# **Causal Inference Under Interference And Network Uncertainty**

**Rohit Bhattacharya** 

Daniel Malinsky Department of Computer Science Johns Hopkins University {rbhattacharya@, malinsky@, ilyas@cs.}jhu.edu

## Abstract

Classical causal and statistical inference methods typically assume the observed data consists of independent realizations. However, in many applications this assumption is inappropriate due to a network of dependences between units in the data. Methods for estimating causal effects have been developed in the setting where the structure of dependence between units is known exactly [12, 40, 24], but in practice there is often substantial uncertainty about the precise network structure. This is true, for example, in trial data drawn from vulnerable communities where social ties are difficult to query directly. In this paper we combine techniques from the structure learning and interference literatures in causal inference, proposing a general method for estimating causal effects under data dependence when the structure of this dependence is not known a priori. We demonstrate the utility of our method on synthetic datasets which exhibit network dependence.

# **1 INTRODUCTION**

In many scientific and policy settings, research subjects do not exist in isolation but in interacting networks. For instance, data drawn from an online social network will exhibit *homophily* (friends are similar, because they are friends), and *contagion* (friends may causally influence each other) [19, 33, 15, 34]. Similarly, vaccinating some subset of a population may confer immunity to the entire population – a well-documented phenomenon known as *herd immunity* in infectious disease epidemiology. This implies that a treatment given to one unit affects outcomes for another. Finally, resource constraints in allocation problems may also induce data dependence. In the context of causal inference, methods for dealing with data dependence are developed under the heading of *interference* [36, 10, 31, 12, 40, 33, 24, 39]. Most such work assumes the structure of the dependence (which units depend on which others, and how) is known precisely. For example, [40] assumes units in the data may be organized into equal sized blocks, where units within a block are pairwise dependent and units across blocks are not. Some work makes alternative assumptions, e.g., [39] assumes that blocks are drawn from a known random field.

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In many applications, the network inducing dependence between units may not be known exactly. For instance, in vulnerable, stigmatized, or isolated communities (such as groups of drug users, or remote villages), we may have no way of reconstructing the precise social ties between individuals. Some online databases of social media users may be anonymized, with friendship ties deliberately omitted. There has been some work in such settings that involves adapting the data collection method itself in order to discover the underlying networks: e.g., snowball sampling in [5] and [3]. Unfortunately, such study designs are not always possible to arrange in advance, and most data available on networks of interacting units is not collected under such designs.

While there is a rich literature on model selection from observational data in the context of causal inference (e.g., [37, 4, 35, 27]), to our knowledge all previous work has assumed the absence of interference. We explore learning the dependence structure using graphical model selection methods. Techniques for structure learning from probabilistic relational models are also related to this work [21, 18].

The contributions of our paper may be viewed in one of two ways. From the point of view of causal inference under interference, our paper contributes to methods for estimating causal effects when there is substantial uncertainty about network structure. From the point of view of structure learning, we introduce novel algorithms for model selection when units are dependent due to a network, the structure of which is unknown.

# 2 MOTIVATING EXAMPLE AND BACKGROUND ASSUMPTIONS

To motivate our work, we discuss an example application. Consider a public health program aimed at lowering the incidence of blood-borne diseases such as HIV in atrisk individuals who are addicted to heroin and share needles when injecting intravenously. An example of such a program is described in [38]. The program creates popup clinics around the city where disposable needles are distributed for free to individuals in need, but due to limited resources only a limited number of individuals will actually receive these needles. We would like to know, in this restricted resource setting, if the use of disposable needles spreads amongst the rest of the population. Additionally, we would like to detect the phenomenon of herd immunity, i.e., whether some members of the population being protected due to taking advantage of the clean needles confer this protection to others who do not.

Data on heroin users was collected via such program, with users arranged by neighborhood or municipality. Users in different neighborhoods are assumed independent, but users within the same neighborhood are likely dependent. This setting is known as *partial interference* [12]. For each individual *i*, data is collected on their use of disposable needles  $A_i$ , their subsequent health outcome  $Y_i$  (risk of obtaining blood-born disease), along with a vector of pre-treatment covariates  $\mathbf{L}_i = (L_{1,i}, ..., L_{p,i})$ . We may be interested in quantifying the causal effects of  $A_i$  on  $Y_j$ , for arbitrary *i* and *j* within a neighborhood, or network-averaged versions of such effects [24].

We may assume that background knowledge or study design implies a "known" individual-level causal structure for each *i*, namely that  $A_i \to Y_i$  and  $A_i \leftarrow \mathbf{L}_i \to Y_i$ , but that we are uncertain about network ties among users. One approach is to assume the least restrictive model, where all users in a neighborhood are arbitrarily dependent. This would correspond to a complete network, where every pair of vertices is directly connected. However, assuming a complete network when the true network is sparse ignores useful structure in the problem and leads to inefficient estimates of target quantities. In addition, complete networks often lead to likelihoods that are intractable to evaluate. An alternative is to a select a sparse network supported by the data. In addition to enabling tractable and statistically efficient inference, such an approach may also rule out the presence of cer-



Figure 1: A chain graph over three variables (L, A, and Y) on 4 individuals, representing possible relationships between disposable needle use and risk of blood-borne disease among heroin-users.

tain causal effects without explicitly estimating them, if corresponding pathways are absent in the selected network.

