Collaborative Causal Discovery
with Atomic Interventions

Abstract

1 We introduce a new Collaborative Causal Discovery problem, through which we
2 model a common scenario in which we have multiple independent entities each
3 with their own causal graph, and the goal is to simultaneously learn all these causal
4 graphs. We study this problem without the causal sufficiency assumption, using
5 Maximal Ancestral Graphs (MAG) to model the causal graphs, and assuming
6 that we have the ability to actively perform independent single vertex (or atomic)
7 interventions on the entities. If the M underlying (unknown) causal graphs of the
8 entities satisfy a natural notion of clustering, we give algorithms that leverage this
9 property, and recovers all the causal graphs using roughly logarithmic in M number
10 of atomic interventions per entity. These are significantly fewer than n atomic
11 interventions per entity required to learn each causal graph separately, where n is
12 the number of observable nodes in the causal graph. We complement our results
13 with a lower bound and discuss various extensions of our collaborative setting.

1 Introduction

15 In this paper, we introduce a new model for *causal discovery*, the problem of learning all the causal
16 relations between variables in a system. Under certain assumptions, using just observational data,
17 some ancestral relations as well as certain causal edges can be learned, however, many observationally
18 equivalent structures cannot be distinguished [27]. Given this issue, there has been a growing interest
19 in learning causal structures using the notion of an *intervention* described in the Structural Causal
20 Models (SCM) framework introduced by Pearl [20].

21 As interventions are expensive (require carefully controlled experiments) and performing multiple
22 interventions is time-consuming, an important goal in causal discovery is to design algorithms
23 that utilize simple (preferably, single variable) and fewer interventions [24]. However, when there
24 are latents or unobserved variables in the system, in the worst-case, it is not possible to learn the
25 exact causal DAG without intervening on every variable at least once. Furthermore, multivariable
26 interventions are needed in presence of latents [1].

Figure 1: Examples of M causal graphs constructed from Lung Cancer dataset [15]. Here, the causal graphs differ only in the presence of latents (nodes with dotted square box), but they could differ elsewhere too.

27 On the other hand, in a variety of applications, there is no one true causal structure, different entities
28 participating in the application might have different causal structures [5, 21, 11]. For example, see
29 figure 1. In these scenarios, generating a single causal graph by pooling data from these different
30 entities might lead to flawed conclusions [23]. Allowing for interventions, we propose a new model
31 for tackling this problem, referred here as *Collaborative Causal Discovery*, which in its simplest form
32 states that: given a collection of entities, each associated with an individual unknown causal graph
33 and generating their own independent data samples, learn all the causal graphs while minimizing the
34 number of interventions for every entity. An underlying assumption is that each entity on its own
35 generates enough samples in both the observational and interventional settings so that conditional

independence tests can be carried out *accurately* on each entity separately. To motivate this model of collaborative causal discovery, let us consider two different scenarios.

(a) Consider a health organization interested in controlling incidence of a particular disease. The organization has a set of M individuals (entities) whose data it monitors and can advise interventions on. Each individual is an independent entity that generates its own set of separate data samples[1]. In a realistic scenario, it is highly unlikely that all the M individuals share the same causal graph (e.g., see Figures 3a and 3b from Joffe et al. [11] in Appendix A). It would be beneficial for the organization to collaboratively learn all the causal graphs together. The challenge is, *a priori* the organization does not know the set of possible causal graphs or which individual is associated with which graph from this set.

(b) An alternate setting is where, we have M companies (entities) wanting to work together to improve their production process. Each company generates their own data (e.g., from their machines) which they can observe and intervene on [18]. Again if we take the M causal graphs (one associated with each company) it is quite natural to expect some variation in their structure, more so because we do not assume *causal sufficiency* (i.e., we allow for latents). Since interventions might need expensive and careful experimental organization, each company would like to reduce their share of interventions.

The collaborative aspect of learning can be utilized if we assume that there is some underlying (unknown) clustering/grouping of the causal graphs on the entities.

Our Contributions. We formally introduce the collaborative causal discovery problem in Section 2. We assume that we have a collection of M entities that can be partitioned into k clusters such that any pair of entities belonging to two different clusters are separated by large distance (see Definition 2.1) in the causal graphs. Due to presence of latents variables, we use a family of mixed graphs known as *maximal ancestral graphs* (MAGs) to model the graphs on observed variables. Each entity is associated with a MAG.

In this paper, we focus on designing algorithms that have *worst-case* guarantees on the number of atomic interventions needed to recover (or approximately recover) the MAG of each entity. We assume that there are M MAGs one for each entity over the same set of n nodes. Learning a MAG with atomic interventions, in worst case requires n interventions (see Proposition 3.2). We show that this bound can be substantially reduced if the M MAGs satisfy the property that every pair of MAGs from different clusters have *at least* αn nodes whose direct causal relationships are different. We further assume that entities belonging to same cluster have similar MAGs in that every pair of them have *at most* βn ($\beta < \alpha$) nodes whose direct causal relationships are different. We refer to this clustering of entities as (α, β)-clustering (Definition 2.2). A special but important case is when $\beta = 0$, in which case all the entities belonging to the same cluster have the same causal MAG (referred to as α-clustering, Definition 2.3). An important point to notice is that while we assume there is a underlying clustering on the entities, it is *learnt* by our algorithms. Similar assumptions are common for recovering the underlying clusters, in many areas, for e.g., crowd-sourcing applications [3, 4].

