Combining Linear Non-Gaussian Acyclic Model with Logistic Regression Model for Estimating Causal Structure from Mixed Continuous and Discrete Data

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Abstract
Estimating causal models from observational data is a crucial task in data analysis. For continuous-valued data, Shimizu et al. have proposed a linear acyclic non-Gaussian model to understand the data generating process, and have shown that their model is identifiable when the number of data is sufficiently large. However, situations in which continuous and discrete variables coexist in the same problem are common in practice. Most existing causal discovery methods either ignore the discrete data and apply a continuous-valued algorithm or discretize all the continuous data and then apply a discrete Bayesian network approach. These methods possibly lose important information when we ignore discrete data or introduce the approximation error due to discretization. In this paper, we define a novel hybrid causal model which consists of both continuous and discrete variables. The model assumes: (1) the value of a continuous variable is a linear function of its parent variables plus a non-Gaussian noise, and (2) each discrete variable is a logistic variable whose distribution parameters depend on the values of its parent variables. In addition, we derive the BIC scoring function for model selection. The new discovery algorithm can learn causal structures from mixed continuous and discrete data without discretization. We empirically demonstrate the power of our method through thorough simulations.

1 Introduction
Estimating a causal directed acyclic graph (DAG) model (also known as causal Bayesian network) from observational data is a challenging problem and has applications in many research areas, including bioinformatics, economics and social science [Spirtes et al., 1993; Pearl, 2000; Morgan and Winship, 2007]. Existing methods for causal discovery commonly assume the involved variables are either discrete, or continuous valued. In the discrete case, one of the principled approaches is the constrained-based method, which relies on the results of conditional independence tests. While this approach does not impose any functional assumptions on the dependencies, it can not identify the causal directions from two different DAG models that entail identical set of conditional independencies. To cope with this identifiability problem, [Peters et al., 2011] extend the additive noise model to the discrete case and demonstrate the causal direction in their model can be identified in general. However, the model imposes linear dependence assumptions on the data and this assumption is not often satisfied in practice, especially for binary categorical data. For the multivariate count data, [Park and Raskutti, 2015] proposed Poisson DAG model in which each node corresponds to a Poisson random variable with rate parameters depending only on its parent variables. Again, the model can be applied only on count data instead of categorical data.

For the continuous-valued data, the traditional methods for causal discovery are based on linear model with Gaussian noise [Geiger and Heckerman, 1994; Spirtes et al., 1993]. However, the linear Gaussian approach usually outputs a set of possible models which belong to the Markov equivalence class of the true model. To avoid this limitation, [Shimizu et al., 2006] proposed linear non-Gaussian acyclic model (LiNGAM) and showed that the full causal structure is identifiable given sufficiently large number of data. To relax the assumption of all variables are non-Gaussian, [Hoyer et al., 2008] proposed the PClingam algorithm which combines the independence based PC algorithm [Spirtes et al., 1993] and the ICA-based LiNGAM algorithm [Shimizu et al., 2006]. The algorithm first use the PC algorithm to obtain a set of candidate DAG models, and then apply a scoring directions scheme for model selection.

While real data often contains a mixture of discrete and continuous variables, all approaches so far we described have assumed data are either discrete or continuous. One of the commonly employed approach for mixed data is to ignore the discrete variable and apply a linear causal network approach for only continuous data. The causal analysis losses sight of some important information due to ignorance of discrete data. Another one is to discretize the continuous variables and then apply the discrete Bayesian network to analysis causal relationships, since many efficient Bayesian network learning algorithm [Spirtes et al., 1993; Yehezkel and Lerner, 2009; Yuan and Malone, 2013] has been proposed for discrete data. The choice of discretization policy has significant impact on the resulting model and the discretization may lead to wrong
model if much information is lost due to discretization process. Recently, [Chen et al., 2017] proposed a new discretization strategy to mitigate these problem. Nevertheless, these traditional methods learn a Markov equivalence class and therefore the causal directions of some edges can not be determined.

