A Fast Non-parametric Approach for Causal Structure Learning in Polytrees

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Abstract

We study the problem of causal structure learning with no assumptions on the functional relationships and noise. We develop DAG-FOCI, a computationally fast algorithm for this setting that is based on the FOCI variable selection algorithm in [1]. DAG-FOCI requires no tuning parameter and outputs the parents and the Markov boundary of a response variable of interest. We provide high-dimensional guarantees of our procedure when the underlying graph is a polytree. Furthermore, we demonstrate the applicability of DAG-FOCI on real data from computational biology [2] and illustrate the robustness of our methods to violations of assumptions.

1 Introduction

Estimation of the causal structure is challenging using observational data only. In general, one can only infer the Markov equivalence class which can be encoded as a PDAG (e.g., [3, 4]). Prior work on causal structure learning can be categorized into two groups: score-based algorithms (e.g., [5]) and constraint-based approaches using conditional independence testing (e.g., [6, 3]). The latter is focusing mostly on the Gaussian case ([7, 8, 9, 10]) and transformable to Gaussian case ([11, 12, 13]). Score-based methods have been worked out for the Gaussian case ([14, 15]) and there is a substantial amount of work when putting additional restrictions on the functional forms (e.g. nonlinear but additive errors [16, 17]), or on the error distributions (e.g. non-Gaussian error [18] and equal error noise variances [19]). There are also methods that combine the two approaches, score-based and constraint-based, e.g., [20, 21].

In addition to requiring distributional assumptions, score-based methods can become computationally infeasible in high-dimensional settings. Improving the speed of score-based methods involves either using ad-hoc optimization [22, 23] or adding extra assumptions on the model such as additive noise on trees [24].

The difficulty with constraint-based methods (e.g. the PC and IC algorithms [6, 25]) is that they require conditional independence testing, which is known to be a hard problem [26]. Although there has been a large body of research exploring different ideas for conditional independence testing, there is no
model-free and non-parametric method with theoretical guarantees for this purpose. This makes many of constraint-based methods vulnerable in applications where the data may not satisfy the properties for the validity of conditional independence test. A recent work [27] introduce a different constraint-based algorithm using entropy and local Markov boundary estimation. The proposed algorithm in [27] is polynomial both in sample and computational complexity. However, their specific assumptions on the magnitude of the conditional entropy of parents seem very strong. Polynomial time algorithms (in the number of nodes) includes [6], [28] for linear Gaussian models, [29] for a special family of distributions with quadratic variance functions, and extensions of [28] such as [30, 31, 32, 33]. A recent work [27] introduce a different constraint-based algorithm using entropy and local Markov boundary estimation. The proposed algorithm in [27] is polynomial both in sample and computational complexity. However, their specific assumptions on the magnitude of the conditional entropy of parents seem very strong.

In this paper, we propose a computationally efficient algorithm for causal structure learning without placing any restrictions on the function forms or error distributions. We provide finite sample guarantees for our algorithm under mild assumptions of δ-Gap and parent-cycle-free, which are implied when the underlying DAG is a polytree.

1.1 Our Contribution

We consider a setting where the variables satisfy the Causal Markov property with respect to a DAG and are generated according to a structural equation model. As mentioned earlier, no assumptions or restrictions are imposed on the functional forms or error distribution.

We focus on recovering the parental sets of a given target variable (may be multiple since the Markov equivalence class can entail more than one set of parents). Estimating the entire DAG can be viewed as combining the local neighborhood structures of all the nodes [34, 35]. Our proposed algorithm, dubbed DAG-FOCI, consists of two stages. In the first stage, we identify the local structure around the target variable. In the second stage, we combine the result of some pairwise independence tests with the output of the first stage to determine the parents of the target variable.

To obtain the local structure of a target node, we estimate its Markov boundary, i.e., the parents, children, and spouses of the target variable. By definition, conditional on the Markov boundary, the target variable is independent of the rest of the variables. To estimate the Markov boundary, one can use any variable selection technique [34, 36, 14]. We deploy the non-parametric variable selection algorithm FOCI, introduced in [1]. FOCI is a computationally efficient greedy algorithm that does not require a tuning parameter. Furthermore, it does not rely on conditional independence testing or density estimation. Under very mild assumptions, FOCI yields a Markov blanket with high probability [1]. We prove that under an extra assumption, dubbed by δ-Gap, FOCI obtains the Markov boundary, the smallest Markov blanket, of the target node. Informally, the δ-
Gap assumption requires that the target node has a higher dependency on its Markov boundary members compared to the rest of the nodes.

In contrast to methods that rely on conditional independence testing, like the PC algorithm, our method does not require the faithfulness assumption to estimate the Markov boundary.

After estimating the Markov boundary of a given node, we deploy simple independence testing to recover all the possible parental sets. When there is no cycle in the skeleton of the underlying DAG containing edge \((X_i, Y)\) where \(X_i\) is a parent of \(Y\), we guarantee that with high probability, DAG-FOCI estimates the set of parents correctly. If all the nodes satisfy this parent-cycle-free assumption, the DAG is a polytree, and our procedure is guaranteed to recover the underlying Markov equivalence class. When the parent-cycle-free assumption is not satisfied, the output of our algorithm does not contain any non-parent node. On the other hand, if our algorithm does output an estimate, it is guaranteed to be correct with high probability. As such, DAG-FOCI can be viewed as a conservative algorithm and its estimates, when non-empty, can be trusted with high probability.

The algorithm DAG-FOCI is presented in Section 2. Our main theoretical results are presented in Section 3. In Sections 4, we discuss how the violation of our assumptions affects the result of DAG-FOCI. Applications to simulated and real data are presented in Section 5. The proofs of the Theorems and Lemmas and a discussion on interventional data are presented in the Appendix.

1.2 Notations and Definitions

We represent a DAG \(G = (V, E)\) with node set \(V = [p + 1]\) and a collection of directed edges \(E\). We denote a directed edge by \((i, j)\) or \(i \rightarrow j\). In this case \(i\) is a parent of \(j\), and \(j\) is a child of \(i\). If there is any \(k\) such that \(k \rightarrow j\), then \(k\) is a spouse of \(i\). If there is a directed path \(i \rightarrow \cdots \rightarrow j\), then \(j\) is a descendent of \(i\), and \(i\) is an ancestor of \(j\). The skeleton of \(G\) is the undirected graph obtained from \(G\) by substituting directed edges by undirected edges. Nodes \(i\), \(j\), and \(k\) form a v-structure in a DAG if \(i \rightarrow k \leftarrow j\).

For the joint probability distribution \(P\) on \((X, Y)\), the Causal Markov property holds if every variable is independent of its non-descendants conditional on its parents in \(P\). The Markov equivalence class of \(G\) is the set of all DAGs that encode the same set of conditional independencies. Two DAGs are Markov equivalent if and only if they have the same skeleton and the same v-structures [37]. In observational studies, one generally cannot identify the underlying DAG but can potentially identify the Markov equivalence class.