We first start with the observation that under (α, β)-clustering, even entities belonging to the same cluster could have a different MAG, which makes exact recovery hard without making a significant number of interventions per entity. We present an algorithm that using at most $O(\Delta \log(M/\delta)/(\alpha - \beta)^2)$ many interventions per entity, with probability at least $1 - \delta$ (over only the randomness of the algorithm), can provably recover an *approximate* MAG for each entity. The approximation is such that for each entity we generate a MAG that is at most βn node-distance from the true MAG of that entity (see Section 3). Here, Δ is the maximum undirected degree of the causal MAGs. Our idea here is to first recover the underlying clustering of entities by using a randomized set of interventions. Then, we distribute the interventions across the entities in each cluster, thereby, ensuring that the number of interventions per entity is small. By carefully combining the results learnt from these interventions we construct the approximate MAGs.

Under the slightly more restrictive α-clustering assumption, we present algorithms that can *exactly* recover all the MAGs using at most $\min \left\{ O(\Delta \log(M/\delta)/\alpha), O(\log(M/\delta)/\alpha + k^2) \right\}$ many interventions per entity (see Section 4). Again, randomization plays an important role in our approach.

Complementing these upper bounds, we give a lower bound using Yao's minimax principle [26] that shows for any (randomized or deterministic) algorithm $\Omega(1/\alpha)$ interventions per entity is required

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[1]As is common in causal discovery, for the underlying conditional independence tests, the data is assumed to be i.i.d. samples from the interventional/observational distributions.

90 for this causal discovery problem. This implies the $1/\alpha$ dependence in our upper bound in the
91 α-clustering case is optimal.

92 Finally, a note about parameters. The (α, β)-clustering is universal, in the sense that *any* collection
93 of MAGs will satisfy the (α, β)-clustering property for some value of α, β (with $\alpha > \beta$). Ideally,
94 we would like in our problem instance, α to be close to 1 and β to be close to 0. In most real-world
95 applications, we would also expect k to be relatively small and $M \gg n, k$.

96 In Section 5, we show experiments on data generated from both real and synthetic networks with
97 added latents and demonstrate the efficacy of our algorithms for learning the underlying clustering
98 and the MAGs.

99 **Related Work.** A number of algorithms, working under various assumptions, for learning causal
100 graph (or a causal DAG) using interventions have been proposed in the literature, e.g., [9, 6, 24, 13,
101 16, 1, 2, 14, 10]. Saeed et al. [23] consider a model where the observational data is from a mixture
102 of causal DAGs, and outline ideas that recover a *union graph* (up to Markov equivalence) of these
103 DAGs, without any interventions. Our setting is not directly comparable to theirs, as we have entities
104 generating data and doing conditional independence tests independently (no pooling of data from
105 entities), but show stronger guarantees for recovering causal graphs, assuming atomic interventions.

2   Our Model and Problem Statement

107 In this section, we introduce the collaborative causal discovery problem. We start with some notations.

108 **Notation.** Following the SCM framework [20], we represent the set of random variables of interest
109 by $V \cup L$ where V represents the set of endogenous (observed) variables that can be measured and
110 L represents the set of exogenous (latent) variables that cannot be measured. We do not deal with
111 selection bias in this paper. Let $|V| = n$.

112 We assume that the causal Markov condition and faithfulness holds for both the observational and
113 interventional distributions [8]. We use conditional independence (CI) tests of the form $u \perp\!\!\!\perp v \mid Z$ or
114 $u \perp\!\!\!\perp v \mid \mathrm{do}(w), Z$, for some $u, v, w \in V$ and $Z \subseteq V$ (See Appendix A for more details).

115 Throughout this paper, unless otherwise specified, a path between two nodes is an undirected path. A
116 path of only directed edges is called a directed path. u is called an ancestor of v and v a descendant
117 of u if $u = v$ or there is a directed path from u to v. A directed cycle occurs in G when $u \to v$ is in
118 G and v is an ancestor of u.

119 **Our Model.** We assume that we have access to M entities labeled $1, \ldots, M$, each of which can
120 independently generate their own observational and interventional data. Each entity i has an associated
121 causal DAG $\mathcal{D}_i$ over $V \cup L_i$, where L_i represents the latent variables of entity i. In modeling the
122 problem of learning $\mathcal{D}_i$, complications arise in at least two ways:

123 **(i) Uniqueness**. First, with just observational data, if $\mathcal{D}_1, \ldots, \mathcal{D}_M$ are Markov equivalent, then
124   without additional strong assumptions they cannot be distinguished even if they are all structurally
125   different. To overcome the problem of being not identifiable within equivalence class, we allow
126   for interventions on observed variables. Our objective will be to minimize these interventions. In
127   particular, since each of these entities independently generate their own data, so we aim to reduce
128   the number of interventions needed per entity. In causal discovery, minimizing the number of
129   interventions while ensuring that they are of small size is an active research area [19, 24, 6, 7].

130 **(ii) Latents**. Second complication comes due to presence of latents in the system. Even with power
131   of single variable interventions, the structure of a causal DAG is not uniquely identifiable. (see,
132   e.g., In Figure 4 in Appendix A). Similarly, we can show that using single vertex interventions, we
133   cannot exactly recover wider class of acyclic graphs like ADMGs (Acyclic Directed Mixed Graphs).
134   We overcome this problem, *by focusing our attention on maximal ancestral graphs (MAGs) of*
135   *these entities.* MAGs are graphs on observed variables that capture the presence of latents through
136   bidirected edges [22]. A mixed graph containing directed ($\leftarrow$) and bidirected ($\leftrightarrow$) edges is said to
137   be *ancestral* if it has no directed cycles, and whenever there is a bidirected edge $u \leftrightarrow v$, then there
138   is no directed path from u to v or from v to u. An ancestral graph on V (observables) is said to be
139   *maximal*, if, for every pair of nonadjacent vertices u, v, there exists a set $Z \subset V$ with $u, v \notin Z$
140   such that u and v are m-separated (similar to d-separation, see Definition A.2) conditioned on Z.
141   Every DAG with latents (and selection variables) can be transformed into a unique MAG over the
142   observed variables [22].

