Discovering Fully Oriented Causal Networks

Osman Mian, Alexander Marx and Jilles Vreeken
CISPA Helmholtz Center for Information Security
{osman.mian, alexander.marx, jv}@cispa.de

Abstract

We study the problem of inferring causal graphs from observational data. We are particularly interested in discovering graphs where *all* edges are oriented, as opposed to the partially directed graph that the state-of-the-art discover. To this end we base our approach on the *algorithmic* Markov condition. Unlike the *statistical* Markov condition, it uniquely identifies the true causal network as the one that provides the simplest—as measured in Kolmogorov complexity—factorization of the joint distribution. Although Kolmogorov complexity is not computable, we can approximate it from above via the Minimum Description Length principle, which allows us to define a consistent and computable score based on non-parametric multivariate regression. To efficiently discover causal networks in practice, we introduce the GLOBE algorithm, which greedily adds, removes, and orients edges such that it minimizes the overall cost. Through an extensive set of experiments we show GLOBE performs very well in practice, beating the state-of-the-art by a margin.

Introduction

Discovering causal dependencies from observational data is one of the most fundamental problems in science (Pearl 2009). We consider the problem of recovering the causal network over a set of continuous-valued random variables $\boldsymbol{X}$ based on an iid sample from their joint distribution. The state-of-the-art does so by first recovering an undirected causal skeleton—which identifies the variables that have a direct causal relation—and then uses conditional independence tests to orient as many edges as possible. By the nature of these tests this can only be done up to Markov equivalence classes, which means that these methods in practice return networks where only few edges are oriented. In contrast, we develop an approach that discovers fully directed causal graphs.

We base our approach on the algorithmic Markov condition (AMC), a recent postulate that states that the factorization of the joint distribution according to true causal network coincides with the one that achieves the lowest Kolmogorov complexity (Janzing and Schölkopf 2010). As an example, consider the case where X causes Y. Whereas the traditional *statistical* Markov condition cannot differentiate between $P(X)P(Y|X)$ and $P(Y)P(X|Y)$ as both are valid factorizations of joint distribution $P(X, Y)$, the *algorithmic* Markov condition takes the complexities of these distributions into account: in this case, the simplest factorization of $P(X, Y)$ is $K(P(X)) + K(P(Y|X))$ as only this factorization upholds the true independence between the marginal and conditional distribution—any competing factorization will be more complex because of inherent redundancy between the terms. As Kolmogorov complexity can capture any physical process (Li and Vitányi 2009) the AMC is a very general model for causality. However, Kolmogorov complexity is not computable, and hence we need a practical score to instantiate it. Here we do so through the Minimum Description Length principle (Grünwald 2007), which provides a statistically well-founded approach to approximate Kolmogorov complexity from above.

We develop an MDL-based score for directed acyclic graphs (DAGs), where we model the dependencies between variables through non-parametric multivariate regression. Simply put, the lower the regression error of the discovered model, the lower its cost, while more parameters mean higher complexity. We show this score is consistent: given sufficiently many samples from the joint distribution, we can uniquely identify the true causal graph if the causal relations are nearly deterministic. To efficiently discover causal networks directly from data we introduce the GLOBE algorithm, which much like the well-known GES (Chickering 2002) algorithm greedily adds and removes edges to optimize the score. Unlike GES, however, GLOBE traverses the space of DAGs rather than Markov equivalence classes—orienting edges during its search based on the AMC—and hence is guaranteed to result in a fully directed network.

Through extensive empirical evaluation we show that GLOBE performs well in practice and outperforms the state-of-the-art conditional independence and score based causal discovery algorithms. On synthetic data we confirm GLOBE does not discover spurious edges between independent variables, and overall achieves the best scores on both the structural hamming distance and the structural intervention distance. Last, but not least, on real-world data we show that GLOBE even works well when it is unlikely that our modelling assumptions are met.

For reproducibility we provide detailed pseudo-code in technical appendix, and make all code and data available.

Preliminaries

First, we introduce the notation for causal graphs and the main information theoretic concepts that we need later on.

Causal Graph We consider data over the joint distribution of m continuous valued random variables $\boldsymbol{X} = \{X_1, \ldots, X_m\}$. As is common, we assume *causal sufficiency*. That is, we assume that $\boldsymbol{X}$ contains all random variables that are relevant to the system, or in other words, that there exist no latent confounders. Under the assumptions of causal sufficiency and acyclicity, we can model causal relationships over $\boldsymbol{X}$ using a *directed acyclic graph* (DAG). A causal DAG G over $\boldsymbol{X}$ is a graph in which the random variables are the nodes and edges identify the causal relationship between a pair of nodes. In particular, a directed edge between two nodes $X_i \to X_j$ indicates that X_i is a *direct cause* or *parent* of X_j. We denote the set of all parents of X_i with $\mathrm{Pa}(X_i)$.