As an example, if neighborhoods have 4 units, we may aim to learn a graphical model such as shown in Figure 1. This model, containing both directed edges (representing direct causal influences) and undirected edges (representing symmetric network ties), is known as a chain graph model [16]. We describe chain graphs in more detail below. This model tells us that we should expect some spread of disposable needle use from one unit to another. However, it also tells us that users in neighborhoods are split into two non-interacting groups:  $\{1, 2\}$ and  $\{3,4\}$ . This implies the absence of contagion from one group to another. In addition, the conditional independences among units implied by this split suggests that contagion effects within groups may be estimated more efficiently as compared to a statistically saturated model, with a complete network across units.

The algorithms we propose are consistent (in the sense that they asymptotically converge on the true model) under a set of assumptions which we now informally summarize. We assume the true data-generating process corresponds perfectly (satisfying Markov and faithfulness conditions) to some unknown chain graph, with two restrictions: (1) the unit-level graph is known, reflecting the aforementioned causal ordering between pretreatment covariates, treatment variables, and outcomes; and (2) the graph respects what we later call tier symmetry, which restricts connections between variables at the same "tier" in the causal ordering to be symmetric. We assume the data is distributed with some (known) likelihood in the exponential family, as well as some weak statistical regularity conditions. We also present algorithms that make an additional simplifying assumption on the graphical structure - namely that influence between units is the same for all unit pairs - but such an assumption is not strictly necessary for consistency.

We begin by describing some technical preliminaries, including chain graph models, causal inference, and graphical model selection. Then we present algorithms to learn graphical models of the sort shown in Figure 1, before estimating causal effects.

# **3 PRELIMINARIES**

## 3.1 Graphical Terminology

Chain graphs (CGs) are a class of mixed graphs containing directed  $(\rightarrow)$  and undirected (-) edges, such that it is impossible to create a directed cycle by orienting any combination of the undirected edges [16]. A CG with no undirected edges is a directed acyclic graph (DAG). A CG with no directed edges is an undirected graph (UG) Vertices of a graph are denoted by capital letters (e.g. *A*), and they correspond to random variables. We use boldface (e.g. **A**) to denote sets of vertices or sets of random variables. Lowercase letters denote specific values of random variables (e.g. *a*) or sets of values (e.g. **a**). We use **V** and  $\mathcal{E}$  to denote the set of all vertices and edges in a graph  $\mathcal{G}$ , respectively.

For a subset of vertices  $\mathbf{A} \subseteq \mathbf{V}$  we define the induced subgraph  $\mathcal{G}_{\mathbf{A}}$  to be the graph with vertices  $\mathbf{A}$  and edges of  $\mathcal{G}$  that have both endpoints in  $\mathbf{A}$ . A block  $\mathbf{B}$  is defined as a maximal set of vertices such that every vertex pair in  $\mathcal{G}_{\mathbf{B}}$  is connected by an undirected path. The set of blocks in a CG  $\mathcal{G}$ , denoted by  $\mathcal{B}(\mathcal{G})$ , partitions the vertices in  $\mathcal{G}$ . A clique  $\mathbf{C}$  is defined as a maximal set of vertices that are pairwise connected by undirected edges. A clique in a CG is always a subset of some block  $\mathbf{B}$ . We denote the set of all cliques in an UG  $\mathcal{G}$  by  $\mathcal{C}(\mathcal{G})$ .

For a graph  $\mathcal{G}$  and vertex  $V \in \mathbf{V}$  we define some standard vertex sets as follows: the set of parents  $\operatorname{pa}_{\mathcal{G}}(V) \equiv \{V' : V' \to V \text{ in } \mathcal{G}\}$ ; the set of neighbors  $\operatorname{nb}_{\mathcal{G}}(V) \equiv \{V' : V' - V \text{ in } \mathcal{G}\}$ ; the boundary  $\operatorname{bd}_{\mathcal{G}}(V) \equiv \operatorname{pa}_{\mathcal{G}}(V) \cup \operatorname{nb}_{\mathcal{G}}(V)$ ; and the closure  $\operatorname{cl}_{\mathcal{G}}(V) \equiv \operatorname{bd}_{\mathcal{G}}(V) \cup V$ . These definitions generalize disjunctively to sets, e.g.  $\operatorname{pa}_{\mathcal{G}}(\mathbf{A}) \equiv \bigcup_{A \in \mathbf{A}} \operatorname{pa}_{\mathcal{G}}(A)$ . Note that for a block  $\mathbf{B}$ ,  $\operatorname{bd}_{\mathcal{G}}(\mathbf{B}) = \mathbf{B} \cup \operatorname{pa}_{\mathcal{G}}(\mathbf{B})$ . Given a CG  $\mathcal{G}$ , define the augmented graph  $\mathcal{G}^a$  to be an UG constructed from  $\mathcal{G}$  by replacing all directed edges with undirected edges and connecting all vertices in  $\operatorname{pa}_{\mathcal{G}}(\mathbf{B})$  for every block  $\mathbf{B}$  in  $\mathcal{G}$ by undirected edges.

We will utilize chain graphs to represent both causal relationships and network dependence among units that form a ("social") network  $\mathcal{N}$ . The undirected network  $\mathcal{N}$  is a graph (distinct from our CG of interest) where the vertices correspond to units (e.g. individuals i, j, ...), not random variables. Units may be adjacent or non-adjacent in  $\mathcal{N}$  based on whether they are "friends" or otherwise directly dependent.