143 Given the M entities, let $\mathcal{M}_i$ denote the MAG associated with entity i (the MAG constructed from
144 the DAG $\mathcal{D}_i$). Our goal is to collaboratively learn all these MAGs $\mathcal{M}_1, \ldots, \mathcal{M}_M$ while minimizing
145 the maximum number of interventions per entity.

146 To facilitate this learning, we make a natural underlying clustering assumption that partitions the
147 entities based on their respective MAGs such that: (i) any two entities belonging to the same cluster
148 have MAGs that are "close" to each other, (ii) any two entities belonging to different clusters have
149 MAGs that are "far" apart. Before stating this assumption formally, we need some definitions.

150 For MAG $\mathcal{M}_i = (V, E_i)$, we denote the children (through outgoing edges), parent (through incoming
151 edges), and spouse (through bidirected edges) of a node $u \in V$ as

$$\mathrm{ch}_i(u) = \{v \mid u \to v \in E_i\}, \ \mathrm{pa}_i(u) = \{v \mid u \leftarrow v \in E_i\}, \ \mathrm{sp}_i(u) = \{v \mid u \leftrightarrow v \in E_i\}. \quad (1)$$

152 Also, define an incidence set for a vertex $u \in V$ which contains an entry (v, type) for every node v
153 adjacent to u as

$$N_i(u) = \left\{ \begin{array}{ll} (v, \text{tail}) & \text{if } u \to v \in E_i \\ (v, \text{head}) & \text{if } u \leftarrow v \in E_i \\ (v, \text{bidirected}) & \text{if } u \leftrightarrow v \in E_i \end{array} \right\}. \quad (2)$$

154 Note that $|N_i(u)|$ is the undirected degree of u in $\mathcal{M}_i$. We now define a distance measure between
155 MAGs that captures structural similarity between them.

156 **Definition 2.1.** *Given two MAGs $\mathcal{M}_i = (V, E_i)$ and $\mathcal{M}_j = (V, E_j)$, define the node-difference as*
157 *the set:* $\mathrm{diff}(\mathcal{M}_i, \mathcal{M}_j) = \{u \in V \mid N_i(u) \neq N_j(u)\}$*, and the node-distance as the cardinality of*
158 *this set:* $d(\mathcal{M}_i, \mathcal{M}_j) = |\mathrm{diff}(\mathcal{M}_i, \mathcal{M}_j)| = |\{u \in V \mid N_i(u) \neq N_j(u)\}|$.

159 Intuitively, the node distance captures the number of nodes whose incidence relationships differ.
160 It is easy to observe that the node distance is a distance metric, and captures a strong structural
161 similarity between the graphs. Two graphs $\mathcal{M}_i, \mathcal{M}_j$ are identical iff $d(\mathcal{M}_i, \mathcal{M}_j) = 0$. For e.g., in
162 Figure 2, we have two MAGs that satisfy $d(\mathcal{M}_{12}, \mathcal{M}_{13}) = 2$ as $\mathrm{diff}(\mathcal{M}_{12}, \mathcal{M}_{13}) = \{x, z\}$, where
163 $d(\mathcal{M}_{12}, \mathcal{M}_{21}) = 3$ as $\mathrm{diff}(\mathcal{M}_{12}, \mathcal{M}_{21}) = \{x, y, z\}$. We are now ready to define a simple clustering
164 property on MAGs.

Figure 2: MAGs with $(\alpha = 0.75, \beta = 0.5)$-clustering. Every pair of graphs in $C_1^\star$ and $C_2^\star$ differ in at least $3(= 0.75 \times 4)$ nodes, while pairs of graphs within clusters differ by at most $2(= 0.5 \times 4)$ nodes.

165 **Definition 2.2** ((α, β)-clustering)**.** *Let $\mathcal{M}_1, \ldots, \mathcal{M}_M$ be a set of M MAGs. We say that this set of*
166 *MAGs satisfy the (α, β)-clustering property, with $\alpha > \beta \geq 0$, if there exists a partitioning of $[M]$*
167 *into sets (clusters) $C_1^\star, \ldots, C_k^\star \subset [M]$ (for some $k \in \mathbb{N}$) such that for all $(i, j) \in [M] \times [M]$:*

168   *(i) if i and j belong to same set (cluster), then $d(\mathcal{M}_i, \mathcal{M}_j) \leq \beta n$;*

169   *(ii) if i and j belong to different sets (clusters), then $d(\mathcal{M}_i, \mathcal{M}_j) \geq \alpha n$.*

170 Under this definition, all the M MAGs could be different. See, e.g., Figure 2. With right setting of
171 $\alpha > \beta$ we can capture any set of possible M MAGs. Therefore, an algorithm such as FCI [25], that
172 constructs PAGs might not be able to recover the clusters, as all the PAGs could be different, and the
173 node-distance between PAGs does not correlate well with the node-distance between corresponding
174 MAGs (e.g., see Figure 5 in Appendix A). We use the PAGs generated by FCI as a starting point for
175 all our algorithms that is then refined. With this discussion, we introduce our collaborative causal
176 graph learning problem as follows:

> **Assumption:** MAGs $\mathcal{M}_1, \ldots, \mathcal{M}_M$ (associated with entities $1, \ldots, M$ respectively) satisfy-
> ing the (α, β)-clustering property
> **Access to each entity:** Through conditional independence (CI) tests on observational and
> interventional distributions. Each entity generates their own (independent) data samples.
> **Goal:** Learn $\mathcal{M}_1, \ldots, \mathcal{M}_M$ while minimizing the max. number of interventions per entity.

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178 An interesting case of the Definition 2.2 is when $\beta = 0$.