When working on causal DAGs, we assume the common assumptions, the *causal Markov condition* and the *faithfulness condition*, to hold. Simply put, the combination of both assumptions implies that each separation present in the true graph G implies an independence in the joint distribution P over the random variables $\boldsymbol{X}$ and vice versa (Pearl 2009).

Identifiability of Causality A causal relationship is said to be *identifiable* if it is possible to unambiguously recover it from observational data alone. In general, causal dependencies are not identifiable without assumptions on the causal model. The common assumptions for discovering causal DAGs allow identification up to the Markov equivalence class (Pearl 2009). Given additional assumptions, such as that the relation between cause and effect is a non-linear function with additive Gaussian noise (Hoyer et al. 2009), it is possible to identify causal directions within a Markov equivalence class (Glymour, Zhang, and Spirtes 2019). This is the causal model we investigate.

Kolmogorov Complexity The Kolmogorov complexity of a finite binary string x is the length of the shortest binary program p^* for a universal Turing machine $\mathcal{U}$ that outputs x and then halts (Kolmogorov 1965; Li and Vitányi 2009). Simply put, p^* is the most succinct *algorithmic* description of x, and therewith Kolmogorov complexity of x is the length of its ultimate lossless compression. Conditional Kolmogorov complexity, $K(x \mid y) \leq K(x)$, is then the length of the shortest binary program p^* that generates x, and halts, given y as input.

The Kolmogorov complexity of a probability distribution P, $K(P)$, is the length of the shortest program that outputs $P(x)$ to precision q on input $\langle x, q \rangle$ (Li and Vitányi 2009). More formally, we have

$$K(P) = \min \left\{ |p| : p \in \{0,1\}^*, |\mathcal{U}(p, x, q) - P(x)| \leq \frac{1}{q} \right\}.$$

The conditional, $K(P \mid Q)$, is defined similarly except that the universal Turing machine $\mathcal{U}$ now gets the additional information Q. For more details on Kolmogorov complexity see Li and Vitányi (2009).

Minimum Description Length Principle Although Kolmogorov complexity is not computable, we can approximate it from above through lossless compression (Li and Vitányi 2009). The Minimum Description Length (MDL) principle (Rissanen 1978; Grünwald 2007) provides a statistically well-founded and computable framework to do so. Conceptually, instead of all programs, *ideal MDL* considers only those programs for which we know that they output x and halt, i.e., lossless compressors. Formally, given a model class $\mathcal{M}$, MDL identifies the best model $M \in \mathcal{M}$ for data D as the one minimizing $L(D, M) = L(M) + L(D \mid M)$, where $L(M)$ is the length in bits of the description of M, and $L(D \mid M)$ is the length in bits of the description of data D given M. This is known as two-part, or *crude* MDL. There also exists one-part, or *refined* MDL. Although refined MDL has theoretically appealing properties, it is efficiently computable for a small number of model classes. Asymptotically, there is no difference between the two (Grünwald 2007).

To use MDL in practice we need to define a model class, and how to encode a model, resp. the data given a model, into bits. Note that we are only concerned with optimal code *lengths*, not actual codes—our goal is to measure the *complexity* of a dataset under a model class, after all (Grünwald 2007). Hence, all logarithms are to base 2, and we use the common convention that $0 \log 0 = 0$.

Theory

In this section, we will first introduce the algorithmic model of causality which is based on Kolmogorov complexity. To put it into practice, we need to introduce a set of modelling assumptions that allow us to approximate it using MDL. We conclude this section by providing consistency guarantees.

Algorithmic Model of Causality

Here we introduce the main concepts of algorithmic causal inference as introduced by Janzing and Schölkopf (Janzing and Schölkopf 2010), starting with the causal model.

Postulate 1 (Algorithmic Model of Causality)**.** *Let G be a DAG formalizing the causal structure among the strings $x_1, \ldots, x_m$. Then, every x_j is computed by a program q_j with constant length from its parents $Pa(x_j)$ and an additional input n_j. That is*

$$x_j = q_j(Pa(x_j), n_j) \ ,$$

where the inputs n_j are jointly independent.

As any mathematical object x can be described as a binary string, and a program q_j can model any physical process (Deutsch 1985) or possible function h_j (Li and Vitányi 2009), this is a particularly general model of causality. Equivalent to the statistical model, we can derive that the algorithmic model of causality fulfils the *algorithmic* Markov property (Janzing and Schölkopf 2010), that is

$$K(x_1, \ldots, x_m) \stackrel{+}{=} \sum_{j=1}^{m} K(x_j \mid \mathrm{Pa}^*(x_j)) \ ,$$

where $\stackrel{+}{=}$ denotes equality up to an additive constant. Meaning, to most succinctly describe all strings, it suffices to know

what are the parents and additional inputs n_j for each string x_j. Unlike its statistical counterpart which can only identify the causal network up to Markov equivalence, the *algorithmic* Markov property can identify a single DAG as the most succinct description of all strings. As any mathematical object, including distributions, can be described by a binary string, Janzing and Schölkopf (2010) define the following postulate.