In this contribution, we propose a novel hybrid causal model which consists of both continuous and discrete variables. Our model is based on the LiNGAM model and logistic regression model. In our model, we assume:

1. The data generating process can be represented by a directed acyclic graph.
2. Each continuous variable is generated from a linear function of its parent variables plus a non-Gaussian noise.
3. Each discrete variable is a logistic variable which depends on its parent variables.

An important features of this model is that the model can handle continuous and discrete variables simultaneously without using discretization. In addition, we derive the BIC scoring function for evaluating possible model and we also propose to use the BIC score for causal discovery. Most constraint-based discovery algorithms, e.g. the PC algorithm [Spirtes et al., 1993], find a Markov equivalent class which is a set of DAG models. In contrast, our method leverage the identifiability of the LiNGAM model, are expected to be able to identify the full causal structure from observational data. Finally, we empirically demonstrate the power of our method through thorough simulations.

The remainder of this paper is structured as follows: Section 2 summaries the necessary notation and reviews the LiNGAM model and logistic model. Section 3 defines our hybrid causal model and derives the BIC scoring function for model selection. Section 4 empirically evaluates our methods. Section 5 concludes this paper.

2 Background

In this section, we first introduce some necessary notation and definitions for directed acyclic graph (DAG) models. Then we briefly review the two building blocks of our model: the linear non-Gaussian acyclic model (LiNGAM) and logistic conditional probability distribution.

2.1 DAG Models

Let us consider a set of random variables \( X = \{X_1, X_2, \ldots, X_p\} \) with index set \( V = \{1, 2, \ldots, p\} \). Following the convention of previous studies, a causal graph over a set of variables \( X \) is a DAG \( G = (V, E) \) with node set \( V = \{1, 2, \ldots, p\} \), which represents the random variables \( X = \{X_1, X_2, \ldots, X_p\} \), and edge set \( E \) (or lack of them), which represents direct dependency relationships (or conditional independence relationships) between variables. A directed edge from node \( i \) to node \( j \) is denoted by \((i, j)\) or \( i \rightarrow j \). A node \( i \) is called a parent of \( j \) if \((i, j) \in E \) and the parent set \( \text{PA}(i) \) of a node \( i \) consists of all nodes \( j \) such that \((j, i) \in E \). The joint probability distribution \( p(X) \) of variables \( X \) can be factorized in terms of the conditional probability distributions as follows:

\[
P(X) = P(X_1, X_2, \ldots, X_p) = \prod_{i=1}^{p} P(X_i | X_{\text{PA}(i)}),
\]

where \( P(X_i | X_{\text{PA}(i)}) \) refers to the conditional probability distribution of \( X_i \) given its parents variables \( X_{\text{PA}(i)} \). For the variables \( X_i \) without parents (called root variables), \( P(X_i | X_{\text{PA}(i)}) \) stands for marginal distribution \( P(X_i) \).

The set of all independence constraints imposed by the structure of a DAG model can be characterized by the Markov conditions, which are the constraints that each variable is independent of its non-descendants given its parents. Two DAG structures are Markov equivalent if the set of conditional independence constraints imposed by one DAG is identical to that of another DAG. A Markov equivalence class is a set of DAGs that encode the same set of conditional independencies. The constraint based causal discovery algorithm requires a faithfulness assumption: the conditional independencies in the data distribution exactly equal the ones encoded in the causal structure. Because the constraint based approach to causal inference considers only independence constraints, these methods find a Markov equivalent class of the true causal structure.

To identify more edge directions of estimated causal structure, we propose to combine the LiNGAM model and logistic model for causal discovery. Therefore, we review these two concepts in the next two subsections.

![Figure 1](image.png)

Figure 1: (a) An example of the LiNGAM model, and (b) the Markov equivalence class of the DAG on the left.