Algorithm 1 IDENTIFY-OUTNBR $(\mathcal{U}_i, u)$	**Algorithm 2** IDENTIFY-BIDIRECTED $(\mathcal{U}_i, u)$
1: **Input:** node $u \in V$, PAG $\mathcal{U}_i$ of entity i	1: **Input:** node $u \in V$, PAG $\mathcal{U}_i$ of entity i
2: **Output:** $\mathrm{ch}_i(u)$	2: **Output:** $\mathrm{sp}_i(u)$
3: $\mathrm{ch}_i(u) = \{v \mid u \rightarrow v \in \mathcal{U}_i\}$	3: $\mathrm{sp}_i(u) = \{v \mid u \leftrightarrow v \in \mathcal{U}_i\}$
4: **for** $v \in \Gamma_i(u)$ such that $u\circ\!\!-\!\!\circ v$ or $u\circ\!\!\rightarrow v \in \mathcal{U}_i$ **do**	4: **for** $v \in \Gamma_i(u)$ such that $u\circ\!\!-\!\!\circ v$ or $u\leftarrow\!\!\circ v$ or $u\circ\!\!\rightarrow v \in \mathcal{U}_i$ **do**
5: **if** $u \not\perp\!\!\!\perp v \mid \mathrm{do}(u)$ **then**	5: **if** $u \perp\!\!\!\perp v \mid \mathrm{do}(u)$ and $u \perp\!\!\!\perp v \mid \mathrm{do}(v)$ **then**
6: $\mathrm{ch}_i(u) \leftarrow \mathrm{ch}_i(u) \cup \{v\}$	6: $\mathrm{sp}_i(u) \leftarrow \mathrm{sp}_i(u) \cup \{v\}$
7: **end if**	7: **end if**
8: **end for**	8: **end for**
9: Return $\mathrm{ch}_i(u)$	9: Return $\mathrm{sp}_i(u)$

Definition 2.3 (α-clustering). *We say a set of MAGs $\mathcal{M}_1, \ldots, \mathcal{M}_M$ satisfy the α-clustering property, if and only if they satisfy $(\alpha, 0)$-clustering property.*

Note that α-clustering is a natural property, wherein each cluster is associated with a single unique MAG, and all entities in the cluster have the same MAGs, and same conditional independences.

3 Causal Discovery under (α, β)-Clustering Property

In this section, we present our main algorithm for collaboratively learning causal MAGs under the (α, β)-clustering property. Missing details from this section are presented in Appendix C.

Definition 3.1 (Partial Ancestral Graph (PAG)). *Let $[\mathcal{M}_i]$ denote the Markov equivalence class of the MAG $\mathcal{M}_i$ and represented by the Partial Ancestral Graph (or PAG) $\mathcal{U}_i = (V, \widehat{E}_i)$. Edges $\widehat{E}_i$ have three kinds of endpoints given by arrowheads $(\leftarrow)$, circles $(\circ\!-)$ and tails $(-)$.*

All our algorithms are randomized, and succeed with high probability over the randomness introduced by the algorithm. The idea behind all our algorithms is to first learn the true clusters $C_1^\star, \ldots, C_k^\star$ using very few interventions. Once the true clusters are recovered, the idea is to distribute the interventions across the entities in each cluster and merge the results learned to recover the MAGs (Section 3.2). For our algorithms, a lower bound for α and upper bound for β is sufficient. In practice, a clustering of the PAGs (generated from FCI algorithm) can provide guidance about these bounds on α, β, or if we have additional knowledge that $\alpha \in [1 - \epsilon, 1]$ and $\beta \in [0, \epsilon]$ for some constant $\epsilon > 0$, then, we can use a binary search based guessing strategy that increases our intervention bounds by $\log^2(n\epsilon)/(1 - 2\epsilon)^2$ factor. It is important to note that none of our algorithms require the knowledge of the number of underlying clusters k.

Helper Routines. Let $\Gamma_i(u)$ denote all nodes that are adjacent to u in the PAG $\mathcal{U}_i$, i.e., $\Gamma_i(u) = \{v \mid (u, v) \in \widehat{E}_i\}$. Given the PAG $\mathcal{U}_i$, Algorithm IDENTIFY-OUTNBR identifies all the outgoing neighbors of any node u in $\mathcal{M}_i$. We look at edges of the form $u\circ\!\!-\!\!\circ v$ or $u\circ\!\!\rightarrow v$ in $\mathcal{U}_i$ incident on u, and identify if $u \rightarrow v$ using the CI-test $u \not\perp\!\!\!\perp v \mid \mathrm{do}(u)$. This is based on the observation that any node v that is a descendant of u (including $\mathrm{ch}_i(u)$) satisfies $u \not\perp\!\!\!\perp v \mid \mathrm{do}(u)$. Algorithm IDENTIFY-BIDIRECTED identifies all the bidirected edges incident on u. If there is an edge of the form $u\circ\!\!-\!\!\circ v$ or $u\leftarrow\!\!\circ v$ or $u\circ\!\!\rightarrow v$ in the PAG, and $v \notin \mathrm{ch}_i(u)$ and $u \notin \mathrm{ch}_i(v)$, then it must be a bidirected edge.

Using these helper routines, we give an Algorithm RECOVERG (in Appendix B) that recovers any MAG $\mathcal{M}_i$ using n atomic interventions. Complementing this, we show that n interventions are also required. The missing details are presented in Appendix B.