Postulate 2 (Algorithmic Markov Condition)**.** *A causal DAG G over random variables $\boldsymbol{X}$ with joint density P is only acceptable if the shortest description of P factorizes as*

$$K(P(X_1, \ldots, X_m)) \stackrel{+}{=} \sum_{j=1}^{m} K(P(X_j \mid Pa(X_j))) \ . \quad (1)$$

Hence, under the assumption that the true causal graph can be modelled by a DAG, it has to be the one minimizing Eq. (1). As K is not computable we cannot directly compute this score. What we can however, restrict our model class from allowing all possible functions to a subset of these and then approximate K using MDL.

Causal Model

As causal model we consider a rich class of structural equation models (Pearl 2009) (SEMs) where the value of each node is determined by a linear combination of functions over all possible subsets of parents and additional independent noise. Formally, for all $X_i \in \boldsymbol{X}$ we have

$$X_i := \sum_{\mathcal{S}_j \in \mathcal{P}(\mathrm{Pa}(X_i))} h_j(\mathcal{S}_j) + N_i \ , \quad (2)$$

where h_j is a non-linear function of the j-th subset over the power set, $\mathcal{P}(\mathrm{Pa}(X_i))$, of parents of X_i, and N_i is an independent noise term. We assume that all noise variables are jointly independent, Gaussian distributed and that $N_i \perp\!\!\!\perp \mathrm{Pa}(X_i)$.

MDL Encoding of the Causal Model

Next, we specify our MDL score for DAGs. Given an iid sample $\boldsymbol{X}^n$ drawn from the joint distribution P over $\boldsymbol{X}$, our goal is to approximate Eq. (1) using two-part MDL, which means we need to define a model class $\mathcal{M}$ for which we can compute the optimal code length. Here, we define $\mathcal{M}$ to include all possible DAGs over $\boldsymbol{X}$ and their corresponding parametrization according to our causal model. That is, for each node X_i a model $M \in \mathcal{M}$ contains an index indicating the parents of X_i, which is equivalent to storing the DAG structure, and the corresponding functional dependencies.

Building upon Eq. (1), we want to find that model $M^* \in \mathcal{M}$ such that

$$\begin{aligned} M^* &= \operatorname*{argmin}_{M \in \mathcal{M}} L(\boldsymbol{X}^n, M) \\ &= \operatorname*{argmin}_{M \in \mathcal{M}} \left(L(M) + \sum_{i=1}^{m} L(X_i^n \mid \mathrm{Pa}(X_i), M) \right) \\ &= \operatorname*{argmin}_{M \in \mathcal{M}} \left(L(M) + \sum_{i=1}^{m} L(\epsilon_i) \right) \end{aligned}$$

where $\mathrm{Pa}(X_i)$ are the parents of X_i according to the model M. In the last line, we replace $L(X_i^n \mid \mathrm{Pa}(X_i), M)$ with $L(\epsilon_i)$ to clarify that encoding a node given M and its parents comes down to encoding the residuals ϵ_i.

Encoding the Model The model complexity $L(M)$ for a model $M \in \mathcal{M}$, comprises of the parameters of the functional dependencies and the graph structure. The total cost is simply the sum of the code lengths of the individual nodes

$$L(M) = \sum_{i=1}^{m} L(M_i) \ .$$

To encode the individual nodes X_i, we need to transmit its parents, the form of the functional dependency, and the bias or mean shift μ_i. We encode the model M_i for a node X_i as

$$L(M_i) = L_{\mathbb{N}}(k) + k \log m + L_F(f_i) + L_p(\mu_i) \ ,$$

where we first encode the number of parents using $L_{\mathbb{N}}$, the MDL-optimal encoding for integers $z \geq 0$ (Rissanen 1983). It is defined as $L_{\mathbb{N}}(z) = \log^* z + \log c_0$, where $\log^* z = \log z + \log\log z + \ldots$ and we consider only the positive terms, and c_0 is a normalization constant to ensure the Krafft-inequality holds (Kraft 1949). Next, we identify which out of the m random variables these are, and then proceed to encode the function f_i over these parents, where f_i represents the summation term on the right hand side of Eq. (2). Last, we encode the bias term using L_p, defined later in Eq.(3).

