bidirected edges only and an estimate of $B$.

Identify multi-directed edges

$X = Y - BY$

Remove directed edges

Obtain samples $Y$ from LSEM on true graph

Figure 6

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Given a $p \times n$ data matrix $Y$ whose columns are i.i.d. samples from a LSEM on an unknown bow-free acyclic mixed graph $G = (V, D, \mathcal{H})$ with an unknown direct effects matrix $B$, we aim to recover the graph $G$ and the matrix $B$. The first step is to apply the BANG procedure and obtain the coefficient matrix $B$ together with a bow-free acyclic mixed graph $G_1 = (V, D, B)$. The directed edges and bidirected edges are obtained from $\mathcal{H}$ by replacing each multi-directed edge $h = (i_1, \ldots, i_k) \in \mathcal{H}$ by $\binom{k}{2}$ bidirected edges, one for each pair $i_s, i_t \in \{i_1, \ldots, i_k\}$. We call such a set $B$ the bidirected subdivision of $\mathcal{H}$. We then, "remove" the directed edges by removing the direct effects given by $B$. This is done by replacing the original data matrix $Y$ with $X = Y - BY$. This new matrix $X$ can be thought of as observations from a LSEM corresponding to the acyclic mixed graph $G' = (V, \emptyset, \mathcal{H})$ which is the same as $G$ with the directed edges removed. However, we only know the bidirected subdivision $B$ of $\mathcal{H}$. Finally, using the higher order cumulants of $X$ and a clique-finding algorithm on the graph $G'_1 = (V, 0, B)$, we identify all multi-directed edges in $\mathcal{H}$. The algorithm is summarized below.

**Algorithm 1: MBANG procedure**

1: Input: $Y \in \mathbb{R}^{p \times n}$ arising from an unknown LSEM on $G = (V, D, \mathcal{H})$ with unknown direct effects matrix $B$.

2: Apply the BANG procedure to estimate the coefficient matrix $B$ and the mixed graph $G_1 = (V, D, B)$.

3: Let $X = Y - BY$ be the new observation matrix, corresponding to the graph $G' = (V, \emptyset, \mathcal{H})$ which has no directed edges.

4: Initiate $R = Q = \emptyset$, $P = \{1, 2, \ldots, p\}$.

5: Apply Algorithm 2 to $X, G'_1 = (V, 0, B), R, P$ and $Q$ to recover the set $\mathcal{H}$ of multidirected edges.

6: Output: the graph $G = (V, D, \mathcal{H})$ and the matrix $B$. 

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Algorithm 2 finds those multi-directed edges that contain the most vertices and are consistent with the cumulant structure of the data matrix $X$. It is based on the Bron-Kerbosh algorithm [1] for finding all cliques in an undirected graph, applied to the bidirected edges in $G_1' = (V, \emptyset, B)$.

### 3.1 The BANG procedure

In this section we briefly describe the BANG Procedure [14]. It is an algorithm which takes as input a $p \times n$ data matrix $Y$, and returns a bow-free acyclic mixed graph $G$ which contains directed and bidirected edges only, consistent with $Y$ as well as a direct effects matrix $B$.

Suppose the observed data is drawn from a LSEM whose corresponding graph is the one in Figure 7a. Figure 7b shows how the BANG algorithm works.

It first identifies sibling and ancestor relations, and then it distinguishes parent and non-parent ancestors. Recall that two vertices are siblings if there is a multi-directed edge between them, a vertex $i$ is a parent of a vertex $j$ if there is a directed edge $i \rightarrow j$, and a vertex $i$ is an ancestor of a vertex $j$ if there is a directed path $i \rightarrow i_0 \rightarrow \cdots \rightarrow i_k \rightarrow j$.

![Figure 7: BANG algorithm example](image)

However, the BANG algorithm returns bow-free acyclic mixed graphs in which the latent variable structure is recorded using bidirected edges only, i.e., it recovers the bidirected subdivision of the true set of multi-directed edges $\mathcal{H}$. This means it cannot determine whether more than two vertices have a common cause. We resolve this problem using cumulant information.

### 3.2 Finding the multidirected edge structure

Consider the two models in Figure 8. By Theorem 1, we know that $C_{2,3,4}^{(3)} = 0$ in Case 1 whereas $C_{2,3,4}^{(3)} \neq 0$ in Case 2. In other words, the exact model can be recovered by testing whether $C_{2,3,4}^{(3)} = 0$. 


More generally, as depicted in Figure 6, we first apply the BANG algorithm to the data matrix \( Y \in \mathbb{R}^{p \times n} \) arising from a LSEM on \( G = (V, \mathcal{D}, \mathcal{H}) \), to obtain an estimate of the direct effects matrix \( B \) and the bow-free acyclic mixed graph \( G_1 = (V, \mathcal{D}, B) \) with directed and bidirected edges only, where there is a bidirected edge between \( i \) and \( j \) in \( G_1 \) if and only if there is a multidirected edge in \( G \) containing both \( i \) and \( j \), i.e., \( B \) is the bidirected subdivision of \( H \).