Proposition 3.2. *There exists a causal MAG $\mathcal{M}$ such that every adaptive or non-adaptive algorithm requires $\Omega(n)$ many atomic interventions to recover $\mathcal{M}$.*

3.1 Recovering the Clusters

From the (α, β)-clustering definition, we know that a pair of entities belonging to the same cluster have higher structural similarity between their MAGs than a pair of entities across different clusters. Let us start with a simplifying assumption that $\beta = 0$ (i.e., α-clustering). So, all the MAGs are separated by a distance of at least αn. We make the observation that to identify that two MAGs, say $\mathcal{M}_i$ and $\mathcal{M}_j$ belong to different clusters, it suffices to find a node u from the node-difference set $\mathrm{diff}(\mathcal{M}_i, \mathcal{M}_j)$ and checking their neighbors using Algorithms IDENTIFY-OUTNBR and IDENTIFY-BIDIRECTED. We argue that (see Claim D.3, Appendix D.2), with probability at least $1 - \delta$, we can identify one such node $u \in \mathrm{diff}(\mathcal{M}_i, \mathcal{M}_j)$ by sampling $2\log(M/\delta)/\alpha$ nodes uniformly from

220   V as $|\mathrm{diff}(\mathcal{M}_i, \mathcal{M}_j)| = d(\mathcal{M}_i, \mathcal{M}_j) \geq \alpha n$.[2] However, this approach will not succeed when $\beta \neq 0$ because now we have MAGs in the same cluster that are also separated by non-zero distance.

Algorithm 3 (α, β)-BOUNDEDDEGREE

1: **Input:** $\alpha > 0, \beta \geq 0 \, (< \alpha)$, confidence parameter $\delta > 0$, PAGs $\mathcal{U}_1, \ldots, \mathcal{U}_M$ of M entities
2: **Output:** Partition of $[M]$ into clusters
3: Let S denote a uniform sample of $\frac{4 \log(M/\delta)}{(\alpha - \beta)^2}$ nodes from V selected with replacement.
4: **for** every entity $i \in [M]$ and $u \in S$ **do**
5:     $\mathrm{ch}_i(u) \leftarrow$ IDENTIFY-OUTNBR$(\mathcal{U}_i, u)$
6:     $\mathrm{sp}_i(u) \leftarrow$ IDENTIFY-BIDIRECTED$(\mathcal{U}_i, u)$
7:     $\mathrm{pa}_i(u) \leftarrow \Gamma_i(u) \setminus (\mathrm{ch}_i(u) \cup \mathrm{sp}_i(u))$
8:     Construct $N_i(u)$ (defined in (2))
9: **end for**
10: Let $\mathcal{P}$ denote an empty graph on set of entities $[M]$
11: **for** every pair of entities i, j **do**
12:     Let $\mathrm{COUNT}(i, j) = \sum_{u \in S} \mathbf{1}\{N_i(u) = N_j(u)\}$
13:     **if** $\mathrm{COUNT}(i, j) \geq \left(1 - \frac{\alpha + \beta}{2}\right) |S|$ **then**
14:         Include an edge between i and j in $\mathcal{P}$
15:     **end if**
16: **end for**
17: Return connected components in $\mathcal{P}$

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222 **Overview of Algorithm (α, β)-BOUNDEDDEGREE.** We now build upon the above idea, to recover
223 the true clusters $C_1^\star, \ldots, C_k^\star$ when $\beta \neq 0$. As identifying a node $u \in \mathrm{diff}(\mathcal{M}_i, \mathcal{M}_j)$ is not sufficient,
224 we maintain a count of the number of nodes among the sampled set of nodes S that the pair of entities
225 i, j have the same neighbors, i.e., $\mathrm{COUNT}(i, j) = \sum_{u \in S} \mathbf{1}\{N_i(u) = N_j(u)\}$. Based on a carefully
226 chosen threshold value for the $\mathrm{COUNT}(i, j)$, that arises through the analysis of our randomized
227 algorithm, we classify whether a pair of entities belong to the same cluster correctly.

228 Overall, the idea here is to construct a graph $\mathcal{P}$ on entities (i.e., the node set of $\mathcal{P}$ is $[M]$). We include
229 an edge between two entities i and j if $\mathrm{COUNT}(i, j)$ is above the threshold $(1 - (\alpha + \beta)/2)|S|$.
230 Using Lemma 3.3, we show that this threshold corresponds to the case where if the entities are from
231 same true clusters, then the COUNT value corresponding to the pair is higher than the threshold; and
232 if they are from different clusters it will be smaller, with high probability. This ensures that every
233 entity is connected only to the entities belonging to the same true cluster. We return the connected
234 components in $\mathcal{P}$ as our clusters.

235 **Theoretical Guarantees.** In Algorithm (α, β)-BOUNDEDDEGREE, we construct a uniform sample
236 S of size $O(\log(M/\delta)/(\alpha - \beta)^2)$, and identify all the neighbors of S for every entity $i \in [M]$. As
237 we use IDENTIFY-BIDIRECTED to identify all the bi-directed edges, the total number of interventions
238 used by an entity for this step is at most $\Delta \cdot |S|$. Combining all the above, using the next lemma, we
239 show that with high probability Algorithm (α, β)-BOUNDEDDEGREE recovers all the true clusters.
240 **Lemma 3.3.** *If the underlying MAGs $\mathcal{M}_1, \ldots, \mathcal{M}_M$ satisfy (α, β)-clustering property with true*
241 *clusters $C_1^\star, \ldots, C_k^\star$ and have maximum undirected degree Δ. Then, the Algorithm (α, β)-*
242 BOUNDEDDEGREE *recovers the clusters $C_1^\star, \ldots, C_k^\star$ with probability at least $1 - \delta$. Every entity*
243 $i \in [M]$ *uses at most $4(\Delta + 1) \log(M/\delta)/(\alpha - \beta)^2$ many atomic interventions.*

244 **3.2   Learning Causal Graphs from (α, β)-Clustering**

245 In this section, we outline an approach to recover a close approximation of the causal MAGs of all
246 the entities, after correctly recovering the clusters using Algorithm (α, β)-BOUNDEDDEGREE. First,
247 we note that since the (α, β)-clustering allows the MAGs even in the same cluster to be different, the
248 problem of exactly learning all the MAGs is challenging (with a small set of interventions) as causal
249 edges learnt for an entity may not be relevant for another entity in the same cluster.