For an arbitrary node \(X_i\), \(X_i\) is the set of all \(X_j\)'s excluding \(X_i\). For an index set \(S \subseteq [p + 1]\), the vector of corresponding features is shown as \(X_S\). For \(S \subseteq [p + 1] \setminus \{i\}\), \(X_S\) is a Markov blanket or a sufficient set for \(X_i\) if and only if \(X_i \perp X_{[p+1] \setminus (S \cup \{i\})} | X_S\). A minimal Markov blanket is called a Markov boundary, i.e., a Markov blanket is a Markov boundary if no strict subset of it is a Markov blanket. Under mild assumptions, the Markov boundary of a node is unique [38]; we denote the unique Markov boundary of \(X_i\) by \(\text{MB}(X_i)\).
In this work, we focus on discovering the causal structure of $Y$. For simplicity in the notation, we show the set of parents, children, and spouses of $Y$ respectively by $X_P$, $X_C$, and $X_{PC}$. It is well-known that $\text{MB}(Y) = X_P \cup X_C \cup X_{PC}$. Node $Y$ satisfies a parent-cycle-free property if no cycle in the skeleton of $G$ contains edge $(X_i, Y)$ for any $X_i \in X_P$. Node $Y$ satisfies a tree-neighborhood property if any cycle in the skeleton of $G$, contains at most one member of $\text{MB}(Y)$. Thus, the tree-neighborhood property is a stronger condition than the parent-cycle-free property: if the tree-neighborhood property is satisfied, then the parent-cycle-free property is also satisfied. A polytree is a DAG whose skeleton is a tree.

2 The algorithm DAG-FOCI

We consider random vectors $X = (X_1, \ldots, X_p, X_{p+1}) \in \mathbb{R}^{p+1}$ and denote by $Y = X_{p+1} \in \mathbb{R}$ a response variable of special interest. We posit that the distribution underlying $X$ satisfies the Causal Markov property with respect to a DAG and is parameterized by the following structural equation model (SEM):

$$X_i = f_i(X_{i_1}, \ldots, X_{i_k}, \varepsilon_i), \ i \in \{p + 1\}. \ (1)$$

Here, $f_i$ is a measurable function, $X_{i_1}, \ldots, X_{i_k}$ are the direct parents of $X_i$, and $\varepsilon_i$’s are independent noise variables from non-degenerate probability laws.

Given $n$ observations of $X$ generated independent and identically distributed according to the distribution of the SEM in (1), we identify the Markov boundary of node $Y$, and output the parental set(s) of $Y$. As described in the introduction, our algorithm DAG-FOCI consists of two stages. In the first stage, we deploy the non-parametric variable selection procedure FOCI [1] to obtain the local Markov structures around the node $Y$: the Markov boundary of $Y$ as well as the Markov boundary of each of the variables inside the Markov boundary of $Y$. In the second stage, we combine the local Markov structures around $Y$ to identify the parents of $Y$. In particular, we identify set(s) of variables inside the Markov boundary of $Y$ that are pairwise independent, and that are in each other’s Markov boundaries. A high-level description of DAG-FOCI is presented in Algorithm 1.

2.1 Stage I of DAG-FOCI: Finding the Markov Boundary

To discover the Markov boundary for any given variable, we use the model-free variable selection algorithm FOCI [1]. FOCI is based on the non-parametric and distribution-free measure of dependence CODEC [1]. For random variable $Y$ and random vectors $X \in \mathbb{R}^q$ and $Z \in \mathbb{R}^s$ where $s \geq 0$ and $q \geq 1$, CODEC quantifies the dependency of $Y$ on $Z$ given $X$ as

$$T(Y, Z \mid X) = \frac{\int \mathbb{E}(\text{Var}(P(Y \geq t \mid Z, X) \mid X))d\mu(t)}{\int \mathbb{E}(\text{Var}(1_{\{Y \geq t\}} \mid X))d\mu(t)}. \ (2)$$

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Algorithm 1 sketch of DAG-FOCI

Input: \( n \) samples of \((X_1, \cdots, X_p, Y)\)

Output: set of all possible parental sets

1: **Markov boundary search**: estimate \( \hat{\text{MB}}(Y) \) as well as \( \hat{\text{MB}}(X_j) \) for all \( X_j \in \hat{\text{MB}}(Y) \), where the Markov boundary search is fully non-parametric

2: **Finding connected components**: find maximal set(s) \( S \subseteq \hat{\text{MB}}(Y) \) such that for every \((X_i, X_j) \in S\): \( X_i \in \hat{\text{MB}}(X_j) \), \( X_j \in \hat{\text{MB}}(X_i) \), \( X_i \perp X_j \)

3: **Output**: if all but one set(s) \( S \) is a singleton, return the non-singleton set. Otherwise return all set(s) \( S \)

When \( q = 0 \) or in other words \( X \) does not have any components, \( T(Y, Z \mid X) = T(Y, Z) \) which measures the dependency of \( Y \) on \( Z \) without any conditioning.

Using \( n \) samples, the following estimator \( T_n \) for \( T \) was introduced in [1]. This estimator is defined as

\[
T_n(Y, Z \mid X) = \frac{\sum_{j=1}^{n} \min\{R_j, R_{M(j)}\} - \min\{R_j, R_{N(j)}\}}{\sum_{j=1}^{m} R_j - \min\{R_j, R_{N(j)}\}}.
\]

The summation in the numerator and denominator is over the index set of the sample, \( R_j := \sum_{k=1}^{n} 1\{Y_k \leq Y_j\} \) is the rank of \( Y_j \) among all the other \( Y_k \)’s, \( N(j) \) is the index of the nearest neighbor of \( X_j \) among the rest of \( X_k \)'s, and finally \( M(j) \) is the index of the nearest neighbor of \( (X_j, Z_j) \) among the rest of \( (X_k, Z_k) \)'s. Since this estimator only relies on the rank of \( Y_j \)'s and the nearest neighbor indices, it is computationally efficient and can be estimated in \( O(n \log n) \). Finally, note that this estimator does not require any assumption or estimation of the joint density functions and is free of any tuning parameters.

For target variable \( Y \), and features \( X_1, \cdots, X_p \), FOCI proceeds in the following forward step-wise manner: In each step, FOCI selects one of the remaining variables until none of the remaining variables adds any “predictive power”. Let \( S_t \subseteq [p] \) be the set of selected variables by FOCI up to an including step \( t \) with \( S_0 = \emptyset \). In step \( t + 1 \), FOCI selects \( \arg\max_{i \not\in S_t} T_n(Y, X_i \mid X_{S_t}) \), if the maximum value is positive. Otherwise FOCI stops and returns \( \hat{S} = S_t \). Note that FOCI possesses a natural stopping rule and does not require the user to specify any stopping criterion. Below is a summary of FOCI.

Algorithm 2 FOCI

Input: \( n \) samples of \((X_1, \cdots, X_p, Y)\)

Output: \( \hat{S} \)

1: \( \hat{S} = \emptyset \)

2: while \( \min_{i \not\in \hat{S}} T_n(Y, X_i \mid X_{\hat{S}}) > 0 \) do

3: \( \hat{S} = \hat{S} \cup \{\arg\max_{i \not\in \hat{S}} T_n(Y, X_i \mid X_{\hat{S}})\} \)

4: end while
In [1, Th.6.1] it is shown that under mild assumptions, and for large enough sample size $n$, $X_\hat{S}$ is with high probability a Markov blanket for $Y$. In general, there is no bound on the size of this Markov blanket, and it may not be the minimal one. In Theorem 3.1 we show that under the $\delta$-Gap assumption A.3 the estimated Markov blanket by FOCI is minimal and hence is the Markov boundary.