Then, we form a new data matrix \( X = Y - BY \) and we consider the graph \( G' = (V, \emptyset, H) \) which contains only multi-directed edges. In other words, the data matrix \( X \) can be thought of as a matrix of samples coming from a LSEM on the graph \( G' \). However, we only know the graph \( G'_1 = (V, \emptyset, B) \). The bidirected edges \( B \) recovered by the BANG algorithm can now be "merged" together to obtain the true multi-directed edge structure \( H \). Since \( G'_1 \) contains only bidirected edges, we look for all cliques (of bidirected edges) \( \{i_1, \ldots, i_k\} \) in \( G' \) such that \( C^{(k)}_{i_1 \ldots i_k} \neq 0 \), where \( C^{(k)} \) is the \( k \)-th cumulant of \( X \). We do this by adapting the Bron-Kerbosch algorithm \([1]\), which is used for finding all cliques in an undirected graph.

**Algorithm 2:** Determine Multidirected Edges

1. **Input:** \( X \in \mathbb{R}^{p \times n}, G'_1 = (V, \emptyset, B), R, P \) and \( Q \). Denote the elements of \( R \) to be \( i_1, \ldots, i_k \).
2. **if** \( P \) and \( Q \) are both empty **then**
3. **Report** \( R \) as a multidirected edge.
4. **end if**
5. **for all** vertex \( v \in P \) **do**
6. **if** \( N(v) \neq \emptyset \), where \( N(v) \) is the set of vertices adjacent to \( v \) in \( B \) **then**
7. **if** \( C^{(k+1)}_{i_1 \ldots i_k, v} \neq 0 \) or \( \exists j \in \{i_1, \ldots, i_k\} \) s.t. \( C^{(k+2)}_{i_1 \ldots i_k, v, j} \neq 0 \) **then**
8. **call** Algorithm 2 \( X, R \cup \{v\}, P \cap N(v), Q \cap N(v) \)
9. **end if**
10. **end if**
11. \( P = P \setminus \{v\} \)
12. \( Q = Q \cup \{v\} \)
13. **end for**

Algorithm 2 is a direct modification of the Bron-Kerbosch algorithm \([1]\). It is a recursive algorithm, that maintains three disjoint sets of vertices \( R, P, Q \subset V \), and aims to output all cliques in the graph which contain all vertices in \( R \), do not contain any of the vertices in \( Q \), and could contain some of the vertices in \( P \). The only addition to the Bron-Kerbosch algorithm

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**Figure 8:** The same bidirected edge structure depicts two different hidden variable models.
that Algorithm 2 does is the test of whether or not specific cumulants are nonzero in Line 7.

In practice, since Theorem 1 holds for generic distributions, sometimes random variables consistent with a model that has a multi-directed edge between \( i_1, \ldots, i_k \) may still have a zero cumulant. For example, if \( i_1, i_2, \) and \( i_3 \) are all caused by a hidden parent variable whose distribution is symmetric around 0, then \( C_{i_1,i_2,i_3}^{(3)} = 0 \). To solve this problem, we relax the criterion \( C_{i_1,\ldots,i_k}^{(k)} \neq 0 \). In our implementation, we also check if there exists \( j \in \{i_1,\ldots,i_k\} \) such that \( C_{i_1,\ldots,i_{k-1},j}^{(k+1)} \neq 0 \). If there is a multidirected edge \( h \) such that \( i_1,\ldots,i_k \in h \) but due to non-genericity of the model \( C_{i_1,\ldots,i_k} = 0 \), we find that often times \( C_{i_1,\ldots,i_{k-1},j}^{(k+1)} \neq 0 \) which allows us to reach the correct conclusion.

### 3.3 Theoretical results

In this section we show that Algorithm 1 recovers the correct bow-free acyclic mixed graph given enough samples. We begin with a population moment result.

**Theorem 2.** Suppose \( Y \) is generated from a linear structural equation model corresponding to a bow-free acyclic mixed graph \( G = (V,D,H) \). Then for a generic choice of the coefficient matrix \( B \) and generic error moments, when given the population moments of \( Y \), Algorithm 1 produces the correct graph \( G \).