2.2 LiNGAM

To estimate a causal structure from continuous data, [Shimizu et al., 2006] proposed a linear non-Gaussian acyclic model (LiNGAM), which is a special case of structural equation models and continuous-valued Bayesian networks. The LiNGAM model assumes that the observed data are generated from a process which is represented graphically by a directed acyclic graph (DAG). Moreover, it assumes that the relations between the variables are linear. Let us denote a connection strength from a variable \( x_j \) to another variable \( x_i \) in the DAG by \( b_{ij} \), then the model can be represented by

\[
X_i = e_i + b_{i0} + \sum_{j \in \text{PA}(i)} b_{ij} X_j \text{ with } e_i \sim \text{non-Gaussian}
\]
where $e_i$ is called an noise variable. All noise variables $e_i$ are continuous random variables having non-Gaussian distributions with zero means and non-zero variances, and $e_i$ are independent of each other so that there are no latent confounding variables [Spirtes et al., 1993]. See Figure 1 for a concrete example of LINGAM model, the data is generated by first drawing the $e_i$ independently from their respective non-Gaussian distributions, and subsequently setting (in an chronological order) $X_2 = e_2$, $X_1 = 0.5 \times X_2 + e_1$, $X_4 = X_2 + e_4$, and $X_3 = -1 \times X_1 - 2 \times X_4 + e_3$. (Here, we have assumed for simplicity that all the $b_{ij}$ are zero, but this may not be the case in general.) A remarkable result was shown in [Shimizu et al. 2006] is that under the non-Gaussian assumption about the noise distribution, the full causal structure and associated parameters are identifiable. In contrast, the constraint-based algorithms estimate the Markov equivalence class and thus the directions of some edges can not be estimated (see Figure 1).

2.3 Logistic Conditional Probability Distribution

In this section, we describe the logistic regression model as a local causal structure. Consider a discrete variable $Y$ whose distribution depends on some set of causes $X_1, X_2, \ldots, X_k$. In this study, we restrict our analysis on binary variables for $Y$ which takes two values $\{1, 2\}$. We assume that the conditional probability distribution of $Y$ given its dependent variables is a logistic CPD, which is defined as follows.

Let $Y$ be a binary-valued random variable defined over the domain $\{1, 2\}$, with $k$ parents $X_1, X_2, \ldots, X_k$ that take on numerical values. The conditional probability distribution (CPD) $P(Y \mid X_1, X_2, X_k)$ of $Y$ is a logistic CPD if there are $k + 1$ weights $b_0, b_1, \ldots, b_k$ such that:

$$P(Y = 1 \mid X_1, X_2, \ldots, X_k) = \frac{e^{b_0 + \sum_{j=1}^{k} b_j X_j}}{1 + e^{b_0 + \sum_{j=1}^{k} b_j X_j}},$$

where the sigmoid function stands for:

$$\text{sigmoid}(z) = \frac{e^z}{1 + e^z} \quad (4)$$

The logistic CPD is a natural model for many real-world applications, because it naturally aggregates the influence of different parents. [Koller and Friedman 2009] also provide a variant of binary logistic CPD which can handle the multivalued variables, however, we have not implemented this feature in our software, yet.

3 The Hybrid Causal Model

In this section, we propose a novel hybrid causal model, i.e., a DAG model consisting of both continuous and discrete variables. Then we discuss two commonly used approaches to causal discovery. Finally, we derive the BIC scoring function to evaluate the fitness of a DAG model to the data.

3.1 Definition of Our Model

We partition the variables of our model in two types: continuous variables and discrete variables. In this paper, we assume that each discrete variable only take two values $\{1, 2\}$ and assume that the observed data has been generated by the following process:

1. The data are generated from a process represented graphically by a directed acyclic graph, in which each variable is directly caused by its parent variables.

2. The value assigned to each continuous variables $X_i$ is a linear function of its parent variables plus a non-Gaussian noise term $e_i$, that is

$$X_i = e_i + b_{i0} + \sum_{j \in \text{PA}(i)} b_{ij} X_j, \quad (5)$$

where the noise term $e_i$ are all continuous random variables with non-Gaussian densities, and the noise variables $e_i$ are independent of each other.