For each unit *i*, we denote the unit-level variables for *i* in the CG  $\mathcal{G}$  (e.g.,  $L_i$ ,  $A_i$ , and  $Y_i$  in Figure 1) by  $\mathbf{V}_i$ , and edges among those variables by  $\mathcal{E}_i$ . Similarly, for a pair of units *i*, *j* which are adjacent in  $\mathcal{N}$ , we represent the set of edges from  $\mathbf{V}_i$  to  $\mathbf{V}_j$  (and vice versa) by  $\mathcal{E}_{ij}$ . It is the presence of these edges that induces data dependence between *i* and *j* in our analysis. The set of  $\mathcal{E}_{ij}$  for all pairs *i*, *j* adjacent in  $\mathcal{N}$  (i.e., the set of all cross-unit edges) will be denoted by  $\mathcal{E}_{\mathcal{N}}$ .

## 3.2 Chain Graph Models

A statistical chain graph model associated with a LWF (Lauritzen-Wermuth-Frydenberg) chain graph G is a set of distributions that factorize as:

$$p(\mathbf{V}) = \prod_{\mathbf{B} \in \mathcal{B}(\mathcal{G})} p(\mathbf{B} \mid \text{pa}_{\mathcal{G}}(\mathbf{B}))$$
  
and (1)

$$p(\mathbf{B} \mid \mathrm{pa}_{\mathcal{G}}(\mathbf{B})) = \frac{\prod_{\{\mathbf{C} \in \mathcal{C}((\mathcal{G}_{\mathrm{bd}_{\mathcal{G}}(\mathbf{B})})^a): \mathbf{C} \not\subseteq \mathrm{pa}_{\mathcal{G}}(\mathbf{B})\}}{Z(\mathrm{pa}_{\mathcal{G}}(\mathbf{B}))} \phi_{\mathbf{C}}(\mathbf{C})$$

for each block **B** in  $\mathcal{G}$ , where  $\phi_{\mathbf{C}}(\mathbf{C})$  is a clique potential function for a clique **C** in the UG  $(\mathcal{G}_{\mathrm{bd}_{\mathcal{G}}(\mathbf{B})})^a$  defined as above and  $Z(\mathrm{pa}_{\mathcal{G}}(\mathbf{B}))$  is a normalizing function [16].

A CG without undirected edges is a DAG, which has a simpler factorization:  $p(\mathbf{V}) = \prod_{V \in \mathbf{V}} p(V \mid \text{pa}_{\mathcal{G}}(V))$ . If it is the case that for every block **B** in CG  $\mathcal{G}$ ,  $\mathcal{G}_{\text{bd}_{\mathcal{G}}(\mathbf{B})}$  has missing edges only among elements of  $\text{pa}_{\mathcal{G}}(\mathbf{B})$ , then  $(\mathcal{G}_{\text{bd}_{\mathcal{G}}}(\mathbf{B}))^a$  has a single clique containing all elements in  $\text{bd}_{\mathcal{G}}(\mathbf{B})$ . In other words, the model corresponding to such a CG may be viewed as a DAG model with entire blocks **B** acting as vertices in a DAG.

## 3.3 Causal Models

A causal model is a set of distributions over counterfactual random variables, a.k.a. potential outcomes. For  $Y \in \mathbf{V}$  and  $\mathbf{A} \subseteq \mathbf{V} \setminus Y$ , the counterfactual  $Y(\mathbf{a})$  denotes the value of Y when the "treatment" variables  $\mathbf{A}$  are fixed to values  $\mathbf{a}$  by an intervention. Sometimes interventions are formalized by the 'do'-operator: do( $\mathbf{a}$ ) denotes the assignment  $\mathbf{a}$  to  $\mathbf{A}$  [25]. The counterfactual distribution corresponding to the intervention where  $\mathbf{A}$  is set to  $\mathbf{a}$  is written  $p(Y(\mathbf{a}))$  or  $p(Y | do(\mathbf{a}))$ .

A causal model of a DAG  $\mathcal{G}$  is a set of distributions defined on counterfactual random variables  $V(\mathbf{a})$  for each  $V \in \mathbf{V}$  and where  $\mathbf{a}$  is a set of values for  $pa_{\mathcal{G}}(V)$ . Equivalently, a causal model can be understood as the set of distributions induced by a system of structural equations (one equation for each vertex) equipped with the do(.) operator [25, 29]. In a causal model of a DAG G, all counterfactual distributions are *identified*, i.e., they can be expressed as functions of the observed data, by the g-formula [30]:

$$p(\mathbf{V} \setminus \mathbf{A} \mid do(\mathbf{a})) = \prod_{V \in \mathbf{V} \setminus \mathbf{A}} p(V \mid pa_{\mathcal{G}}(V)) \Big|_{\mathbf{A}=\mathbf{a}}.$$

Counterfactual responses to interventions are often contrasted on a mean difference scale under two possible interventions **a** and **a**', representing cases and controls. For example, the average causal effect (ACE) is given by  $\mathbb{E}[Y(\mathbf{a})] - \mathbb{E}[Y(\mathbf{a}')]$ .