2.2 Stage II of DAG-FOCI: Combining Markov boundaries to identify parents

We next describe how DAG-FOCI combines the information of Markov boundaries obtained from the first stage to identify the set(s) of causal parents. In particular, suppose that the Markov equivalence class of the population DAG consists of $K$ members where $X_{p(1)}, X_{p(2)}, \ldots, X_{p(K)}$ represent the parental sets of $Y$ for each DAG in the equivalence class. The procedure we describe relies on the following properties. For any $k \in [K]$

(p1) For all $X_i, X_j \in X_{p(k)}$: $X_i \in MB(X_j)$

(p2) For all $X_i, X_j \in X_{p(k)}$: $X_i \perp X_j$

(p3) For all $X_i \in X_{p(k)}, X_j \in MB(Y \setminus X_{p(k)}) : X_i \notin MB(X_j)$

Properties [p2] and [p3] relies on the assumption that $Y$ satisfies the parent-free-cycle property. Properties [p1] and [p2] require $|X_{p(k)}| \geq 2$ and property [p3] requires $MB(Y \setminus X_{p(k)}) \neq \emptyset$.

We prove the relationships in [p1], [p2], and [p3] in the supplementary material Section A.1. These relationships motivate the following algorithm to identify the parental sets $X_{p(1)}, X_{p(2)}, \ldots, X_{p(K)}$: First, we generate an empty undirected graph among all nodes in the Markov blanket of $Y$. In the second step, for every pair of nodes $X_i, X_j \in MB(Y)$, we connect them in the graph if $X_i \in MB(X_j)$. Relations [p1] and [p2] will conclude that the parental nodes $X_{p(1)}, X_{p(2)}, \ldots, X_{p(K)}$ form $K$ fully connected subgraphs that are disconnected from each other and the remaining nodes in the Markov blanket of $Y$. In the third step of the algorithm, we identify the connected subgraphs that contain pairwise independent nodes. Indeed, appealing to relation [p2], we will conclude that some of these identified subgraphs will correspond to the parental sets $X_{p(1)}, X_{p(2)}, \ldots, X_{p(K)}$.

Naturally, the following question arises: are all the sets outputted in the third step of the Algorithm 1 parental? In general, the answer is no, and there is only a single exception. Consider the scenario with multiple parents, no spouses, and at least one child, where the children are only connected in the graph via $Y$. Then, the output of step 3 in Algorithm 1 will consist of the parental set as well as singletons containing each of the children. Thus, to account for this scenario, we add a final step to the algorithm that checks whether all but one of the subgraphs in step 3 are singletons. In such a case, the non-singleton subgraph is returned as the only parental set.
Below we describe Algorithm 3, called DAG-FOCI, in all details to reconstruct the causal structure. Note that we do not need to perform any conditional testing to identify the parents under the parent-cycle-free assumption. This algorithm takes as an input a sample of all the nodes with the target node being specified, here $Y$. DAG-FOCI outputs $\mathcal{P}$ which is the collection of all possible sets of parents, possibly empty.

Algorithm 3 DAG-FOCI

**Input:** $n$ samples of $(X_1, \ldots, X_p, Y)$

**Output:** parental set(s) $\mathcal{P}$

1. **Stage I: Markov boundary search**: Apply Algorithm 1 to estimate $\hat{\text{MB}}(Y)$ as well as $\hat{\text{MB}}(X_j)$ for all $X_j \in \hat{\text{MB}}(Y)$.

2. **Stage II: combining local Markov structures**
   1. Create $\tilde{G}_Y = (\tilde{V} = \hat{\text{MB}}(Y), \tilde{E})$ where $(i,j) \in \tilde{E}$ iff $X_i \in \hat{\text{MB}}(X_j)$ and $X_j \in \hat{\text{MB}}(X_i)$.
   2. Initialize $\mathcal{P}_{\text{temp}} = \emptyset$, $\text{count} = 0$
   3. Decompose $\tilde{G}_Y$ to its connected components $G_1 \cup \cdots \cup G_R$.
   4. **for** $i = 1$ to $R$ **do**
   5.  **if** for every $(X_i, X_j) \in G_i$, $X_i \perp X_j$ **then**
   6.   $\mathcal{P}_{\text{temp}} = \mathcal{P}_{\text{temp}} \cup \{V(G_i)\}$
   7.   $\text{count} = \text{count} + |V(G_i)|$
   8.   **end if**
   9. **end for**
   10. **if** $\text{count} > |\mathcal{P}_{\text{temp}}|$ **then** $\mathcal{P}$ : only non-singleton set in $\mathcal{P}_{\text{temp}}$
   11. **else** $\mathcal{P} = \mathcal{P}_{\text{temp}}$
   12. **end if**

**Remark 2.1.** If $\mathcal{P} = \emptyset$, Algorithm 3 has not recognized any of the $G_i$’s as the parental component. In the population setting, this can be interpreted in two ways, either $Y$ is a source node and therefore does not have any parents or $Y$ does not satisfy the parent-cycle-free property and hence some of its parents are not independent.

**Remark 2.2.** If $|\mathcal{P}| > 1$, i.e. DAG-FOCI recognizes more than one of the $G_i$’s as the parental component (this happens only when all the possible parental components are singletons), with high probability there is $|\mathcal{P}| + 1$ possibilities for the parent node. Either one of the singleton members of $\mathcal{P}$ is the parent set or $Y$ does not have any parent.

**Remark 2.3.** To recover the whole DAG, one can apply Algorithm 3 to all the nodes.
Remark 2.4. One can use the idea of stability selection in [32] to enhance the performance of FOCI for estimating the Markov boundary. For this purpose simply choose a probability threshold \( \pi \in [0, 1] \) and take \( m \) a positive integer. For \( i \in [m] \), take a subset of size \( \lfloor n/2 \rfloor \) of data, run FOCI on this subsample and set the result as \( \hat{MB}_i(Y) \). Finally let \( \hat{MB}^\pi(Y) \) be the set of variables which appeared at least \( \lfloor m \pi \rfloor \) times in the estimated \( \hat{MB}_i(Y) \).

\[
\hat{MB}^\pi(Y) := \{ Z \in \bigcup \hat{MB}_i(Y) \mid \frac{1}{m} \sum_{i=1}^{m} 1\{ Z \in \hat{MB}_i(Y) \} \geq \pi \}.
\]

In Algorithm 3 one can use this stabilized estimation of Markov boundaries for a choice of \( \pi \).

3 Theoretical Guarantees

Let \((Y, X)\) be as in the previous section. For any nonempty set \( S \subseteq \{1, \cdots, p\} \) consider function \( Q \) defined as in (6.1) in [1], where \( Q(\emptyset) = 0 \) and

\[
Q(S) := Q(Y, X_S) = \int \Var(P(Y \geq t \mid X_S))d\mu(t). \tag{4}
\]

Note that \( Q(Y, X_S) \) is the numerator of \( T(Y, X_S) \).

Let \( \delta \) be the largest number such that for any insufficient subset \( S \), there is some \( i \notin S \) such that \( Q(S \cup \{i\}) \geq Q(S) + \delta \). In other words adding \( i \) to \( S \) increases the “predictive power” by at least \( \delta \). The definition of \( \delta \) ensures that there is at least one sufficient subset of size at most \( 1/\delta \).

To prove our result, we need the following three technical assumptions on the joint distribution of \((Y, X)\).