3. For a discrete variable $X_i$, the conditional probability distribution of variable $X_i$ is the logistic CPD, such that,

$$P(X_i = 1 \mid X_{\text{PA}(i)}) = \text{sigmoid}(b_{i0} + \sum_{j \in \text{PA}(i)} b_{ij} X_j),$$

$$P(X_i = 2 \mid X_{\text{PA}(i)}) = 1 - P(X_i = 1 \mid X_{\text{PA}(i)}), \quad (6)$$

3.2 Discovery Algorithms

Causal discovery consists in finding the causal model that best fits the sample data according to certain criterion. Since a causal model consists of a causal graph structure (a DAG) and associated parameters, the discovery algorithms often need to deal with two highly related tasks: search for a causal graph and estimation of the parameters. That is, in order to estimate the parameters, we must know the causal structure; in order to evaluate a candidate causal structure, we must estimate the parameters from the data and the causal graph. In this paper, we are mainly interested in algorithms for learning the causal structure, and view the parameter estimation part as a subroutine of the search algorithm.

The constraint-based algorithms typically apply statistical tests to identify conditional independence relations and attempt to find a causal graph that represents these relations as precise as possible. Since the accuracy of the statistical test is sensitive to the number of data and the complexity of the independence tests, the constraint-based algorithms may not work well when there are insufficient data. Another issue in the constraint-based algorithm is that independence test based approach can not distinguish two DAGs in the same Markov equivalence class. Since most of Markov equivalence classes contain more than one graph, conditional independence based methods leave some arrows undirected and cannot uniquely identify the true causal graph. Recently, [Hoyer et al. 2008] use constraint-based methods to infer the Markov equivalence class of the true causal model and then score each DAG belonging to the equivalence class.

3.3 Scoring the Hybrid Causal Model

In order to evaluate the hybrid causal model, we derive the Bayesian information criterion (BIC) scoring function [Schwarz, 1978] of our model. The basic idea of the BIC is to select the causal structure that maximizes the log-likelihood
In the data generating process, each continuous variable has a distribution 
\( X_i \sim \text{logistic} \) for each pair of possible nodes under constraints that are enforced.
Each edge of the graph is denoted as \( b_{ij} \), and \( M \) denotes the number of data points.

The BIC score of a structure \( G \) can be defined as:

\[
\text{Score}_{BIC}(G) = \log \mathcal{L}(\hat{B}_G : D) - \frac{\log(M)}{2} \text{Dim}[G],
\]

where \( \mathcal{L}(\hat{B}_G : D) \) is the log-likelihood of the model, \( \hat{B}_G \) is the maximum likelihood estimated (MLE) parameters for \( G \), \( M \) stands for the number of data points, and \( \text{Dim}[G] \) signifies the number of free parameters of the model.

Since in our model, each conditional probability distribution \( P(X_i \mid X_{PA(i)}) \) have the number of its parent variables plus one constant parameter, the total number of parameters \( \text{Dim}[G] \) is the number of edges plus the number of variables.

Next, we discuss the methods for obtaining the MLE parameters. For the logistic variables, it is easy to estimate the coefficients by the maximum likelihood principle [Bishop, 2006]. However, for the continuous variables, as we do not assume the Gaussian noise, to obtain the exact MLE parameters, we have to estimate the noise distribution first. This would be very complicated and not easy for implementation. For simplicity of the estimation, we obtain the coefficients \( b_{ij} \) estimated using ordinary least-square regression. Note this provide a consistent estimates. When the number of data is sufficiently large, the approximation error becomes zero.

Finally, for the continuous variable \( X_i \), the local log-likelihood \( \log L(X_i) \) of the variable \( X_i \) is given by [Hyvärinen et al., 2010]. For the discrete variable, we just use canonical likelihood function for logistic regression [Bishop, 2006].