250 In the scenarios mentioned in the introduction, we expect the clusters to be more homogeneous, with
251 many entities in the same cluster sharing the same MAG. We provide an overview of Algorithm (α, β)-

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[2]For theoretical analysis, our intervention targets are randomly chosen, even with the knowledge available from PAGs, because in the worst-case the PAGs might contain no directed edges to help decide which nodes to intervene on. In practice, though if we already know edge orientations from PAG we do not have to relearn them, and a biased sampling based on edges uncertainties in PAGs might be a reasonable approach.

RECOVERY that recovers one such MAG called *dominant MAG* for every cluster. Consider a recovered cluster $C_a^\star$, and a partitioning $S_a^1, S_a^2, \cdots$ of MAGs such that all MAGs in a partition S_a^i are equal for all i. We call the MAG $\mathcal{M}_a^{\text{dom}}$ corresponding to the largest partition S_a^{dom} as the *dominant MAG* of $C_a^\star$. The dominant MAG of a cluster is parameterized by $\gamma_a = |S_a^{\text{dom}}|/|C_a^\star|$ (fraction of the MAGs in the cluster that belong to the largest partition). We defer additional details of Algorithm (α, β)-RECOVERY to Appendix C.1.

Overview of Algorithm (α, β)-RECOVERY. Consider a cluster $C_a^\star$. We recover the dominant MAG of this cluster, $\mathcal{M}_a^{\text{dom}}$, by recovering all the neighbors of every node and carefully merging them. Our idea is to assign a node, selected uniformly at random, to every entity in $C_a^\star$, and recover the neighborhood of the node using Algorithms IDENTIFY-OUTNBR and IDENTIFY-BIDIRECTED. If the clusters are large such that $|C_a^\star| \gg n$ (see Theorem 3.4 for a precise bound), we can show a large number of entities T_u are assigned node u, and many of them will share the dominant MAG. We maintain a count NCOUNT(i, u) of the number of times the entity i agrees with other entities in T_u about neighbors of u, and guarantee (with high probability) that the entity with the highest count will be that of dominant MAG. After merging the neighbors recovered for every node, we assign the resulting graph to every entity in the cluster.

As the entities satisfy (α, β)-clustering property, for all entities the recovered MAGs (dominant MAGs) are close to the true MAGs, and within a distance of at most βn. Note that any MAG from the cluster is within a distance of at most βn due to (α, β)-clustering property, but naively generating a valid MAG from a cluster will require n interventions on one entity from Proposition 3.2. Our actual guarantee is somewhat stronger, as in fact, for the entities whose MAGs are dominant in their cluster, we do recover the exact MAGs. We have the result:

Theorem 3.4. *Suppose $\mathcal{M}_1, \mathcal{M}_2, \cdots \mathcal{M}_M$ satisfy (α, β) clustering property. If $C_a^\star = \Omega(n \log(n/M\delta)(2\gamma_a - 1)^2)$ for all $a \in [k]$, then, Algorithm (α, β)-RECOVERY recovers graphs $\widehat{\mathcal{M}}_1, \cdots \widehat{\mathcal{M}}_M$ such that for every entity $i \in [M]$, we have $d(\mathcal{M}_i, \widehat{\mathcal{M}}_i) \leq \beta n$ with probability $1 - \delta$. Every entity uses at most $(\Delta + 1) + 4(\Delta + 1) \log(M/\delta)/(\alpha - \beta)^2$ many atomic interventions.*

4 Causal Discovery under α-Clustering Property

In the previous section, we discussed the more general (α, β)-clustering scenario where we manage to construct a good approximation to all the MAGs. Now, we show that we can in fact recover all the MAGs exactly, if we make a stronger assumption. Suppose the MAGs $\mathcal{M}_1, \ldots, \mathcal{M}_M$ of the M entities satisfy the α-clustering property (Defn. 2.3). Firstly, we can design an algorithm similar to Algorithm (α, β)-BOUNDEDDEGREE (see Algorithm α-BOUNDEDDEGREE, Appendix D.3) that recovers the causal MAGs exactly with $O(\Delta \log(M/\delta)/\alpha)$ many interventions per entity, succeeding with probability $1 - \delta$. Note that this has a better $1/\alpha$ term in the intervention bound, instead of $1/\alpha^2$ (when $\beta = 0$) term arising in Theorem 3.4.

In this section, we present another approach (Algorithm α-GENERAL) with an improved result that requires fewer number of interventions, even when Δ is big, provided that each cluster has at least $\Omega(n \log(M/\delta))$ entities. Missing details of Algorithm α-GENERAL are in Appendix D.4.

Overview of Algorithm α-GENERAL. First, using a similar approach as Algorithm (α, β)-BOUNDEDDEGREE, we construct a uniform sample $S \subseteq V$, and find all the outgoing neighbors of nodes in S, for every entity $i \in [M]$. Then, we construct a graph on entities denoted by $\mathcal{P}$, where we include an edge between a pair of entities if the outgoing neighbors of the set of sampled nodes S, and the set of neighbors in PAGs associated with the entities (obtained from FCI) are the same. However, due to the presence of bidirected edges, it is possible that the connected components of $\mathcal{P}$ may not represent the true clusters $C_1^\star, \ldots, C_k^\star$.