Encoding the Functions We will instantiate the framework using non-parametric functions h_i that also allow for non-linear transformations of the parent variables. To this end, we fit non-parametric Multivariate Adaptive Regression Splines (Friedman 1991). In essence, we estimate X_i as

$$\hat{X}_i := \sum_{j=1}^{|H|} h_j(\mathcal{S}_j) \ ,$$

where h_j is called a hinge function that is applied to a subset of the parents, $\mathcal{S}_j$, with size $|\mathcal{S}_j|$, that is associated with the j-th hinge. A hinge takes the form

$$h(\mathcal{S}) = \prod_{i=1}^{T} a_i \cdot \max(0, g_i(s_i) - b_i) \ ,$$

where T denotes the number of multiplicative terms in h, $s_i \in \mathcal{S}$ is the parent associated with the i-th term, g_i is a non-linear transformation applied to s_i where g_i belongs to the function class $\mathcal{F}$, e.g. the class of all polynomials up to a certain degree. We specify $\mathcal{F}$ in more detail in the supplementary section, but the encoding can be very general and can include any regression function as long as we can describe the parameters and $|\mathcal{F}| < \infty$. If $T = 1$ for all hinges, the above definition simplifies to an additive model over individual parents. We encode a hinge function as follows

$$L_F(h) = \ L_{\mathbb{N}}(|H|) + \sum_{h_j \in H} \Big[\ L_{\mathbb{N}}(T_j) + \log \binom{|\mathcal{S}| + T_j - 1}{T_j} + T_j \log(|\mathcal{F}|) + L_p(\theta(h_j)) \ \Big]$$

First, we use $L_{\mathbb{N}}$ to encode the number of hinges and the number of terms per hinge. We then transmit the correct assignment of terms T_j to parents in $\mathcal{S}$, and finally need $\log(|\mathcal{F}|)$ bits to identify the specific non-linear transformation that is used for each of the T_j terms in the hinge.

Encoding Parameters To encode the bias we use the proposal of Marx and Vreeken (2017) for encoding parameters up to a user specified precision p. We have

$$L_p(\theta) = |\theta| + \sum_{i=1}^{|\theta|} L_{\mathbb{N}}(s_i) + L_{\mathbb{N}}(\lceil \theta_i \cdot 10^{s_i} \rceil) \ , \qquad (3)$$

where s_i is the smallest integer such that $|\theta_i| \cdot 10^{s_i} \geq 10^p$. Simply put, $p = 2$ implies that we consider two digits of the parameter. We need one bit to store the sign of the parameter, then we encode the shift s_i and the shifted parameter θ_i.

Encoding Residuals Last, we need to encode the residual term, $L(\epsilon_i)$. Since we use regression functions, we aim to minimize variance of the residual—and hence should encode the residual ϵ as Gaussian distributed with zero-mean (Marx and Vreeken 2017; Grünwald 2007)

$$L(\epsilon) = \frac{n}{2}\left(\frac{1}{\ln 2} + \log 2\pi\hat{\sigma}^2\right) \ ,$$

where we can compute the empirical variance $\hat{\sigma}^2$ from ϵ.

Combining the above, we now have a lossless MDL score for a causal DAG.

Consistency

Since MDL can only upper bound Kolmogorov complexity, but not compute it, it is not possible to directly derive strict guarantees from the AMC. We can, however, derive consistency results. We first show that our score allows for identifying the Markov equivalence class of the true DAG i.e. the partially directed network for which each collider is correctly identified. Then, we show that under slightly stricter assumptions, we can orient the remaining edges correctly.

The main idea for the first part is to show that our score is consistent—simply put, *the likelihood term dominates in the limit*. For a score with such properties e.g. BIC (Haughton 1988), Chickering (2002) showed that it is possible to identify the Markov equivalence class of the true DAG. To show that our score behaves in the same way, we need to make two light weight assumptions for $n \to \infty$:

1. the number of hinges of $|H|$ is bounded by $\mathcal{O}(\log n)$, and
2. the precision of the parameters θ is constant w.r.t. to n and hence $L_p(\theta) \in \mathcal{O}(1)$.

Based on these assumptions, we can show that our score is consistent as it asymptotically behaves like BIC, meaning that the penalty term for the parameters only grows with $\mathcal{O}(\log n)$ complexity, while the likelihood term grows linearly with n and hence is the dominating term as $n \to \infty$.

Theorem 1. *Given a causal model as defined in Eq.* (2) *and corresponding data $\boldsymbol{X}^n$ drawn iid from joint distribution P. Under Assumptions (1) and (2), $L(\boldsymbol{X}^n, M)$ asymptotically behaves like BIC.*

Algorithm 1: The GLOBE Algorithm

Data: Data $\boldsymbol{X}^n$ over $\boldsymbol{X}$
Result: Causal DAG G

```
Q ← EdgeScoring(X^n)
G ← ForwardSearch(Q, X^n)
G ← BackwardSearch(G)
return G
```

With the above, we know that given sufficient data our score will identify the correct Markov equivalence class.