For the discrete Bayesian network, it is well known that the BIC scoring function assigns the same score to structures in the same equivalence class. However, under assumptions described in subsection 3.1, using BIC scoring function we are expected to be able to find the unique true causal structure as well as the associated parameters.

4 Experiments

In this section, we evaluated our proposed algorithm with respect to accuracy rate of discovering causal structure through extensive experiments. We also showed that our algorithm has better performance compared to the state of the art algorithm.

4.1 Simulations

The simulation study was conducted on a set of random DAG models with both continuous and discrete variables. Each random graph was generated by adding an edge with probability 0.5 for each pair of possible nodes under constraints that the newly added edge will not introduce any directed cycle. In the data generating process, each continuous variable \( X_i \) is caused by the function \( X_i = b_{0i} + e_i + \sum_{j \in PA(i)} b_{ij} X_j \); each discrete variable \( X_i \) was sampled from the probability distribution \( P(X_i \mid X_{PA(i)}) = \text{sigmoid}(b_{0i} + \sum_{j \in PA(i)} b_{ij} X_j) \).

In all results presented, parameters \( b_{ij} \) were chosen uniformly at random in the range \([-1, -0.5] \) or \([0.5, 1] \).

Using the BIC scoring function in equation (8), we searched for the structure with maximum score among all possible structures. Our search algorithm is implemented in Python 3. We compared our algorithm against the PC algorithm which is implemented in the latest versions of the pgmpy library. Since the discrete PC algorithm can not directly apply on the mixed continuous and discrete data, we discretized all the continuous data using mean value [Yuan and Malone, 2013]. Since the PC algorithm does not recover all directions of the DAG, we only measure how often the PC algorithm can correctly infer the skeleton of the true DAG, which is the undirected graph resulting from removing all arrowheads from the DAG.

Procedures used for the simulation experiments are described below.

1. For different number of continuous variables \( c \in \{1, 2, 3\} \), we simulated 100 random DAGs with 4 variables. In total, we generated 300 random graphs.

2. Using BIC score as we described previously, the causal structures were estimated based on \( n \in \{100, 300, 1000, 3000, 10000, 300000\} \) samples, respectively.

3. The accuracy rate of recovering causal structure was calculated based on 100 iterations.

Figure 3 provides a comparison of our proposed algorithm and the PC algorithm in terms of skeleton accuracy. First, we observed that our proposed method learns the correct causal structure as the number of data increases. The results empirically show that our method has the asymptotic consistency. In contrast, the discrete PC algorithm was not able to estimate the correct causal structure even for large numbers of samples. Second, as the number of continuous variables increases, the performance of the PC algorithm decreases. The reason is considered that some information might be lost due to discretization. The more number of continuous variables are discretized, the more information loses.

In another experiment, we assume that the skeleton of the DAG model can be obtained from some oracle procedure. Then we score each DAG which is consistent with the skeleton. Figure 4 reported the accuracy rate of this hybrid-oracle approach on the previous generated 300 DAG models. In comparison, we also reported the performance analysis of full search approach. A key observation is that when we know the undirected structure, the hybrid-oracle can learn full causal structure with 80% accuracy, even for only 100 data samples.

This insight is quite important in practical case. Because in many analysis we might know some pair of variables are correlate but do not know the causal direction. Our BIC score and search approach can get efficiency if we know the undirected structure. On they other hand, if we start from undirected structure instead of scratch, the necessary number of data samples decreases, which is a huge advantage for practice.
Causal discovery from a mixture of continuous and discrete data is an important research problem and has practical value. Most existing causal discovery methods either ignore the discrete data or discretize all the continuous data. In this paper we proposed a hybrid causal model and derived the BIC scoring function for evaluating our model.

5 Summary

Figure 2: The accuracy rate of estimating skeleton from mixed continuous and discrete data for increasing number of samples and the number $c \in \{1, 2, 3\}$ of continuous variables involved.

Figure 3: A comparison of the hybrid algorithm and the hybrid-oracle algorithm with respect to the accuracy rate of estimating the DAG structure.

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