We make the observation that a pair of entities i, j that have an edge in this $\mathcal{P}$ and from different true clusters, can differ only if there is a node u such that u has a bidirected edge $u \leftrightarrow v$ in $\mathcal{M}_i$, and a directed edge $u \leftarrow v$ in $\mathcal{M}_j$ (or vice-versa). Intervening on both u and v will separate these entities, our main idea is to ensure that this happens. First, we show how to *detect* if there are at least two true clusters in any connected component of $\mathcal{P}$. Then, we identify all the entities belonging to these two clusters and remove the edges between these entities in $\mathcal{P}$ and continue.

More formally, let $T_1, \ldots, T_{k'}$ be the partition of $[M]$ provided by the k' connected components of $\mathcal{P}$ and some of these can contain more than one true cluster, hence $k' \leq k$ and we focus on detecting such events. Let $\pi : [M] \to V$ denote a mapping from the set of entities to the nodes in V such

306 that $\pi(i)$ is chosen uniformly at random from V for every entity i. For every entity i, we intervene
307 on the node $\pi(i)$. To detect that there are at least two clusters in a given subset T_a of entities, we
308 show that there are two entities i, j with an edge in $\mathcal{P}$ and for some node $u \in S$, we can identify the
309 neighbor $v \in \Gamma_i(u) \cap \Gamma_j(u)$ such that $u \leftrightarrow v$ is an edge in $\mathcal{M}_i$ and $u \leftarrow v$ is an edge in $\mathcal{M}_j$ (or
310 vice-versa). As there are at least $\Omega(n \log(M/\delta))$ entities in each of these two true clusters in T_a, for
311 some $i, j \in T_a$, we can show that $\pi(i) = \pi(j) = v$ with probability at least $1 - \delta$.

312 After detecting the event that a component T_a of $\mathcal{P}$ contains entities from at least two different true
313 clusters (say, $C_b^\star$ and $C_c^\star$) due to an edge (u, v) as above, we intervene on v for every entity in T_a.
314 By intervening on v (and $u \in S$), we can separate all entities in T_a that belong to true clusters $C_b^\star$
315 and $C_c^\star$, and remove edges between such entity pairs from $\mathcal{P}$. We repeat this above procedure of
316 refining $\mathcal{P}$. In each iteration, we will have removed all edges between every pair of entities belonging
317 to at least two different true clusters. Since there are at most k^2 different true cluster pairs, after k^2
318 iterations the connected components remaining correspond to the true clusters (with high probability).
319 This can be done without knowing the value of k, by checking whether the connected components in
320 $\mathcal{P}$ change or not after each iteration of the above idea.

321 **Going from Clustering to MAGs.** The idea of going from clusters to MAGs is simple and is based
322 on distributing the interventions across the entities in the cluster. Since, under α-clustering, all the
323 entities belonging to the same cluster share the same MAG, combining the results is relatively simpler
324 (see Appendix D.1). Combining the best of the guarantees obtained using Algorithms α-GENERAL
325 and α-BOUNDEDDEGREE, we have:

326 **Theorem 4.1.** *If MAGs* $\mathcal{M}_1, \ldots, \mathcal{M}_M$ *satisfy* α-*clustering property with true clusters* $C_1^\star, \ldots, C_k^\star$
327 *such that* $\min_{b \in [k]} |C_b^\star| = \Omega(n \log(M/\delta))$. *Then, there is an algorithm that exactly*
328 *learns all these MAGs with probability at least* $1 - \delta$. *Every entity* $i \in [M]$ *uses*
329 $\min \left\{ O(\Delta \log(M/\delta)/\alpha), O(\log(M/\delta)/\alpha + k^2) \right\}$ *many atomic interventions.*

330 **Lower Bound on the Number of Interventions**. We now give a lower bound on the number
331 of atomic interventions needed for every algorithm that recovers the true clusters on the MAGs
332 $\mathcal{M}_1, \mathcal{M}_2, \cdots \mathcal{M}_M$. Since a lower bound under α-clustering is also a lower bound under (α, β)-
333 clustering, we work with the α-clustering property here. First, we show that to identify whether a
334 given pair of entities i, j belong to the same true cluster or not, every (randomized or deterministic)
335 algorithm must make $\Omega(1/\alpha)$ interventions for both i and j.

336 Our main idea here is to use the famous Yao's minimax theorem [26] to get lower bounds on
337 randomized algorithms. Yao's theorem states that an *average case* lower bound on a deterministic
338 algorithm implies a *worst case* lower bound on randomized algorithms. To show a lower bound
339 using Yao's minimax theorem, we construct a distribution μ on MAG pairs and show that every
340 deterministic algorithm requires $\Omega(1/\alpha)$ interventions for distinguishing a pair of MAGs drawn from
341 μ. The construction of this distribution is presented in Appendix D.5. We summarize the result:

342 **Theorem 4.2.** *Suppose the underlying MAGs* $\mathcal{M}_1, \ldots, \mathcal{M}_M$ *satisfy* α-*clustering property. In order*
343 *to recover the clusters with probability* $2/3$, *every (randomized or deterministic) algorithm requires*
344 $\Omega(1/\alpha)$ *interventions for every entity in* $[M]$.

5 Experimental Evaluation

346 In this section, we provide an evaluation of our approaches on data generated from real and synthetic
347 causal networks for learning MAGs satisfying (α, β)-clustering property. We defer additional details,
348 results, and evaluation for α-clustering to Appendix E.

349 **Causal Networks.** We consider the following real-world Bayesian networks from the *Bayesian*
350 *Network Repository* which cover a wide variety of domains: *Asia* (Lung cancer) (8 nodes, 8 edges),
351 *Earthquake* (5 nodes, 4 edges), *Sachs* (Protein networks) (11 nodes, 17 edges), and *Survey* (6 nodes,
352 6 edges). For the synthetic data, we use Erdös-Rényi random graphs (10 nodes). We use the term
353 "causal network" to refer to these ground-truth Bayesian networks.