(A.1) There are nonnegative real numbers \( \beta \) and \( C \) such that for any set \( S \subseteq \{1, \cdots, p\} \) of size \( \leq 1/\delta + 2 \), any \( x, x' \in \mathbb{R}^S \) and any \( t \in \mathbb{R} \),

\[
|P(Y \geq t \mid X_S = x) - P(Y \geq t \mid X_S = x')| \leq C(1 + \|x\|^\beta + \|x'\|^\beta)\|x - x'\|.
\]

(A.2) There are positive numbers \( C_1 \) and \( C_2 \) such that for any \( S \) of size \( \leq 1/\delta + 2 \) and any \( t > 0 \), \( P(\|X_S\| \geq t) \leq C_1 e^{-C_2 t} \).

(A.3) (\( \delta \)-Gap) For any subset \( S \subset [p] \) such that \( X_S \) is a strict subset of \( MB(Y) \), there exists \( i \) with \( X_i \in MB(Y) \setminus X_S \), such that for any \( j \) with \( X_j \notin MB(Y) \)

\[
Q(S \cup \{i\}) - Q(S \cup \{j\}) \geq \delta/4.
\]

The value \( \delta > 0 \) is the same for A.1 - A.3. The first two assumptions A.1 and A.2 are identical to the ones in [1] for identifying a Markov blanket. Assumption A.3 which we call \( \delta \)-Gap assumption for future reference, ensures
that the estimated Markov blanket is minimal (i.e., equal to Markov boundary).
More specifically, assumption A.3 requires the members of the Markov boundary
to have strictly higher predictive power compared to the rest of the variables.
It is not hard to see that this assumption is valid when \( Y \) satisfies the tree-
neighborhood property, Proposition 3.3.

**Theorem 3.1.** Suppose that assumptions A.1, A.2, and A.3 hold for some \( \delta > 0 \).
Let \( S \) be the subset selected by FOCI with a sample of size \( n \).
There are positive real numbers \( L_1, L_2, \) and \( L_3 \) depending only on \( C, \beta, C_1, C_2, \) and \( \delta \) such that
\[
\Pr(X_S \text{ is the Markov boundary}) \geq 1 - L_1p^{L_2}e^{-L_3n}.
\]

The following theorem gives a lower bound on the probability of the event
that DAG-FOCI gives the correct set of parents.

**Theorem 3.2.** Suppose that assumptions A.1, A.2, and A.3 hold for some \( \delta > 0 \).
In addition assume that \( Y \) satisfies the parent-cycle-free property. We have
\[
\Pr(X_P = X_P) \geq 1 - (|MB(Y)| + 1)(L_1p^{L_2}e^{-L_3n}) - (|MB(Y)| - 1)(1 - \beta(n)) - \left(\frac{|X_P|}{2}\right)^\alpha.
\]

Constants \( \alpha \) and \( \beta(n) \) are the size and power of the independence test
in Algorithm 3 for a sample of size \( n \) (i.e., the minimal power across all tests performed).
The positive real numbers \( L_1, L_2, \) and \( L_3 \) are depending only on \( C, \beta, C_1, C_2, \) and \( \delta \).

Note that the probability bound in Theorem 3.2 depends on some values
that are usually unknown, namely \(|MB(Y)|\), and \(|X_P|\). They can be bounded
as follows. Denote by \( d \) the maximal degree of the graph. Then we have:
(i) \(|MB(Y)| \leq d(d - 1)\) as \( Y \) has at most \( d \) directly connected neighbors
and each of those have at most \( d - 1 \) nodes connected to them besides \( Y \);
(ii) \(|X_P| \leq d \) since \( Y \) has degree at most \( d \); Putting these together shows
that DAG-FOCI correctly estimates parents of \( Y \) with probability at least
\( 1 - d^2\max(L_1p^{L_2}e^{-L_3n}, \alpha, 1 - \beta(n)) \).
Thus, for \( n \) large enough we have a guarantee that DAG-FOCI estimates the parents correctly with high probability,
even for high-dimensional cases where \( p \) can grow polynomially fast with sample size
but the graph is sparse with maximal degree \( d \) being constant or growing
sufficiently slowly with \( n \).

**Proposition 3.3.** Assume there exists \( \delta > 0 \) such that for any insufficient set
\( S \) there exists \( i \) such that
\[
Q(S \cup \{i\}) \geq Q(S) + \delta.
\]
If \( Y \) has the tree-neighborhood property then there exist \( 0 < \delta' \leq \delta \) such that \( Y \)
has the \( \delta' \)-Gap property with \( \delta' \).
Combining 3.3 and 3.2 gives us immediately the following corollary.

**Corollary 3.4.** Suppose that assumptions \(A.1\), \(A.2\) holds, and DAG \(G\) is a polytree with bounded degree \(d\). Then DAG-FOCI estimates \(G\) correctly with probability at least \(1 - |V(G)| (d^2 \max(L_1 p^{L_2 e^{-L_3 n}} \alpha, 1 - \beta(n)))\).

Therefore for large enough sample size, when our DAG is a polytree DAG-FOCI estimates the whole DAG structure correctly with high probability.

The following Theorem guarantees that even if \(Y\) does not satisfy the parent-cycle-free property, DAG-FOCI with high probability does not return any non-parental node as the parent.

**Theorem 3.5.** Suppose that assumptions \(A.1\), \(A.2\), and \(A.3\) hold for \(Y\) for some \(\delta > 0\) and \(A.1\), \(A.2\) hold for all members of \(MB(Y)\). Let \(P\) be the output of DAG-FOCI for \(Y\). Let \(E\) be the event that \(\exists P \in P\) such that \(|P| > 1\) and \(P\) contains a non-parent node. Then

\[
P(E) \leq \frac{1}{2} |MB(Y)|^2 (1 - \beta(n)) + (|MB(Y)| + 1)L_1 p^{L_2 e^{-L_3 n}}.
\]

Theorem 3.5 put an emphasize on the conservative nature of DAG-FOCI. If the data meets our assumption then with high probability DAG-FOCI estimates the true set of parents. Otherwise with high probability it does not return any false discovery.

We study in Section 4.2 why the \(\delta\)-Gap assumption is necessary to estimate the Markov boundary. We also show how the violation of the parent-cycle-free property affects the result of DAG-FOCI in identifying the parents.

## 4 Violation of Assumptions

In this section, first, we explain the necessity of the \(\delta\)-Gap assumption for discovering the Markov boundary using FOCI. We also study why we require the parent-cycle-free assumption to distinguish the upstream and downstream nodes.

### 4.1 The \(\delta\)-Gap assumption

Consider the DAG structure in Figure 1. The Markov boundary of \(Y\) is \(\{X_1, X_2\}\). Note that since FOCI works in a greedy fashion, it is not hard to build distributions such that FOCI selects \(X_3\) earlier than \(X_1\) or \(X_2\). For example let

\[
X_1 = \text{sign}(X_3) + \alpha \varepsilon_1, \\
X_2 = |X_3| + \alpha \varepsilon_2,
\]

\[
Y = X_1 X_2,
\]

where \(X, \varepsilon_1, \varepsilon_2\) are i.i.d \(N(0, 1)\), and \(\alpha\) is a non-negative constant. We only assume for simplicity of exposition that the structural equation for \(Y\) has no noise term.
By choosing \( \alpha \) small, one can enforce that
\[
\max \{ T(Y, X_1), T(Y, X_2) \} \leq T(Y, X_3)
\]
and that then the \( \delta \)-Gap assumption does not hold. In this case, FOCI selects \( X_3 \) earlier than \( X_1, X_2 \). Further details are given in Appendix B.