**Proof.** Algorithm 1 first applies the BANG procedure to produce a bow-free acyclic mixed graph \( G_1 = (V,D,E) \) containing bi-directed edges and directed edges only as well as the coefficient matrix \( B \). In [14] the authors show that the BANG algorithm recovers the correct bow-free acyclic mixed graph (with directed and bidirected edges only) and the correct coefficient matrix \( B \). Note that this means that the graph \( G_1 \) will have a bidirected edge \( b \in E \) between two nodes \( i \) and \( j \) which are part of a multi-directed edge \( h \in H \) in \( G \). Consider the data matrix \( X = Y - BY \) which corresponds to a graph \( G' = (V,\emptyset,H) \) obtained by removing all directed edges in \( G \), and the graph \( G'_1 = (V,\emptyset,B) \) obtained from \( G_1 \) by removing all directed edges. Our task is to merge together some of the bidirected edges in \( G'_1 \) in order to obtain the graph \( G' \).

There is a multi-directed edge between \( i_1,\ldots,i_k \) in \( G' \) (or, equivalently, in \( G \)), if and only if any two of \( i_1,\ldots,i_k \) are joined by a bidirected edge in \( G'_1 \), i.e., they will form a clique, AND

\[
C_{i_1,\ldots,i_k}^{(k)} \neq 0, \tag{2}
\]

where \( C_{i_1,\ldots,i_k}^{(k)} \) is the \( k \)-th cumulant of \( X \) (assuming the distribution of \( X \) is generic). Therefore, finding all multi-directed edges is equivalent to finding all maximal cliques in \( G'_1 \), which holds. This is precisely what Algorithm 2 does – it applies the Bron-Kerbosch algorithm for finding all cliques in an undirected graph (which can equally well be applied to the graph \( G'_1 \) since it only has bidirected edges) and for each such clique it checks whether (2) holds.

Therefore, Algorithm 1 produces the correct graph \( G \).

**Theorem 3.** Suppose \( Y_1, Y_2, \ldots, Y_n \) are generated by a linear structural equation model which corresponds to a bow-free acyclic mixed graph \( G = (V,D,H) \). Then, for generic choices of the effects coefficient matrix \( B \), and generic error moments, there exist \( \delta_1, \delta_2, \delta_3 > 0 \) such that if the sample moments are within a \( \delta_1 \) ball of the population moments of \( Y \), then Algorithm 1 will produce the correct graph \( G \) when comparing the absolute value of the sample statistics to \( \delta_2 \) as a proxy for the independence tests in the BANG procedure and when comparing the absolute value of the cumulants to \( \delta_3 \) as a proxy in the tests for the vanishing of cumulants in Algorithm 2.
Proof. First, consider the data matrix \( X = Y - B Y \). Note that by definition the cumulants of \( X \) have the form

\[
C_{i_1, \ldots, i_k}^{(k)} := \text{cum} \left( X_{i_1}, \ldots, X_{i_k} \right) = \sum_{(A_1, \ldots, A_L)} \frac{(-1)^L}{L!} \left( \prod_{j \in A_1} X_j \right) \cdots \left( \prod_{j \in A_L} X_j \right) ,
\]

which is a rational function of the moments of \( X \), which are rational functions of the moments of \( Y \) and of the matrix \( B \). Thus, it is also a continuous function of the population moments of \( Y \). For the population cumulants \( PC^{(k)} \) of \( X \) let

\[
\delta_3 = \frac{1}{2} \min_{PC^{(k)}_{i_1, \ldots, i_k} \neq 0} \left| PC^{(k)}_{i_1, \ldots, i_k} \right| , \quad 1 \leq k \leq p.
\]

Thus, there exists \( \delta' > 0 \) such that whenever the empirical moments of \( Y \) are within a \( \delta' \) ball of its population moments and the estimated \( B \) is within \( \delta' \) of the true one, all of the estimated cumulant entries of \( X \) are within an \( \delta_3 \) ball of the entries of its population cumulants \( C^{(k)} \).

Next, we know from \([14]\) that there exist \( \delta, \delta_2 > 0 \) such that if the sample moments are within a \( \delta \) ball of the population moments BANG will output the correct graph \( G_1 = (V, D, B) \) (where \( B \) is the bidirected subdivision of \( H \)) if it uses \( \delta_2 \) as a proxy for its independence tests. Furthermore, if the sample moments are within a \( \delta \) ball of the population moments, the estimated directed effects matrix \( B \) will be within a \( \delta' \) ball from the true direct effects matrix. This is because the estimated matrix \( B \) is a rational function of the sample moments \([14]\).

Thus, choosing \( \delta_1 = \min(\delta, \delta') \), we see that if the sample moments of \( Y \) are within \( \delta_1 \) of its population moments, and if we use \( \delta_2 \) as a proxy for its independence tests in BANG and \( \delta_3 \) as as a proxy in the tests for vanishing cumulants, Algorithm \([4]\) will yield the correct graph \( G = (V, D, H) \).

4 Numerical Results

In this section we examine how well Algorithm \([4]\) performs numerically.