To infer the complete DAG, we need to be able to infer the direction for those edges that cannot be inferred using collider structures—i.e. single edges like $X - Y$. Closest to our approach is the work of Marx and Vreeken (2019) who showed that it is possible to distinguish between $X \to Y$ and $Y \to X$ using any L_0 regularized score—e.g. BIC, if we assume that the underlying causal function is near deterministic i.e. $Y := f(X) + \alpha N$, where f is a non-linear function and N is an unbiased, unit-variance noise regulated by a small constant $\alpha > 0$. Since our score in the limit behaves like an L_0-based score (ref. Theorem 1), we can distinguish between Markov equivalent DAGs under these stricter assumptions. For a detailed discussion, readers are directed to the proof of Theorem 1 in technical appendix.

Although our score is consistent and can be used to distinguish Markov equivalent DAGs, these guarantees only hold if we were to score all DAGs over $\boldsymbol{X}$. Since this is infeasible for large graphs, we propose a modified greedy DAG search algorithm to minimize $L(\boldsymbol{X}^n, M)$.

The GLOBE Algorithm

We now present GLOBE, a score-based method for discovering directed acyclic causal graphs from multivariate continuous valued data. GLOBE consists of three steps: edge scoring, forward and backward search, as shown in Algorithm 1.[1]

Edge Scoring To improve the forward search where we greedily add the edge that provides the highest gain, we first order all potential edges in a priority queue by their causal strength. We measure the causal strength of an edge, using the absolute gain in bits for orienting an edge in either direction in our model. Formally, let $e = (X_i, X_j)$ be an undirected edge between X_i and X_j, and further let $\vec{e}$ refer to the directed edge $X_i \to X_j$ and $\overleftarrow{e}$ the directed edge in the reverse direction. Now, let M be the current model. We write $M \oplus \overleftarrow{e}$ to refer to the model where we add edge $\overleftarrow{e}$, and $M \oplus \vec{e}$ for the model where we add $\vec{e}$. We define the gain in bits, δ, associated with edge $\overleftarrow{e}$ as

$$\delta(\ \overleftarrow{e}\ ) = \max\{0, L(\boldsymbol{X}^n, M) - L(\boldsymbol{X}^n, M \oplus \overleftarrow{e})\}$$

where $L(\boldsymbol{X}^n, M)$ is defined according to the causal model specified in the theory section, and define $\delta(\ \vec{e}\ )$ analogously. Based on $\delta(\ \overleftarrow{e}\ )$ and $\delta(\ \vec{e}\ )$, we define the directed gain $\Psi(\overleftarrow{e})$ for a given edge as

$$\Psi(\overleftarrow{e}) = \delta(\overleftarrow{e}) - \delta(\vec{e}) \ ,$$

[1] We provide detailed pseudocodes in the technical appendix

where $\Psi(\overleftarrow{e}) = -\Psi(\vec{e})$. The higher the value of $\Psi(\overleftarrow{e})$, the higher edge $\overleftarrow{e}$ is ranked. Intuitively, the larger the difference between the edge direction, the more certain we are that we inferred the correct direction. The algorithm for this step is straightforward, we pick each undirected edge e, calculate δ and Ψ for $\overleftarrow{e}$ and $\vec{e}$, and add the edges to a priority queue.

Forward Search For forward search phase, we use the priority queue obtained from the edge ranking step to build the causal graph by iteratively adding the highest ranked edge. We reject edges that would introduce a cycle. After adding an edge $X_i \to X_j$ we need to update the score of all edges pointing towards X_j and re-rank them in the priority queue. Due to the greedy nature of the algorithm, we may add edges in the wrong direction when we do not yet know all the parents of a node. Hence, after adding edge $X_i \to X_j$ to the current model—i.e. discovering a new parent for X_j—we check for all children of X_j, whether flipping the direction of the edge improves the overall score. If so, we delete that edge $\vec{e}$ from our model, re-calculate δ and Ψ for $\vec{e}$ and $\overleftarrow{e}$, and push them again to the priority queue (see Fig. 1). The forward search stops when the priority queue is empty.

To avoid spurious edges, we check for significance of the gain. Let $k = \delta(\overleftarrow{e})$, based on the no-hypercompression inequality (Grünwald 2007), the probability to gain k bits over the null model is smaller or equal to 2^{-k}. If for an edge the gain k is not significant—i.e. $2^{-k} > \alpha$, where α is a user defined significance threshold, we disregard the edge.

Backward Search To further refine the graph discovered in the forward search, we iteratively remove superfluous edges. In particular, for each node X_j with $|\text{Pa}(X_j)| = k \geq 2$ we score all graphs for which we only use a subset of the parents of size $k-1$. If any of these graphs provides a gain in compression, we select the one that provides the largest gain and update the model accordingly. We continue this process until we cannot find such a subset for any node and output the current graph as our predicted causal DAG.