4.2 The parent-cycle-free property

The parent-cycle-free property is important for our causal orientation algorithm to work. If node \( Y \) does not satisfy the parent-cycle-free property, then by definition, there exists \( X_i \in X_P \) such that edge \((X_i, Y)\) belongs to a cycle \( J \) in \( G \). In this case cycle \( J \) contains another member of the \( \mathbf{MB}(Y) \) as well, either another parent node, or a child or spouse.

\[
\begin{align*}
\text{V.1} & \quad \left| V(J) \cap X_P \right| \geq 2 \\
\text{V.2} & \quad \left| V(J) \cap X_P \right| \geq 1 \quad \text{and} \quad \left| V(J) \cap \{ X_{PC} \cup X_C \} \right| \geq 1
\end{align*}
\]

If any of V.1 or V.2 happens one will not be able to distinguish the set of parents using DAG-FOCI.

**Case V.1** Assume there exists a cycle \( J \) in \( G \) such that \( \left| V(J) \cap X_P \right| \geq 2 \). Therefore there exists \( X_{ij}, X_{i\ell} \in X_P \) such that both belong to the cycle \( J \). In this case \( X_{ij} \) and \( X_{i\ell} \) may not be independent of each other anymore. The independence is violated because of at least one of the following.

1. There exists a directed path from/to \( X_{ij} \) to/from \( X_{i\ell} \) in \( G \) where all its nodes belong to \( J \). See for example Figure 2a.

2. There exists a node \( Z \) in \( J \) such that two directed paths from \( Z \) to \( X_{ij} \) and \( X_{i\ell} \) with all their nodes belong to \( J \). See for example Figure 2b.

**Case V.2** In this case there exists a cycle \( J \) in \( G \) such that it has at least one node from the set of parents, say \( X_{ij} \) and one node from the set of children or spouses, say \( X_{i\ell} \). Consequently, the subgraph containing the set of all parents in \( \tilde{G}_Y \) may contain children or spouse nodes as well. Without the parent-cycle-free property, we need to perform conditional independence testing, which makes the process more difficult.
5 Empirical results

In this section we study our proposed FOCI and DAG-FOCI algorithms on both synthetic and real data examples.

5.1 Simulated Data

**Setting 5.1.** We consider the DAG structure in Figure 3 with the corresponding relationship between the nodes described in the following set of equations.

\[
\begin{align*}
X_1, X_2, X_3, X_4, X_8, X_{10}, X_{12}, \varepsilon_i & \sim \mathcal{N}(0, 1) \\
X_5 &= X_1 - \arctan(X_2) + \varepsilon_5 \\
X_6 &= X_2 + X_4 + X_3^2 + \varepsilon_6 \\
X_7 &= \sin(X_3) + \varepsilon_7 \\
X_9 &= \sin(X_6 + \varepsilon_9) + |X_{10}| \\
X_{11} &= X_9(X_{12} - X_8) + \varepsilon_{11} \\
X_{13} &= \arctan(X_5^2 + \varepsilon_{13}) \\
X_{14} &= \sin(X_{11}) + \varepsilon_{14} \\
X_{15} &= \sqrt{|X_{12}|} + \varepsilon_{15} \\
X_{16} &= \sin(X_{12}) + \varepsilon_{16}.
\end{align*}
\]
We use DAG-FOCI to estimate the set of parents of $X_6$ and $X_{11}$. We study the performance of DAG-FOCI for this purpose over 100 independent runs for sample sizes $n = 2000, 4000, 6000, 8000, 10000$. For each $n$ and each run we generate a sample according to Eq. and estimate the set of parents of $X_6$ and $X_{11}$. We evaluate our estimations using the Jaccard index. The Jaccard index between two sets $A$ and $B$ is defined as $|A \cap B|/|A \cup B|$ and therefore it takes values in $[0, 1]$. 

Figure 3: DAG in Setting 5.1
Figure 4: Histogram of the Jaccard index between the estimated set of parents and true parent set of node $X_6$ in Setting 5.1 for sample sizes $n = 2000, 4000, 6000, 8000, 10000$. 
Figure 5: Histogram of the Jaccard index between the estimated set of parents and true parent set of node $X_{11}$ in Setting 5.1 for sample sizes $n = 2000, 4000, 6000, 8000, 10000$. 
Figures 4 and 5 show the histograms of the Jaccard index between the estimated set of parents and the true set of parents for nodes $X_6$ and $X_{11}$ respectively. As the sample size $n$ grows, the Jaccard index concentrates more on 1 which is expected from Theorem 3.2. Here in the second stage of DAG-FOCI, for pairwise independence test, we perform permutation test using CODEC [1] as the measure of dependence. For each test we generate 100 independent permutations over set of integers $[n]$, where $n$ is the sample size, and we set our threshold to 0.05.

**Setting 5.2.** We consider the DAG structure related to a forest, consists of disjoint trees. For each tree we consider a binary tree with 15 nodes, similar to the tree structure in Figure 6 with the corresponding relationship between the nodes described in 7.

\[ X_i \overset{i.i.d.}{\sim} \mathcal{N}(0,1) \quad \forall i \in \{8, \cdots, 15\} \]
\[ X_i = X_{2i}X_{2i+1} + \varepsilon_i \quad \forall i \leq 7 \tag{7} \]
\[ \varepsilon_i \overset{i.i.d.}{\sim} \mathcal{N}(0,1) \quad \forall i \leq 7 \]

Figure 6: DAG for a single binary tree with 15 nodes in Setting 5.2

We consider forests with $K = 1, 2, 3, 4, 5$ independent trees generated according to 7. For each such forest we estimate the whole forest using DAG-FOCI over 100 independent runs for sample size $n = 2000$. In Figure 7 the histogram of the Jaccard index between the estimated DAGs and true DAG for different values of $K$ corresponding to node size $p = 15, 30, 45, 60, 75$ is shown. Table 1 shows the summary of the statistics of the Jaccard indexes.
Figure 7: Histogram of the Jaccard index between the estimated DAG and true DAG in Setting 5.2 for $p = 15, 30, 45, 60, 75, 90$. 

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Table 1: Summary of the Jaccard index between the estimated DAG and true DAG over 100 independent runs in Setting 5.2.

5.2 Application to Real Data

5.2.1 Analysis of protein signaling data

We consider the dataset in Sachs et al. [2]. This dataset consists of 7466 measurements of the abundance of phosphoproteins and phospholipids recorded under different experimental conditions in primary human immune system cells. Following the setting in [40], we consider only 5846 measurements in which the perturbations of receptor enzymes are identical. The observational distribution then is defined as the model where only the receptor enzymes are perturbed. This results in 1755 observational measurements and 4091 interventional measurements. Table 2 shows the number of samples for each specific intervention and no-intervention.

| Intervention | None | Akt | PKC | PIP2 | Mek | PIP3 |
|--------------|------|-----|-----|------|-----|------|
| # samples    | 1755 | 911 | 723 | 810  | 799 | 848  |

Table 2: Number of samples under each protein intervention for the flow cytometry dataset from Sachs et al. [2]

In the literature, there is an agreement that the interventions in this dataset, cut the dependency of the intervened variable with its original parents. In this case, we cannot simply use the aggregated data. For estimating the set of parents of each node, we only consider observational data. We use the interventional data to evaluate/verify our findings using observational data. In Table 3, each row contains the estimated Markov boundary for the row variable. For the second stage of DAG-FOCI we run permutation test using CODEC to get the p-values of pairwise independent tests between the variables. We use 1000 independent permutations.