Causal models have been generalized from DAGs to CGs (details in the Supplement) and yield the following generalization of the g-formula [17]:

$$p(\mathbf{V} \setminus \mathbf{A} | \operatorname{do}(\mathbf{a})) = \prod_{\mathbf{B} \in \mathcal{B}(\mathcal{G})} p(\mathbf{B} \setminus \mathbf{A} | \operatorname{pa}(\mathbf{B}), \mathbf{B} \cap \mathbf{A}) \Big|_{\mathbf{A} = \mathbf{a}}.$$
(2)

## 3.4 The Conditionally Ignorable Network Model and Network Causal Effects

For the purposes of this paper, we consider CGs decomposed into three disjoint sets of variables: L, representing vectors of baseline (pre-treatment) factors; A, representing treatments; and Y, representing outcomes. For each unit *i*, we assume  $\mathbf{L}_i \subseteq \mathrm{pa}_{\mathcal{G}}(A_i)$ , and  $\mathbf{L}_i \cup \{A_i\} \subseteq$  $pa_{\mathcal{G}}(Y_i)$ . This represents a common assumption (which we call *causal ordering*) in causal inference that for each unit both baseline factors and treatment potentially affect the outcome, and that the baseline factors also affect treatment assignment. Here each unit has one treatment variable  $A_i$ , one outcome variable  $Y_i$ , and possibly many baseline variables  $L_i$ . In interference settings, it is standard to allow that variables for another unit j may influence variables for unit *i*. In our case, there is a further complication: the precise nature of this influence is unknown.

This model implies, for positive  $p(\mathbf{V})$ , the following standard assumptions from the interference literature:  $\mathbf{Y}(\mathbf{a}) \perp \mathbf{L} \mathbf{A} \mid \mathbf{L}$  (network ignorability);  $p(\mathbf{a} \mid \mathbf{L}) > 0$   $\forall \mathbf{a}$  (positivity); and  $\mathbf{Y}(\mathbf{a}) = \mathbf{Y}$  if  $\mathbf{A} = \mathbf{a}$  (consistency). Under these assumptions, the joint counterfactual outcome is identified, regardless of the underlyling network structure, as the following special case of (2):  $p(\mathbf{Y}(\mathbf{a})) = \sum_{\mathbf{L}} p(\mathbf{Y} \mid \mathbf{A} = \mathbf{a}, \mathbf{L})p(\mathbf{L}).$ 

Given a particular treatment assignment probability  $\pi(\mathbf{A})$ , a number of causal effects of interest may be defined, see [40] for an extensive discussion. In this paper, we focus on a single effect, the *population average over*all effect (PAOE), though our results generalize to any identified causal effect of interest in network settings (for example, spillover effects). Consider a block is of size mand two fixed  $\pi_1, \pi_2$  assignment probabilities. Then the PAOE is defined as:

$$\frac{1}{m}\sum_{i=1}^{m}\sum_{\mathbf{A}}\mathbb{E}[Y_i(\mathbf{A})]\{\pi_1(\mathbf{A})-\pi_2(\mathbf{A})\}.$$
 (3)

Under the aforementioned assumptions, this effect is identified by the following functional [40]:

$$\frac{1}{m}\sum_{i=1}^{m}\sum_{\mathbf{L},\mathbf{A}}\mathbb{E}[Y_i \mid \mathbf{A}, \mathbf{L}]p(\mathbf{L})\{\pi_1(\mathbf{A}) - \pi_2(\mathbf{A})\}.$$
 (4)

A number of estimation strategies for (4) are possible under various assumptions on network structure. For example, [40] considered an inverse probability weighted estimator. In this paper, we use the auto-g-computation algorithm in [39] to estimate the PAOE, which allows for arbitrary network structure; we describe this estimator in detail in the Supplement.

# 4 MODEL SELECTION FOR UNKNOWN NETWORKS

We are interested in estimating causal effects like the PAOE under the aforementioned assumptions, where there is uncertainty about the network structure. We give a taxonomy of problems of this type, having different levels of difficulty depending on the degree of uncertainty present.

The most general version of the problem occurs when neither the causal structure of each unit, nor the network structure inducing dependence between units, is known. In this case the problem reduces to a structure learning problem for arbitrary chain graphs, as considered in [20] and [26]. We do not pursue this version of the problem here for two reasons. First, the causal structure for each unit is often known due to background knowledge on temporal ordering and study design, as is the case for our needle-dispensary motivating example. Second, model selection of arbitrary CGs is known to be a very challenging problem which (in the worst case) may require large sample sizes [6].

In many settings, the causal structure for each individual unit is known and is typically assumed to be the same for every unit, i.e.,  $\mathcal{E}_i = \mathcal{E}_j$  for all *i*, *j*. The problem of model selection then amounts to learning the structure of the connections between units i.e.,  $\mathcal{E}_{ij}$  for all *i*, *j*. The search space for such a problem, while much smaller than the general problem, is still exponential. For a block that contains *m* units, there are  $\binom{m}{2}$  possible pairings of units, leading to  $2^{\binom{m}{2}}$  possible networks. The number of possible valid chain graphs is even larger, since units i, j adjacent in a network could be connected in a variety of ways via (undirected or directed) edges in  $\mathcal{E}_{ij}$ . Learning these connections requires a search through all possible combinations of edges that form  $\mathcal{E}_{ij}$  such that the overall graph is a CG.

We may restrict the problem further by requiring that the connections between any two units, if present, are homogenous, meaning that dependence between any two units, if it exists, arises in the same way. Formally, we define homogeneity such that, for all pairs  $(i, j), (k, l) \in$  $\mathcal{N}, \mathcal{E}_{ij} = \mathcal{E}_{kl}$ . Notice that the space of homogenous networks is still fairly large. The problem may be made more tractable by one of the following two assumptions. We may assume the existence of network connections is known, but that their types are unknown, i.e., we know  $\mathcal{N}$  and would like to learn  $\mathcal{E}_{ij}$ . Alternatively, we may assume we know how two adjacent units are connected, but not which pairs are adjacent, i.e., we know  $\mathcal{E}_{ij}$  and would like to learn  $\mathcal{N}$ . We may also have no such background knowledge. In the following, we present algorithms for both homogenous and heterogenous settings.