Complexity Analysis

The edge ranking does one pass over the edges, it has a runtime of $\mathcal{O}(|V|^2)$. In the forward search, each edge can lead to at most $(|V|-1)$ ranking updates due to edge flips. Resulting in a total complexity in $\mathcal{O}(|V|^3)$. The backwards search has a loose upper bound of $\mathcal{O}(|V|^3)$, that results when the forward search returns a fully connected graph and we delete each of those edges in the backwards search. Hence, the overall complexity of GLOBE is in $\mathcal{O}(|V|^3)$. In practice, GLOBE is fast enough for networks as large as 500 nodes.

Instantiation

We instantiate GLOBE[2] using the open-source implementation in R of Multivariate Adaptive Regression Splines framework (Friedman 1991). Since we could face issues like multicollinearity (Farrar and Glauber 1967) and unrealistic run times if we allow for arbitrary many interactions between parents, we restrict the maximum number of interaction terms to 2 for experiments.

[2]GLOBE stems from discovering fully, rather than locally, oriented networks, as well as from it being based on Multivariate Adaptive Regression Splines (MARS), of which the public implementation is known as EARTH.

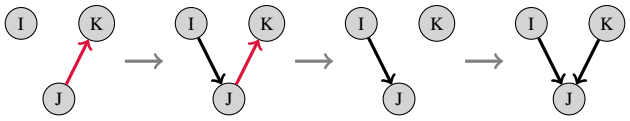

Figure 1: Edge reversal in the forward search: We start with the graph where we wrongly added edge $X_j \to X_k$, then we add the correct edge $X_i \to X_j$. Revisiting the children of X_j we see that flipping $X_j \to X_k$ improves our score and hence delete the edge. In the next step we add the correct edge.

Related Work

Causal discovery on observational data has drawn more attention in recent years (Bühlmann et al. 2014; Huang et al. 2018; Hu et al. 2018; Margaritis and Thrun 2000) and is still an open problem. To give a succinct overview, we focus on the most related methods, ones that aim to recover a DAG or its Markov equivalence class from continuous valued data. We exclude methods that aim at weakening assumptions such as causal sufficiency or acyclicity (Spirtes et al. 2000), or methods for discrete data (Budhathoki and Vreeken 2017).

Most approaches can be classified as constraint based or score based. Both rely on the Markov and faithfulness conditions to recover Markov equivalence classes of the true DAG. Constraint based methods such as the PC and FCI algorithm (Spirtes et al. 2000), their extensions (Colombo and Maathuis 2014; Pearl, Verma et al. 1991) as well as the Grow-Shrink algorithm (Margaritis and Thrun 2000) rely on conditional independence (CI) tests to first recover the undirected causal graph and then infer edge directions only up to the Markov equivalence class using additional edge orientation rules (Meek 1995). The main bottleneck for those approaches is the CI test. The standard choice is the Gaussian CI test (Kalisch and Bühlmann 2007). However, it cannot capture non-linear correlations. The current state-of-the-art uses kernel based tests such as HSIC (Gretton et al. 2005), which can capture non-linear dependencies.

Score based methods define a scoring function, $S(G, \boldsymbol{X}^n)$, that evaluates how well a causal DAG G fits the provided data $\boldsymbol{X}^n$. If the true causal graph G^* is a DAG, then given infinite data the highest scoring DAG is part of the equivalence class of G^* (Chickering 2002). Score based approaches start with an empty graph and greedily traverse to the highest scoring Markov equivalence class that is reachable by adding, deleting or reversing an edge. Well-known algorithms in this category include the greedy equivalence search (GES) (Chickering 2002; Hauser and Bühlmann 2012), its extensions (Ramsey et al. 2017), and the current state-of-the-art, generalized-GES (GGES) (Huang et al. 2018) which uses kernel regression to capture complex dependencies.

In contrast, additive noise models (ANMs) aim to discover the fully directed graph (Hoyer et al. 2009). The primary as-

sumption is that the effect can be written as a function of the cause plus additive noise that is independent of the cause. Under this assumption, the function is only admissible in causal direction and not vice-versa (Hoyer et al. 2009). Methods range from linear non-Gaussian (LINGAM) (Shimizu et al. 2006), non-linear functions (RESIT) (Peters et al. 2014) to mixtures of non-linear additive noise models (Hu et al. 2018). The main caveat of ANMs is also the CI test. Fitting a non-linear function that maximizes the independence between the cause and noise is a slow process which restricts ANMs application to small networks (Hoyer et al. 2009).

Most related to our work are methods based on regression error. Those methods have been shown to successfully decide between Markov equivalent DAGs under the assumption of having a non-linear function and low noise (Marx and Vreeken 2017; Blöbaum et al. 2018; Marx and Vreeken 2019) or proven to correctly identify the causal ordering of all nodes (CAM) (Bühlmann et al. 2014). Directly comparing a causal ordering to a DAG is, however, not straightforward.