To explore the performance of DAG-FOCI on this data we focus on estimating the parent set of the nodes that we have intervened on, Akt, PKC, PIP2, Mek, and PIP3. This way we use the observational data for our estimation purpose using DAG-FOCI and then we evaluate the estimated set using the interventional data.
Table 3: Estimated Markov boundary of each node using only the observational data in protein signaling data in [2].

| Node | MB                                    |
|------|---------------------------------------|
| Raf  | Mek, PIP2                             |
| Mek  | Raf, PIP3, Erk, Akt                   |
| Plcg | PIP2, PIP3, Akt                       |
| PIP2 | PIP3, Plcg, Mek                       |
| PIP3 | Plcg, PIP2, Erk, P38, Jnk             |
| Erk  | Akt, PKA                              |
| Akt  | Erk, PKA                              |
| PKA  | PIP3, Erk, Akt                        |
| PKC  | Mek, P38, Jnk                         |
| P38  | Akt, PKC, Jnk                         |
| Jnk  | PIP2, Erk, PKC, P38                   |

Table 4: p-values of the pairwise independence test using only the observational data in protein signaling data in [2]. Values smaller than or equal to 0.05 are shown in bold. For these values we reject the null hypothesis of independence at level $\alpha = 0.05$.

|      | Raf | Mek | Plcg | PIP2 | PIP3 | Erk | Akt | PKA | PKC | P38 | Jnk |
|------|-----|-----|------|------|------|-----|-----|-----|-----|-----|-----|
| Raf  | 0.99| 0.13| 0.72 | 0.35 | 0.56 | 0.32| 0.56 | 0.49 | 0.45 | 0.27|
| Mek  | 0.13| 0.28| 0.62 | 0.40 | 0.54 | 0.28| 0.60 | 0.80 | 0.37 | 0.19|
| Plcg | 0.72| 0.62| 0.00 | 0.00 | 0.00 | 0.00| 0.00 | 0.00 | 0.00 | 0.00|
| PIP2 | 0.00| 0.00| 0.00 | 0.00 | 0.00 | 0.00| 0.00 | 0.00 | 0.00 | 0.00|
| PIP3 | 0.00| 0.00| 0.00 | 0.00 | 0.00 | 0.00| 0.00 | 0.00 | 0.00 | 0.00|
| Erk  | 0.56| 0.54| 0.92 | 0.06 | 0.66 | 0.00| 0.00 | 0.00 | 0.33 | 0.71|
| Akt  | 0.32| 0.28| 0.07 | 0.01 | 0.35 | 0.00| 0.00 | 0.00 | 0.00 | 0.00|
| PKA  | 0.56| 0.60| 0.69 | 0.95 | 0.50 | 0.00| 0.00 | 0.00 | 0.00 | 0.00|
| PKC  | 0.49| 0.80| 0.20 | 0.85 | 0.89 | 0.15| 0.40 | 0.47 | 0.00 | 0.00|
| P38  | 0.04| 0.37| 0.03 | 0.05 | 0.27 | 0.33| 0.19 | 0.09 | 0.00 | 0.00|
| Jnk  | 0.27| 0.19| 0.67 | 0.88 | 0.58 | 0.71| 0.00 | 0.00 | 0.00 | 0.00|

**Akt:** The p-value of the test between the only members of the estimated Markov boundary of Akt, Erk and PKA is 0.00. Hence we reject the null hypothesis of independence between this pair. Therefore DAG-FOCI returns the empty set as the estimated parent set of Akt. This observation is confirmed by exploring the interventional data with direct intervention on Akt. On this interventional data the estimated Markov boundary of Akt is again \{Erk, PKA\}. This confirms that non of Erk, or PKA can be a parent of Akt.

**PKC:** The first stage of DAG-FOCI gives Mek, Jnk, and P38 as the estimated Markov boundary of PKC. In the second stage DAG-FOCI gives the decomposition \{Mek\}, \{P38, Jnk\}. The p-value for independence test P38 and Jnk suggests that we can reject the hypothesis of independence between Jnk and
Therefore DAG-FOCI does not return pair \(\{P38, \text{Jnk}\}\) as the parent set. For PKC, DAG-FOCI concludes that either Mek is the only parent of PKC or it does not have any parents. On the other hand, looking at the interventional data with direct intervention on PKC, we have P38 as the only member of the estimated Markov boundary. This confirms the finding of DAG-FOCI that pair \(\{P38, \text{Jnk}\}\) is not the parental component.

**PIP2:** The first stage of DAG-FOCI gives PIP3, Plec, and Mek as the estimated Markov boundary of PIP2. In the second stage DAG-FOCI gives the decomposition \(\{\text{Mek}\}, \{\text{Plec, PIP3}\}\). Table 4 that Plec and PIP3 are not independent and therefore DAG-FOCI concludes that either Mek is the only parent of PIP2, or PIP2 does not have any parent. On the other hand, looking at the interventional data with direct intervention on PIP2, we have PKC as the only member of the estimated Markov boundary.

**Mek:** The first stage of DAG-FOCI gives PIP3, Act, Erk, and Raf as the estimated Markov boundary of Mek. In the second stage DAG-FOCI gives the decomposition \(\{\text{PIP3}\}, \{\text{Raf}\}, \{\text{Erk, Akt}\}\). Table 4 that Erk and Akt are not independent and therefore DAG-FOCI concludes that either one of PIP3 or Raf is the only parent of Mek, or Mek does not have any parent. On the other hand, looking at the interventional data with direct intervention on Mek, we have Raf as the only member of the estimated Markov boundary of Mek. This suggests that Raf is not a parent and hence is surely a child. Our observation on existence of edge Mek→Raf is confirmed also by [11, 12, 13, 14].

**PIP3:** The first stage of DAG-FOCI gives Plec, PIP2, Erk, P38, and Jnk as the estimated Markov boundary of Mek. In the second stage DAG-FOCI gives the decomposition \(\{\text{Plec, PIP2}\}, \{\text{P38, Jnk}\}, \{\text{Erk}\}\). Since none of the pairs \(\{\text{Plec, PIP2}\}, \{\text{P38, Jnk}\}, \{\text{Erk}\}\) are independent according to Table 4, DAG-FOCI concludes that PIP3 either does not have any parent or Erk is its only parent. The only member of the estimated Markov boundary of PIP3 on the interventional data with direct intervention on PIP3 is PIP2. This confirms that \(\{\text{Plec, PIP2}\}\) is not the parental component.

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### A Proofs

#### A.1 Proof of \[\text{p1}, \text{p2}\]

**Proof.** For any \(k\) such that \(|X_{p(k)}| \geq 2\) let \(X_i, X_j \in X_{p(k)}\). We have \(X_i \not\perp X_j | Y\), therefore \(X_i \in \text{MB}(X_j)\). This shows the validity of \[\text{p1}\]. For such \(k\), if \(Y\) satisfies the parent-cycle-free property, there is no (undirected) path connecting \(X_i, X_j \in X_{p(k)}\) that does not go through \(Y\). This implies \(X_i \perp \perp X_j\).
This proves $p_2$. Finally, for $X_i \in \mathbf{X}_{p(k)}$ and $X_j \in \mathbf{MB}(Y) \setminus \mathbf{X}_{p(k)}$, if $Y$ satisfies the parent-cycle-free property, conditional $Y$, $X_i$ and $X_j$ are independent. Also $Y \in \mathbf{MB}(X_i)$ and $Y \in \mathbf{MB}(X_j)$, these together imply that $X_i \notin \mathbf{MB}(X_j)$.