Throughout, we make an assumption which we call *tier* symmetry, which is commonly made implicitly or explicitly in the interference literature [40, 39]. That is, we require connections between variables in the same "tier" of causal ordering to represent symmetric relations between the variables. This restricts edges  $L_i - L_j$ ,  $A_i - A_j$ , and  $Y_i - Y_j$  to always be undirected. Also it is natural to extend the known causal ordering of variables to connections between units: while we allow for e.g.,  $A_i \rightarrow Y_j$ , the reverse,  $Y_j \rightarrow A_i$  is ruled out. Finally, we rule out the existence of undirected edges connecting variables across tiers, e.g, edges of the form  $A_i - Y_j$ , since the existence of such edges, coupled with our causal ordering assumption, leads to graphs which are not CGs.

Before presenting algorithms to address the above taxonomy of problems, we introduce some necessary concepts from the graphical model selection literature.

## 4.1 Markov Properties and Faithfulness

If  $p(\mathbf{V})$  is a positive distribution, the factorization (1) is equivalent to a global Markov property which relates certain graphical separation facts in the CG  $\mathcal{G}$  (given by the c-separation criterion) to conditional independence relations in  $p(\mathbf{V})$ ; see [16] for precise definitions. In what follows, we make the *faithfulness* assumption, which is the converse of the global Markov property: if ( $\mathbf{A} \perp \mathbf{B} \mid \mathbf{C}$ ) in  $p(\mathbf{V})$ , then  $\mathbf{A}$  is c-separated from  $\mathbf{B}$  given  $\mathbf{C}$ in  $\mathcal{G}$ . This is directly analogous to the faithfulness assumption made when selecting DAG models from data by constraint-based or score-based methods [37, 4].

## 4.2 Model Scores and the Pseudolikelihood

In this paper, we will learn the structure of the network using a score-based approach to model selection. Scorebased methods proceed by choosing the graph (from among some space of candidates) that optimizes a model score. Exhaustive model search is typically infeasible, so it is popular to employ greedy methods that optimize only "locally," that is, they traverse the space of candidate graphs considering only single-edge additions and deletions. Under some conditions, such greedy procedures can be shown to asymptotically converge to the globally optimal model [4]. Scores used for greedy search typically satisfy three properties that are sufficient for finding the globally optimal model: decomposability, score-equivalence, and consistency.

A score is said to be decomposable if it can be written as a sum of local contributions, each a function of one vertex and its boundary. A score is said to be scoreequivalent if two Markov equivalent graphs (i.e., graphs that imply the same set of conditional independences by the global Markov property) yield the same score. A score is said to be consistent if, as the sample size goes to infinity, the following two conditions hold. First, when two models both contain the true generating model, the model of lower dimension will have a better score. Second, when one model contains the true model and another does not, the former will have a better score.

A popular score satisfying these properties for model selection among DAG models is the Bayesian Information Criterion (BIC) [32]. Given a *d*dimensional data set **D** of size *n* and model likelihood  $\mathcal{L}(\mathbf{D}; \mathcal{G}) \equiv \prod_{i=1}^{n} p(x_{1,i}, \dots, x_{d,i}; \mathcal{G})$ , the BIC is given by  $2 \ln \mathcal{L}(\mathbf{D}; \mathcal{G}) - k \ln(n)$  where *k* is model dimension.

For CG models, the BIC is only decomposable for blocks, not for variables within the block. In addition, the score is not easy to evaluate. Both of these issues arise due to the presence of normalizing functions in the likelihood. Here, we present an alternative score which avoids some of these problems, based on the *pseudolike-lihood function* [2]:

$$\mathcal{PL}(\mathbf{D};\mathcal{G}) \equiv \prod_{i=1}^{n} \prod_{j=1}^{d} p(x_{j,i} \mid \mathbf{x}_{-j,i};\mathcal{G}),$$

where  $\mathbf{x}_{-j}$  is the vector  $(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_d)$ . We define a score based on the pseudolikelihood called Pseudo-BIC (PBIC):  $2 \ln \mathcal{PL}(\mathbf{D}; \mathcal{G}) - k \ln(n)$ .

We propose a greedy score-based model selection proce-

dure based on the PBIC score, which is consistent and obeys a weaker notion of decomposability for exponential families, as we show below. All proofs are deferred to the Supplement.

**Lemma 1.** With dimension fixed and sample size increasing to infinity, the PBIC is a consistent score for curved exponential families whose natural parameter space  $\Theta$  forms a compact set.

Decomposability of a scoring criterion makes greedy search a practical procedure, by limiting the number of terms in the overall score that need to be recomputed for each considered edge modification. While the BIC score for DAG models is decomposable, the PBIC score for CG models is not. Nevertheless, a weaker notion of decomposability holds, which implies that two CG models that differ by a single edge differ by a subset of components of the score, which we now describe. Consider a candidate edge between  $V_i$  and  $V_j$  in a CG  $\mathcal{G}$ . Let  $\mathbf{B}_{\text{loc}}$ denote the block to which  $V_j$  belongs when the edge is directed  $V_i \rightarrow V_j$ , or to which  $V_i$  and  $V_j$  belong when the edge is undirected  $V_i - V_j$ . We use  $\text{loc}(V_i, V_j; \mathcal{G})$  to denote a set of vertices called the *local set*, defined as:

$$\bigcup_{\mathbf{C}} \{ \mathbf{C} \in \mathcal{C}((\mathcal{G}_{\mathrm{bd}_{\mathcal{G}}(\mathbf{B}_{\mathrm{loc}})})^{a}) : V_{i}, V_{j} \in \mathbf{C} \not\subseteq \mathrm{pa}_{\mathcal{G}}(\mathbf{B}_{\mathrm{loc}}) \}.$$

As we show, the score difference for graphs  $\mathcal{G}$  and  $\mathcal{G}'$  which differ by a single edge can be written as the difference between terms that involve only variables in the local set of  $\mathcal{G}$ . The next result, and much subsequent discussion in the paper, is stated for conditional Markov random fields (MRFs). This is because statistical CG models can be equivalently described as sets of conditional MRF models. We elaborate on this relationship in the Supplement.