In this paper, we combine the advantages of score based methods and methods based on regression error by discovering the fully oriented graph and allowing for complex non-linear dependencies, while being fast in practice.

Experiments

We evaluate GLOBE on both synthetic and real-world data with known ground truth. GLOBE is implemented in Python and both the source code, as well as the synthetic data are made available for reproducibility.[3] We compare GLOBE to the state-of-the-art from different classes of algorithms. We compare to RESIT (Peters et al. 2014) and LINGAM (Shimizu et al. 2006) as representative ANM-based methods, to GGES as the best score-based method (Huang et al. 2018), and to PC with the Hilbert Schmidt Independence Criteria, short PC_{HSIC} (Colombo and Maathuis 2014; Gretton et al. 2005), as the state-of-the-art constraint-based method for causal discovery. Comparison with FASTGES (Ramsey et al. 2017) is ommitted since its performance was significantly worse than the other methods. We provide details on experimental setup as well as additional experiments, involving a case-study in the technical appendix. GLOBE finished within ten minutes for each experimental instance except one real-world dataset with 500 nodes, on which it took 3 days. While the competitors could not handle this data.

Evaluation Metrics We evaluate the predicted and the ground truth graphs on the basis of their structural, as well as their *causal* similarity. We justify using our proposed evaluation metrics in the technical appendix.

The Structural Hamming Distance (*SHD*) (Kalisch and Bühlmann 2007), between two partially directed acyclic graphs (PDAGs) G and $\hat{G}$ is the the total number of edges where the two graphs differ. Denoting the edge adjacency matrix of G and $\hat{G}$ with X resp. $\hat{X}$ we have

[3] http://eda.mmci.uni-saarland.de/globe/

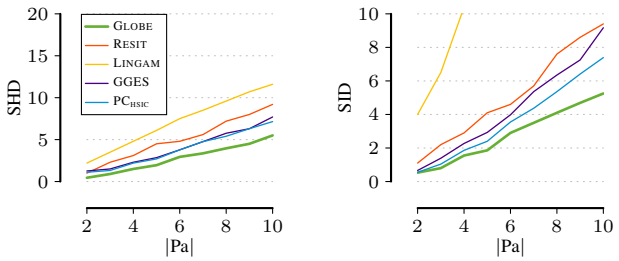

Figure 2: [Lower is better] *SHD* (left) and *SID* (right) for increasing number of parents.

$$SHD(G, \hat{G}) \coloneqq \sum_{1 \leq i < j \leq m} \mathbf{I}((X_{ij} \oplus \hat{X}_{ij}) \vee (X_{ji} \oplus \hat{X}_{ji})) \,,$$

where $\oplus$ denotes an XOR operation and $\mathbf{I}(x)$ is 1 when the expression x is $true$ and 0 otherwise.

However, *SHD* tells us nothing about the causal similarity between two graphs. Hence, we use the Structural Intervention Distance (*SID*) (Peters and Bühlmann 2015) pre-metric. *SID* counts the pairs of nodes u and v such that the effect of intervention from u to v is falsely estimated by $\hat{G}$ with respect to G. In case of a PDAG, *SID* is an interval, with smallest and largest scores indicating the best resp. worst scores for the DAGs in a given Markov equivalence class.

Synthetic Data

We start with a sanity check to ensure that GLOBE can reliably avoid false positives and build up to the case of varying sample sizes over a more complex network. We generated 100 instances each with 1 000 observations for the discussed structures, unless stated otherwise. We standardized the data to have zero mean and unit variance.

Independent Data As a sanity check, we test the methods on instances of a graph containing 10 independent nodes where the value of each node is sampled independently from a Gaussian distribution. We expect all the methods to report empty sets of edges for the instances in this experiment. GLOBE did not report a single spurious edge on *any* of the instances. On the other hand, LINGAM reported at least one spurious edge for 38%, RESIT for 42% and PC_{HSIC} and GGES for half resp. 10% of the instances.

Effect of Multiple Parents Next we test GLOBE on a simple case of a collider where we vary the number of parents from 2 up to 10. The collider node is calculated as a linear combination of non-linear parent functions given as

$$X_j = \sum_{X_i \in \text{Pa}(X_j)} a_i \cdot (X_i + b_i)^{c_i} \quad . \tag{4}$$

Since it is possible to identify a collider structure using conditional independence tests, we expect GGES and PC_{HSIC} to discover a fully directed network. The results for both

n	GLOBE	RESIT	LINGAM	GGES	PC_{HSIC}
100	**0.28**	0.45	0.47	[0.18 , 0.48]	[0.28 , 0.54]
500	**0.26**	0.43	0.43	[0.17 , 0.48]	[0.21 , 0.55]
1000	**0.26**	0.42	0.42	[0.17 , 0.48]	[0.20 , 0.54]
1500	**0.27**	0.40	0.43	[0.17 , 0.48]	[0.19 , 0.53]
2000	**0.26**	0.40	0.40	[0.18 , 0.49]	[0.19 , 0.54]

Table 1: [Lower is Better] Averaged normalized *SID* for the methods. Interval for GGES and PC_{HSIC} indicates the best, resp. worst possible intervention distance for the DAGs in the discovered Markov equivalence class.