This proves $p_3$. \hfill \square

A.2 Proof of Theorem 3.1

Proof. Under assumptions A.1 and A.2, Theorem 6.1 in [1] gives us

$$
\mathbb{P}(\hat{X}_S \text{ is a Markov blanket}) \geq 1 - L_1 p^{L_2} e^{-L_3 n}.
$$

Hence we only need to show that with the additional assumption A.3, $X_\hat{S}$ is exactly the Markov boundary.

Let $j_1, j_2, \ldots, j_p$ be the complete ordering of all variables produced by the stepwise algorithm in FOCI. Let $S_0 = \emptyset$, and $S_k = \{j_1, \ldots, j_k\}$ for all $k \leq p$. Let

$$
Q(Y, Z) = \int \text{Var}(\mathbb{P}(Y \geq t \mid Z)) d\mu(t),
$$

and

$$
Q_n(Y, Z) = \frac{1}{n^2} \sum_{i=1}^{n} \left( \min\{R_i, R_{M(i)}\} - \frac{L_i^2}{n} \right),
$$

be the numerator of $T(Y, Z)$ and $T_n(Y, Z)$ respectively. Remember that $R_i = \sum_{j=1}^{n} 1\{Y_j \leq Y_i\}$, and $L_i = \sum_{j=1}^{n} 1\{Y_j \geq Y_i\}$, and $M(i)$ is the index of the nearest neighbor of $Z_i$ among all the other $Z_j$’s.

As defined in proof of Theorem 6.1 in [1], let $E'$ be the event that for all $1 \leq k \leq K$, $|Q_n(Y, X_{S_k}) - Q(Y, X_{S_k})| \leq \delta/8$ where $K$ is the integer part of $\delta + 2$. Note that $E'$ and assumption A.3 together imply that members of $\mathbf{MB}(Y)$ appear first in the ordering by FOCI. This completes the proof. \hfill \square

A.3 Proof of Proposition 3.3

Proof. Let $S$ be an index set such that $X_S \subset \mathbf{MB}(Y)$. Let $Z \notin \mathbf{MB}(Y)$ be an arbitrary node. Take $W \in \mathbf{MB}(Y)$ the closest member of $\mathbf{MB}(Y)$ on the path between $Y$ and $Z$ in $G$ to $Y$. Since $Y$ has the tree-neighborhood property this path is unique and $W$ is well-defined. First let’s consider the case where $W \notin X_S$. If the path from/to $Y$ to/from $Z$ is directed in $G$ then given $W, Y$ and $Z$ are independent of each other. Since $W \in \mathbf{MB}(Y)$, this implies

$$
\varepsilon_Z := Q(Y, X_S \cup W) - Q(Y, X_S \cup Z) > 0.
$$

If the path between $Y$ and $Z$ in $G$ is not directed let $W'$ be the farthest node on the path between $W$ and $Z$ to $W$ such that the path between $W$ and $W'$ is directed.

(m.1) $Y \leftarrow W \rightarrow \cdots \rightarrow W' \leftarrow \cdots Z$
(m.2) $Y \leftarrow W \leftarrow \cdots \leftarrow W' \rightarrow \cdots \rightarrow Z$

Let $V = (W', \cdots, Z)$ the vector consist of all the nodes on the path between $W'$ and $Z$. Then we replace this part of the path by the single node $V$. This will modify (m.1) and (m.2) into

(n.1) $Y \leftarrow W \rightarrow \cdots \rightarrow V$

(n.2) $Y \leftarrow W \leftarrow \cdots \leftarrow V$

When the path between $Y$ and $V$ is directed again we have

$$Q(Y, X_S \cup W) - Q(Y, X_S \cup V) > 0.$$ 

By monotonicity of $Q$ in its second argument we have $Q(Y, X_S \cup V) \geq Q(Y, X_S \cup Z)$ and this results

$$\varepsilon_Z := Q(Y, X_S \cup W) - Q(Y, X_S \cup Z) > 0.$$ 

When the path between $Y$ and $V$ is not directed but $W$ is the parent of $Y$, i.e., $Y \leftarrow W \rightarrow \cdots \rightarrow V$, we have $Y \perp V \mid W$ and similar to the previous case we get

$$\varepsilon_Z := Q(Y, X_S \cup W) - Q(Y, X_S \cup Z) > 0.$$ 

So the only remaining case is $Y \rightarrow W \leftarrow \cdots \leftarrow V$. In this case there exists $W_2 \in MB(Y)$ such that $W \leftarrow W_2$ and hence $W_2$ is a spouse of $Y$. Then we have $Y \perp V \mid W_2$ and therefore

$$\varepsilon_Z := Q(Y, X_S \cup W_2) - Q(Y, X_S \cup Z) > 0.$$ 

If $W \in S$, then

$$Q(Y, X_S) = Q(Y, X_S \cup W) = Q(Y, X_S \cup Z).$$ 

Since $X_S$ is a strict subset of $MB(Y)$, for any $W' \in MB(Y) \setminus X_S$ we have

$$Q(Y, X_S \cup W') - Q(Y, X_S \cup Z) > 0.$$ 

Let

$$\varepsilon_Z := \max_{W' \in MB(Y) \setminus X_S} Q(Y, X_S \cup W') - Q(Y, X_S \cup Z).$$ 

Therefore $\min(\delta, 4 \min_{Z \in MB(Y), S \subseteq MB(Y)} \{\varepsilon_Z\})$ satisfies the value for the $\delta$-Gap property. This finishes proof of Proposition 3.3.

A.4 Proof of Theorem 3.2

Proof. We divide event $\{X_P \neq X_{\tilde{P}}\}$ into two parts.

$$P(X_P \neq X_{\tilde{P}}) = P(\{X_P \neq X_{\tilde{P}}\} \cap \{MB(Y) = MB(Y)\}) + P(\{X_P \neq X_{\tilde{P}}\} \cap \{MB(Y) \neq MB(Y)\}) \leq P(\{X_P \neq X_{\tilde{P}}\} \cap \{MB(Y) = MB(Y)\}) + P(MB(Y) \neq MB(Y)).$$
Theorem 3.1 gives an upper bound on $\Pr(\{MB(Y) \neq \hat{MB}(Y)\})$. Therefore we need to bound $\Pr(\{X_p \neq \hat{X}_p\} \cap \{MB(Y) = \hat{MB}(Y)\})$. When $MB(Y) = \hat{MB}(Y)$, then the estimation of parents can go wrong if at least one of the following happens

- (F.1) For at least one $X_i \in MB(Y)$, $\hat{MB}(X_i) \neq MB(X_i)$
- (F.2) We falsely reject the independence between at least two parental node.
- (F.3) We falsely accept the independence between all the non-independent pairs in a non-parental component.

Theorem 3.1 gives us a bound to control [F.1]. Note that controlling [F.2] is just controlling the type I error in our independence test procedure.