**Lemma 2.** Let  $\mathcal{G}$  and  $\mathcal{G}'$  be graphs which differ by a single edge between  $V_i$  and  $V_j$ . For conditional MRFs in the exponential family, the local score difference between  $\mathcal{G}$  and  $\mathcal{G}'$  is given by:  $\sum_{V \in \text{loc}(V_i, V_j; \mathcal{G}) \cap \mathbf{B}_{\text{loc}}} \{s_V(\mathbf{D}; \mathcal{G}) - s_V(\mathbf{D}; \mathcal{G}')\}$ , where  $s_V(.)$  denotes the component of the score for V.

Note that the above definition of the local set may simplify further in certain special cases of MRF models in the exponential family. In particular, if we consider an MRF that is multivariate normal, or a log linear discrete model with only main effects and pairwise interactions, then the sum in Lemma 2 reduces to either a sum over elements  $V_i$  and  $V_j$  (for an undirected edge  $V_i - V_j$ ) or only  $V_j$  (for a directed edge  $V_i \rightarrow V_j$ ). We omit the straightforward proofs in the interest of space. We will not consider these special instances of the exponential family in the remainder of this paper, but in the supplement we

Algorithm 1 GREEDY NETWORK SEARCH( $\mathcal{G}^{\text{min}}, \mathbf{D}$ )				
1: $\mathcal{G}^* \leftarrow \mathcal{G}^{\text{init}}$				
2: score change $\leftarrow$ True				
3: while score change do				
4: score change $\leftarrow$ False				
5: $\mathcal{E}^*_{\mathcal{N}} \leftarrow$ network ties in $\mathcal{G}^*$				
6: $E_{max} \leftarrow \operatorname{argmax}_{E \in \mathcal{E}_{\mathcal{N}}^*} \operatorname{PBIC}(\mathbf{D}; \mathcal{G}^* \setminus E)$				
7: <b>if</b> PBIC( $\mathbf{D}; \mathcal{G}^* \setminus E_{max}$ ) > PBIC( $\mathbf{D}; \mathcal{G}^*$ ) <b>then</b>				
8: $\mathcal{G}^* \leftarrow \mathcal{G}^* \setminus E_{max} \qquad \triangleright \text{ deleting edge } E_{max}$				
9: score change $\leftarrow$ True				
10: return $\mathcal{E}_{\mathcal{N}}^*$				

discuss the incurred computational costs for exponential families in general.

### 4.3 Greedy Network Search

While there exist numerous methods that take a pseudolikelihood-type approach to model selection in UGs [28, 13, 7, 1], these have been typically restricted to Ising or Gaussian models. Such methods involve a per-vertex neighbourhood selection procedure using L1regularized regression or the standard BIC, which may yield self-inconsistent results (e.g., find that  $V_i$  in  $nb(V_i)$ ) but not vice versa). Any resulting inconsistencies would need to be resolved post hoc through union or intersection consolidation procedures. Methods that try to enforce self-consistency by explicitly maximizing the pseudolikelihood with a regularization penalty are presented in [9] and [14], but are again restricted to Ising and Gaussian graphical models. The properties of the PBIC described in the previous section allow us to design algorithms for greedy network search that are parallelizable, while also generalizing to all exponential families and circumventing the need for post hoc procedures. While our method covers a more general class of models, it can be computationally expensive to calculate the local scores at each step. A more efficient procedure is possible in some subclasses (including Ising and Gaussian), where we can modify our procedure into a "forwardbackward" algorithm reminiscent of the GES algorithm [4]. Since our focus is on a general procedure for all exponential families, we defer further discussion of these special cases to the Supplement.

We begin by describing a greedy search procedure that learns network ties  $\mathcal{E}_{\mathcal{N}}$ , without imposing homogeneity. Model selection proceeds by solving 3 independent sub problems: learning a Markov random field (MRF) over the baseline covariates **L**, learning a conditional MRF on the treatments **A**, and learning a conditional MRF on the outcomes **Y**. The resulting network ties learned from each of these, are combined to produce the final reAlgorithm 2 HETEROGENOUS( $\mathcal{G}^{\text{complete}}, \mathbf{D}$ )

- 1:  $\mathcal{G}^{L}, \mathcal{G}^{A}, \mathcal{G}^{Y} \leftarrow \text{conditional MRFs on } L, A, \text{ and } Y$ formed from  $\mathcal{G}^{\text{complete}}$
- 2:  $\mathcal{E}^*_{\mathcal{N}_{\mathbf{I}}} \leftarrow \text{Greedy Network Search}(\mathcal{G}^{\mathbf{L}}, \mathbf{D})$
- 3:  $\mathcal{E}_{\mathcal{N}_{A}}^{*} \leftarrow \text{Greedy Network Search}(\mathcal{G}^{A}, \mathbf{D})$
- 4:  $\mathcal{E}_{\mathcal{N}_{\mathbf{V}}}^{*} \leftarrow \text{Greedy Network Search}(\mathcal{G}^{\mathbf{Y}}, \mathbf{D})$
- 5: return  $\mathcal{E}^*_{\mathcal{N}_{\mathbf{L}}} \cup \mathcal{E}^*_{\mathcal{N}_{\mathbf{A}}} \cup \mathcal{E}^*_{\mathcal{N}_{\mathbf{Y}}}$