SHD and *SID* are shown in Figure 2. In case of *SID*, we compare favorably to both GGES and PC_{HSIC} by only reporting the *best possible* achievable score for their predicted graphs' Markov equivalence class. Even with this favorable comparison, GLOBE outperforms the competition.

Data Sampled from a Causal Network Next, we show GLOBE's effectiveness in finding the causal relationships in a more general setting. We consider multiple instances of the graph that contains all possible connections that could exist in a DAG. In this setting, each child node, X_j can alternatively be calculated using more complex multiplicative interactions between the parents given by

$$X_j = a_j \cdot \prod_{X_i \in \text{Pa}(X_j)} {X_i}^{c_i} + b_j \ . \tag{5}$$

We generate data where we choose between Eq. (4) and (5) with probability 0.7 resp. 0.3 and report results over varying sample sizes. We report the values for *SID* in Table 1. Overall we see that GLOBE outperforms RESIT and LINGAM by a margin. The causal networks predicted by GLOBE have *SID* closer to the better end of the range of scores possible for PC_{HSIC} and GGES. In terms of *SHD*, all the methods were found to be consistent over varying sample sizes, with GLOBE slightly outperforming the competition.

Real World Data

For real world data with known ground truth, we consider three distinct networks of sizes 5, 15 and 500 nodes from the reged dataset (Statnikov et al. 2015), each containing 1 000 rows. Looking at the results shown in Figure 3, we see that GLOBE is closest to the true causal network for both the 5 node (REGED5) and the 15 node (REGED15) network. For REGED15, GLOBE reports a better *SID* than all the competitors. We see that for the REGED15 network, GGES fails to orient most of the edges, which results in a graph where both extremes of the *SID* are possible.

For the 500 node network, GLOBE was the *only* algorithm to produce any kind of result in reasonable time (3 days), with a reported normalized *SID* and *SHD* of 0.1 resp. 0.01. While GGES failed to terminate within one month, all other methods could not process the data.

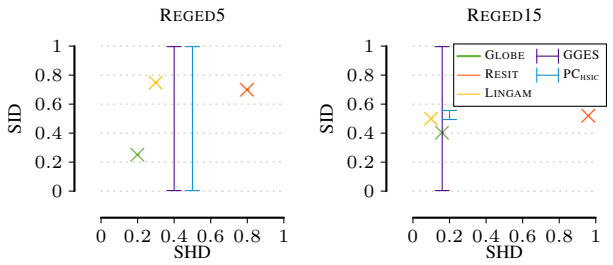

Figure 3: [Closer to Origin is Better] Comparison of Normalized *SHD* and Normalized *SID* for real world networks.

Discussion and Future Work

Instantiating GLOBE using the MARS framework is just one of the many realizations of the algorithm. Other regression approaches, as long as we define a consistent lossless encoding for them, can also be incorporated into GLOBE and may give better results based on the application domain. For proof of concept, we show how to instantiate GLOBE using parametric regression in the technical appendix.

Due to computational reasons, we only traverse the space of DAGs and not the Markov equivalence classes, which could result in a locally optimal solution. We try to mitigate this using the edge flipping step during the forward search. However, by incorporating a more complex search strategy, like the beam search, we could both expand our search space, and eliminate the need for the edge flip.

Our score is specifically defined for continuous valued data. An extension of GLOBE would be to discover causal relationships over discrete and mixed type data. As MDL-based scores have been proposed for inference on discrete (Budhathoki and Vreeken 2017) and mixed (Marx and Vreeken 2018) data, but only for pairs of variables, it would be interesting to extend GLOBE to handle both cases.

Conclusion

We considered discovering fully directed causal graphs from observational data. To tackle this problem, we built upon the algorithmic Markov condition that is based on Kolmogorov complexity. Since the latter cannot be computed directly, we proposed a score based on MDL to approximate it from above. We showed that for non-linear mixture models with additive noise, our score allows for discovering the Markov equivalence class of the true DAG and if the noise term is assumed to have a low variance, we can discover the fully directed causal graph. To minimize our score, we proposed GLOBE, a greedy DAG search algorithm that iteratively builds a DAG to find a locally optimal solution. We modeled functional dependencies using non-parametric regression functions.

Through an extensive set of experiments, we showed that GLOBE beats the state-of-the-art by a margin, reliably orients the edges in the presence of multiple parents, discovers graphs that are *structurally* and *causally* similar to the ground truth and is fast enough to infer networks up to 500 nodes.

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