Assume that for all $X_i \in MB(Y)$, we get $\hat{MB}(X_i) = MB(X_i)$. In this case our estimated $\hat{G}_Y$ is equal to its population version and it has $r$ disjoint connected component. Consider the non-parental component $G_i$ in $\hat{G}_Y$, containing child node $X_j$ and spouse nodes $X_{i_1}, \ldots, X_{i_k}$. DAG-FOCI would falsely recognize $G_i$ as a parental component if and only if all the p-values of independence tests between pairs of nodes in $G_i$ are less than $\alpha$. This means that for all the non-independent pairs $(X_j, X_{i_ℓ})$ the independence test fail to reject the null hypothesis. For node $Y$ with the tree-neighborhood property we expect $|V(G_i)| - 1$ non-independent pairs of nodes in $G_i$, all the $(X_j, X_{i_ℓ})$’s where $X_j$ is the child of $Y$ and $X_{i_ℓ}$ are the spouses. The probability of this event is $(1 - \beta(n))^k$, where $\beta(n)$ is the power of our independence test using a sample of size $n$. Since $k \leq \max_{i \in [r]} |V(G_i)| - 1$, putting all these together using union bound gives us

$$\Pr(X_p \neq \hat{X}_p) \leq (|MB(Y)| + 1)(L_1pL_2e^{-L_3n}) + \left(\frac{|X_p|}{2}\right)\alpha +$$
$$\sum_{i=1}^{r}(1 - \beta(n))^{|V(G_i)| - 1} \{ |V(G_i)| \geq 2 \}$$
$$\leq (|MB(Y)| + 1)(L_1pL_2e^{-L_3n}) + \left(\frac{|X_p|}{2}\right)\alpha +$$
$$(r - 1)(1 - \beta(n))^{\min_{V(G_i)|\neq[1]} |V(G_i)| - 1}$$
$$\leq (|MB(Y)| + 1)(L_1pL_2e^{-L_3n}) + \left(\frac{|X_p|}{2}\right)\alpha + (r - 1)(1 - \beta(n))$$

Since $r \leq |MB(Y)|$ we have

$$\Pr(X_p \neq \hat{X}_p) \leq (|MB(Y)| + 1)(L_1pL_2e^{-L_3n}) + \left(\frac{|X_p|}{2}\right)\alpha +$$
$$(|MB(Y)| - 1)(1 - \beta(n)).$$

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Therefore
\[ P(X_P = X_{P}) \geq 1 - (|MB(Y)| + 1)(L_1p^{L_2}e^{-L_3n}) - \left( \frac{|X_P|}{2} \right) \alpha - (|MB(Y)| - 1)(1 - \beta(n)). \]

This completes the proof of Theorem 3.2.

A.5 Proof of Theorem 3.5

Proof. Note that under assumptions A.1-A.3 with high probability we have \( \hat{MB}(Y) = MB(Y) \). Also under assumptions A.1-A.2 for nodes \( Z \in MB(Y) \) with high probability we have \( MB(Z) \subseteq \hat{MB}(Z) \). Therefore to find an upper bound on \( P(E) \) we can decompose this event into two disjoint parts.

\[ P(E) = P(E \cap \{ \forall Z \in Y \cup MB(Y) \mid \hat{MB}(Z) = MB(Z) \}) + P(E \cap \{ \exists Z \in Y \cup MB(Y) \mid \hat{MB}(Z) \neq MB(Z) \}). \]

By Theorem 3.1 [1, Th.6.1], and union bound we have

\[ P(E \cap \{ \exists Z \in Y \cup MB(Y) \mid \hat{MB}(Z) \neq MB(Z) \}) \leq (|MB(Y)| + 1)L_1p^{L_2}e^{-L_3n}. \]

Now assume for all \( Z \in Y \cup MB(Y) \) we have \( \hat{MB}(Z) = MB(Z) \), and \( E \) occurs. Therefore there exists \( W \in \hat{P} \) such that \( W \notin X_P \) and \( W \notin X_C \). Note that in this case if \( X_P \cap \hat{P} \neq \emptyset \) then \( X_P \subseteq \hat{P} \). Now consider the following two cases:

1. \( X_P \subseteq \hat{P} \). In this case \( W \) is the descendent of one of the members of \( X_P \) like \( V \) and therefore \( W \notin V \).
2. \( X_P \cap \hat{P} = \emptyset \). In this case \( \hat{P} \) contains at least one more child of \( Y \) like \( V \). Again in this case \( W \notin V \).

Therefore when estimating all the Markov boundaries correctly, \( E \) happens if at least for one pair of dependent pairs we wrongly accept the null hypothesis of independence. Therefore

\[ P(E \cap \{ \forall Z \in Y \cup MB(Y) \mid \hat{MB}(Z) = MB(Z) \}) \leq \frac{1}{2}|MB(Y)|^2(1 - \beta(n)). \]

Therefore we have

\[ P(E) \leq \frac{1}{2}|MB(Y)|^2(1 - \beta(n)) + (|MB(Y)| + 1)L_1p^{L_2}e^{-L_3n}. \]

\[ \square \]

B More on Violation of the Assumptions

In Figure 8 we plot the values of \( T_n(Y, X_3) \) and \( \max\{T_n(Y, X_1), T_n(Y, X_2)\} \) for \( \alpha \in [0, 1] \), with \( n = 10^4 \), where \( Y, X_1, X_2, X_3 \) follow the SEM in 5. This shows that for small values of \( \alpha \), the \( \delta \)-Gap assumption is not satisfied and FOCI selects \( X_3 \) earlier than \( X_1, X_2 \).
Figure 8: The values of $T_n(Y, X_3)$ ($\ast$) and $\max\{T_n(Y, X_1), T_n(Y, X_2)\}$ ($\circ$) for different values of $\alpha$, with $n = 10^4$. For small values of $\alpha$ we have $T_n(Y, X_3) > \max\{T_n(Y, X_1), T_n(Y, X_2)\}$.

C Interventions

In recent years, new technological advancements have given scientists better tools to intervene on some of the variables in their experiments. Therefore in some areas of science, researchers now have access to both observational and interventional data.

Interventions are categorized into two groups,

1. Entirely independent interventions that cut off the dependency of $Y$ with its original parents.
2. Dependent interventions that potentially change the distribution of the target variable $Y$ but do not change the Markov boundary.

Practitioners usually have a dataset $D$ which is a mix of observational data, $D_{Ob}$ and interventional data from different interventions/environments, $D_{I_i}$'s, $D = D_{Ob} \cup D_{I_1} \cup \ldots \cup D_{I_m}$. If the interventions are from the first type, i.e., entirely independent interventions, we cannot simply use our method on the union of all datasets $D$, as the interventions change the dependency structure in the data. Therefore one should estimate the Markov boundary on each dataset separately which results in $\hat{MB}_{Ob}(Y)$, and $\hat{MB}_{I_i}(Y)$'s corresponding to datasets $D_{Ob}$, and $D_{I_i}$'s.

Interventions let us gain extra information to find out the upstream and downstream nodes. For example if the $i$-th intervention is of the first type, i.e. this interventions are on $Y$, we already know that $\hat{MB}_{I_i}(Y)$ does not contain any parental node. Specifically in cases that the target node may not have
the tree-neighborhood property, independent intervention are extra helpful, as they block any cycle going connecting the set of up-streams and down-streams. Combining these information from all the environments can even compensate for the cases where our assumptions are not necessarily satisfied.

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