354 **Parameters**. For each causal network, we start from the corresponding DAG, and generate M MAGs
355 (one for each entity) split into k clusters that satisfy the (α, β)-clustering property through random
356 changes to the graph. We also randomly introduce two latents in each graph, and account for them in
357 MAG constructions. For more details, refer Appendix E. We set number of entities $M = 40$, number
358 of clusters $k = 2$, $\alpha = 0.60, \beta = 0.20$, and dominant MAG parameter $\gamma = 0.90$ for both the clusters.
359 For the synthetic data generated using Erdös-Rényi model, we use $n = 10$, probability of edge 0.3.

Evaluation of Clustering. First, we focus on recovering the clustering using Algorithm (α, β)-BOUNDEDDEGREE. As a baseline, we employ the well-studied FCI algorithm based on purely observational data [25]. After recovering the PAGs corresponding to the MAGs using FCI, we cluster them by constructing a similarity graph (similar to (α, β)-BOUNDEDDEGREE) defined on the set of entities (refer Appendix E for more details). For Algorithm (α, β)-BOUNDEDDEGREE, we first construct a sample S, and perform various interventions based on the set S for every entity to obtain the clusters. We also implemented another baseline algorithm (GREEDY) that uses interventions, based on a greedy idea that selects nodes to set S in Algorithm (α, β)-BOUNDEDDEGREE by considering nodes in increasing order of their degree in the PAGs returned by FCI. We use this ordering to minimize the no. of interventions as we intervene on every node in S and their neighbors.

Metrics. We use the following standard metrics for comparing the clustering performance: *precision* (fraction of pairs of entities correctly placed in a cluster together to the total number of pairs placed in a cluster together), *recall* (fraction of pairs of entities correctly placed in a cluster together to the total number of pairs in the same ground truth clusters), and *accuracy* (fraction of pairs of entities correctly placed or not placed in a cluster to the total number of pairs of entities).

Causal Network	FCI			(α, β)-BOUNDEDDEGREE (Alg. 3)			Total # Interventions
	Precision	Recall	Accuracy	Precision	Recall	Accuracy	
Earthquake	0.57 ± 0.18	0.94 ± 0.013	0.58 ± 0.18	0.78 ± 0.24	0.92 ± 0.03	0.77 ± 0.23	4
Survey	0.62 ± 0.21	0.94 ± 0.013	0.62 ± 0.2	0.64 ± 0.23	0.97 ± 0.02	0.63 ± 0.23	5
Asia	0.57 ± 0.18	0.94 ± 0.013	0.58 ± 0.18	0.92 ± 0.14	0.95 ± 0.03	0.91 ± 0.14	5
Sachs	0.52 ± 0.12	0.94 ± 0.01	0.52 ± 0.12	0.89 ± 0.20	0.96 ± 0.02	0.88 ± 0.19	6
Erdös-Rényi	0.62 ± 0.21	0.94 ± 0.02	0.62 ± 0.21	1.0 ± 0.00	0.95 ± 0.02	0.97 ± 0.013	6

Table 1: In this table, we present the precision, recall and accuracy values obtained by our Algorithm (α, β)-BOUNDEDDEGREE and using FCI. Each cell includes the mean value along with the standard deviation computed over 10 runs. The last column represents the maximum number of interventions per entity including both Algorithms (α, β)-BOUNDEDDEGREE and (α, β)-RECOVERY.

Results. In Table 1, we compare Algorithm (α, β)-BOUNDEDDEGREE to FCI on the clustering results. For Algorithm (α, β)-BOUNDEDDEGREE, we use a sample S of size 1, and observe in Figure 6 (Appendix E), that this corresponds to about 2 interventions per entity. With increase in sample size, we observed that the results were either comparable or better. We observe that our approach leads to considerably better performance in terms of the accuracy metric with an average difference in mean accuracy of about 0.25. This is because FCI recovers partial graphs, and clustering based on the partial information results in poor accuracy. Because of the presence of a dominant MAG with in each cluster, we observe that the corresponding entities are always assigned to the same cluster, resulting in high recall for both (α, β)-BOUNDEDDEGREE and FCI. We observe a higher value of precision for our algorithms, because FCI is unable to correctly classify the MAGs that are different from the dominating MAG.

Algorithm (α, β)-BOUNDEDDEGREE outperforms the GREEDY baseline for the same sample(S) size. For example, on the *Earthquake* and *Survey* causal networks, Algorithm (α, β)-BOUNDEDDEGREE obtains the mean accuracy values of 0.77 and 0.63 respectively, while GREEDY for the same number of interventions obtained an accuracy of only 0.487 and 0.486 respectively. For the remaining networks, the accuracy values of GREEDY are almost comparable to our Algorithm (α, β)-BOUNDEDDEGREE.

After clustering, we recover the dominant MAGs using Algorithm (α, β)-RECOVERY, and observe that the additional interventions needed are bounded by the maximum degree of the graphs (see Theorem 3.4). This is represented in the last column in Table 1. We observe that our *collaborative* algorithms use fewer interventions for dominant MAG recovery compared to the number of nodes in each graph. For example, in the Erdös-Rényi setup, the number of nodes $n = 10$, whereas we use at most 6 interventions per entity. Thus, compared to the worst-case, cutting the number of interventions for each entity by 40%.

Concluding Remarks. We introduce a new model for causal discovery to capture practical scenarios where are multiple entities with different causal structures. Under natural clustering assumption(s), we give efficient provable algorithms for causal learning with atomic interventions in this setup and demonstrate its empirical performance. Our model can be naturally extended to the setting where all interventions are non-adaptive, and we plan to study it as part of future work. An interesting future direction would be to extend the interventional equivalence between DAGs studied in [8, 12] to the setting without the causal sufficiency assumption, similar to [10, 14], and exploit that for learning.

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