## Algorithm 3 HOMOGENOUS( $\mathcal{G}^{\text{complete}}, \mathbf{D}, \mathcal{E}_{\text{proto } \mathcal{N}}$ )

- 1:  $\mathcal{G}^* \leftarrow$  graph obtained by removing all edges between units i, j in  $\mathcal{G}^{\text{complete}}$  when  $E_{ij} \notin h(\mathcal{E}_{\text{proto } \mathcal{N}})$ 2: score change  $\leftarrow$  True 3: while score change do
- score change  $\leftarrow$  False 4:
- $\mathcal{N}^* \leftarrow$  network in  $\mathcal{G}^*$ 5:
- $(i, j)_{max} \leftarrow \operatorname{argmax}_{(i, j) \in \mathcal{N}^*} \operatorname{PBIC}(\mathbf{D}; \mathcal{G}^* \setminus \mathcal{E}_{ij})$ 6:
- if  $\operatorname{PBIC}(\mathbf{D}; \mathcal{G}^* \setminus \mathcal{E}_{ij_{max}}) > \operatorname{PBIC}(\mathbf{D}; \mathcal{G}^*)$  then 7:
- $\mathcal{G}^* \leftarrow \mathcal{G}^* \setminus \mathcal{E}_{ij_{max}}$ 8:
- score change  $\leftarrow$  True 9:

10: return  $\mathcal{N}^*$ 

sult (Alg. 2). Each of the above subproblems is solved by a greedy search procedure (Alg. 1) that starts with the complete conditional MRF (or MRF), and deletes the edge that yields the greatest improvement to the PBIC score on each iteration.

We now describe procedures for learning network ties in the homogenous setting, after defining some preliminaries. The homologs of an edge  $E_{ij} \in \mathcal{E}_{\mathcal{N}}$  with endpoints  $U_i, W_j \in \mathbf{V}$ , are defined as:  $h(E_{ij}) \equiv \{E_{kl} \in$  $\mathcal{E}_{\mathcal{N}}$  : endpoints $(E_{kl}) = U_k, W_l$ . The network tie prototypes in a homogenous graph G are defined as:  $\mathcal{E}_{\text{proto }\mathcal{N}} \equiv \{E_{ij} \in \mathcal{E}_{ij} \text{ for any } (i,j) \in \mathcal{N}\}. h(\mathcal{E}_{\text{proto }\mathcal{N}})$ can then be defined as:  $\{h(E) : E \in \mathcal{E}_{\text{proto } \mathcal{N}}\}$ .

When the types of connections  $\mathcal{E}_{\text{proto }\mathcal{N}}$  between any two connected units is known, we start with a CG that is fully connected as  $\mathcal{E}_{\text{proto }\mathcal{N}}$  for every pairwise combination of units. Search proceeds by deleting  $\mathcal{E}_{ij}$  between two units i and j that yields the best improvement in the PBIC on each iteration (Alg. 3). When the social network  $\mathcal{N}$  is known, we start with a CG where pairs of units in  $\mathcal{N}$  are fully connected in network ties. Search proceeds by deleting all homologs of the type of edge in  $\mathcal{E}_{\text{proto }\mathcal{N}}$  that yields the best improvement in the PBIC on each iteration (Alg. 4). Finally, when there is no background knowledge, homogenous search (Alg. 5) can be performed by chaining the operations of Alg. 3 and Alg. 4 (or vice versa) on the CG complete in network ties for every pairwise combination of units.

Clearly we could use the heterogenous procedure even if

Algorithm 4 HOMOGENOUS( $\mathcal{G}^{\text{complete}}, \mathbf{D}, \mathcal{N}$ )

- 1:  $\mathcal{G}^* \leftarrow$  graph obtained by removing all edges between units *i*, *j* in  $\mathcal{G}^{\text{complete}}$  when  $(i, j) \notin \mathcal{N}$
- 2: score change  $\leftarrow$  True
- 3: while score change do
- score change  $\leftarrow$  False 4:
- 5:
- $\begin{array}{l} \mathcal{E}_{\text{proto }\mathcal{N}}^{*} \leftarrow \text{prototypes of network ties in } \mathcal{G}^{*} \\ E_{max} \leftarrow \operatorname{argmax}_{E \in \mathcal{E}_{\text{proto }\mathcal{N}}} \text{PBIC}(\mathbf{D}; \mathcal{G}^{*} \setminus h(E)) \end{array}$ 6:
- if  $\operatorname{PBIC}(\mathbf{D}; \mathcal{G}^* \setminus h(E_{max}) > \operatorname{PBIC}(\mathbf{D}; \mathcal{G}^*)$  then 7:
- $\mathcal{G}^* \leftarrow \mathcal{G}^* \setminus h(E_{max})$ 8:
- 9: score change  $\leftarrow$  True
- 10: return  $\mathcal{E}^*_{\text{proto }\mathcal{N}}$

Algorithm 5 HOMOGENOUS( $\mathcal{G}^{\text{complete}}, \mathbf{D}$ )

- 1:  $\mathcal{E}_{\text{proto }\mathcal{N}} \leftarrow \text{prototypes of network ties in } \mathcal{G}^{\text{complete}}$
- 2:  $\mathcal{N}^* \leftarrow \text{HOMOGENOUS}(\mathcal{G}^{\text{complete}}, \mathbf{D}, \mathcal{E}_{\text{proto } \mathcal{N}})$
- 3:  $\mathcal{E}_{\text{proto }\mathcal{N}}^* \leftarrow \text{HOMOGENOUS}(\mathcal{G}^{\text{complete}}, \mathbf{D}, \mathcal{N}^*)$
- 4: return  $\mathcal{N}^*$ ,  $\mathcal{E}^*_{\text{proto }\mathcal{N}}$

the true underlying network ties are homogenous, since it is most general. However, intuitively we expect the homogenous procedures to fare better in a finite data setting, because the homogeneity assumption allows pooling data from samples across units for each edge deletion test. This intuition is confirmed in our simulations.