4.1 Simulations

We carried out a number of simulations using four different types of error distributions: the uniform distribution on \([-10, 10]\); the student’s \( t \)-distribution with 10 degrees of freedom; the Gamma distribution with shape = 2 and rate = 4; and the chi-squared distribution with 2 degrees of freedom. We shift these distributions to have zero mean. The \( t \)-distribution is used to test the performance of the algorithm in cases when the distribution resembles the Gaussian distribution.

We generate random bow-free acyclic mixed graphs as follows. First, we uniformly select a prescribed number of directed edges from the set \( \{(i, j) | i < j \} \), and we choose the direct effect coefficients for each edge uniformly from \((-1, -0.6) \cup (0.6, 1)\). Afterwards, some of the vertices of this directed acyclic graph which have no parents are regarded as unobserved variables, and bow structures caused by marginalizing these vertices are removed from the graph. The resulting graph is a bow-free acyclic mixed graph with potential multidirected edges.

To evaluate the performance of our method, we calculate the proportion of time that the algorithm recovers the true graph. We generate graphs with 7 vertices, and after some of them are made hidden, the final graphs usually contain 5 or 6 observed variables. We test three settings with different levels of sparsity. Sparse graphs have 5 directed edges before
marginalization, medium graphs have 8, and dense graphs have 12. We do not restrict the number of multidirected edges, however, almost all dense graphs have multidirected edges, and most of the medium graphs have at least one multidirected edge.

In the first step of our algorithm, we perform the BANG procedure, and we set all the nominal levels of the hypothesis test to $\alpha = 0.01$, as suggested by the authors of the BANG algorithm\[14\]. The tolerance value used in our cumulant tests we use is 0.05.

For each of the three settings: sparse, medium, and dense, we tested 100 graphs by taking different numbers of samples: 10000, 25000 and 50000. In Figure 9, we show the percent of correctly identified bidirected and multidirected edges for each setting. The $x$ axis represents the sample size and the $y$ axis represents the percentage.

In Figure 10, we show the proportion of graphs that were recovered precisely by the BANG and MBANG algorithms. For the BANG algorithm, we recognize each multidirected edge as the corresponding set of bidirected edges.

In practice, we normalize the data matrix $X$ by dividing each row by its standard deviation before initiating Algorithm 2 in order to control the variability of its cumulants.

![Random Graph Results - Correct Multidirected Edges](image)

Among all 3600 graphs we tested in this data set, the BANG algorithm recovered 1883 correctly, and the MBANG algorithm recovered 1774 correctly. Hence, given that the BANG result was correct, the MBANG algorithm identified 94.2% of the graphs correctly. Among all dense graphs, this proportion is reduced to 88.0%. However, this drop in accuracy might be expected because in our simulation dense graphs contain more multi-directed edges.

### 4.2 A Real Data Set

In a paper by Grace et al. [3], a LSEM was used to examine the relationships between land productivity and the richness of plant diversity, the full model of which is shown in Figure [11a](image).
Wang and Drton [14] choose a subset of the variables and consider the model in Figure 11b as the ground truth model. Figure 12 shows the graphical model they discover using the BANG procedure with nominal test level 0.01.

Since this is a real data set, it is possible that some of the hidden variables affect more than one bidirected edge, or there exist other hidden variables that can affect the hidden variables detected in the BANG procedure. After applying our MBANG algorithm with 0.05 tolerance, we found that all bidirected edges can be grouped in three 3-directed edges: ("PlotSoilSuit", "PlotProd", "SiteBiomass"), ("PlotSoilSuit", "SiteBiomass", "SiteProd"), and ("PlotSoilSuit", "SiteBiomass", "SiteProd"), see Figure 13.
5 Further Discussion

In this paper we proposed a high-order cumulant based algorithm for discovering hidden variable structure in non-Gaussian LSEMs. Note that our Algorithm 2 can be used on top of any procedure that recovers a mixed graph $G = (V, D, B)$ with directed and bidirected edges only and an estimate of the direct effects matrix $B$. We chose the BANG algorithm as this first step since it applies to a large class of graphs: bow-free acyclic mixed graphs.

Second, the performance of our algorithm is closely related to the error distribution, and the density and size of the graph. For example, when the errors are unif$(-5, 5)$ and the number of vertices is 7, as the edge number increases from 8 to 20, the correct rate drops from 78% to 1%. Also, if the density is medium, as the number of vertices increases from 5 to 7, the correct rate drops from 78% to about 40%. Compared to the uniform distribution, the exponential distribution has a much milder drop in correct rate. For example, when the sample size is 50000, the correct rate for exp(1) drops from 70% to 61% as the graph density increases from sparse to very dense (almost complete). Note, however, that this drop is also present in the output of the BANG algorithm itself.

Last, while we proved that Algorithm 1 finds the true graph given enough samples, it would be interesting to know the exact amount of samples needed in both BANG and Algorithm 2 as well as the nominal levels for the independence tests in BANG and in our cumulant tests.

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