#### 4.4 Size of the Search Space

In the heterogenous case, the search space grows as  $O(|\mathcal{E}_{\text{proto }\mathcal{N}}|\binom{m}{2})$  i.e., as a function of the number of possible edges between two units i and j multiplied by the number of possible pairings on m units. Under homogeneity when  $\mathcal{E}_{\text{proto }\mathcal{N}}$  is known, this reduces to  $O(\binom{m}{2})$ ; when  $\mathcal{N}$  is known, it reduces to  $O(|\mathcal{E}_{\text{proto }\mathcal{N}}|)$ ; and under homogeneity where neither is available, it is  $O(\binom{m}{2}) + O(|\mathcal{E}_{\text{proto }\mathcal{N}}|).$ 

## 4.5 Consistency of Network Search

**Lemma 3.** If the generating distribution is Markov to a CG satisfying tier symmetry and the causal ordering assumption, then the search space of GREEDY NET-WORK SEARCH consists of graphs belonging to their own equivalence classes of size 1.

**Theorem 1.** If the generating distribution is in the exponential family (with compact natural parameter space  $\Theta$ ) and is Markov and faithful to a CG satisfying tier symmetry and causal ordering, then GREEDY NETWORK SEARCH is consistent.

Under the same assumptions in the theorem above, we

have the following corollary results.

**Corollary 1.1.** *The* HETEROGENOUS *procedure is consistent.* 

**Corollary 1.2.** When the true network ties are homogenous, the HOMOGENOUS procedure is consistent.

# **5 EXPERIMENTS**

We evaluate the performance of our proposed algorithms on networks of varying size, for various block sizes, and for different regularity settings. (Regularity refers to the number of neighbors for each unit *i* in the dependency network  $\mathcal{N}$ . This setting thus controls the density of the graph.) We consider blocks of size 4, 8, 16, and 32, with regularity 2 or 3. The ground truth models are homogenous and of the form shown in Figures 2 and 3, where we display the case of block size 4. Data is generated from each network via a Gibbs sampler with a burn-in period of 1000 iterations and thinning every 100 iterations using the following equations:

$$p(L_i = 1) = \operatorname{expit}(\tau_1),$$

$$p(A_i = 1|L_i, \{A_j : j \in \operatorname{nb}_{\mathcal{N}}(i)\}) =$$

$$\operatorname{expit}(\beta_1 L_i + \beta_2 \sum_{j \in \operatorname{nb}_{\mathcal{N}}(i)} A_j),$$

$$p(Y_i = 1|L_i, A_i, \{A_j : j \in \operatorname{nb}_{\mathcal{N}}(i)\}) =$$

$$\operatorname{expit}(\nu_1 L_i + \nu_2 A_i + \nu_3 \sum_{j \in \operatorname{nb}_{\mathcal{N}}(i)} A_j),$$

where  $\exp(x) = (1 + \exp(-x))^{-1}$ . We emphasize that some of these networks are quite large; for example, the network with block size 32 and 2000 iid blocks has an effective size of 64,000 individuals. For each network setting we run 100 bootstraps of structure learning in order to get an average estimate of precision and recall as shown in Figure 4. However, to spare computation time, we use only Algorithm 3 on the latter two block settings. An interesting feature of the results in Figure 4, which matches our earlier intuition, is the faster convergence of the homogenous procedures to the true model – which we attribute to the parameter sharing (effectively using of more data when testing each edge deletion).

In order to demonstrate the utility of learning the structure in dealing with network uncertainty, we consider the population average overall effect (3). We first execute structure learning, and then estimate the PAOE, contrasting a treatment assignment determined with probability 0.7 with the naturally observed probability. We do this for 2-regular networks with 2000 realizations of iid blocks of varying size. We use the heterogenous procedure and one of the homogenous procedures (Alg. 3) to learn the structure of the networks. Estimation of the causal effect is done by the auto-g-computation algorithm described in [39] and the Supplement. We perform a 1000 bootstraps of both structure learning and effect estimation to compare the bias and variance of the estimates from the learned graphs to the estimates provided by utilizing the maximally uninformative complete graph. Unfortunately the auto-g-computation procedure is also computationally intensive because it requires Gibbs sampling. Again, to spare computation time we do not run the heterogenous procedure on the larger graphs with block sizes 16 and 32 (networks with 32,000 and 64,000 individuals). We also only perform 8 bootstraps for these larger networks. In order to emphasize the need to deal with interference and network uncertainty appropriately, we additionally estimated the bias for 200 bootstraps of the network with blocks of size 8 using the empty graph (a complete iid assumption), and an incorrect graph where  $\mathcal{N}$  is shuffled randomly to have incorrect adjacencies. In both cases the bias turned out to be approximately .06, an order of magnitude higher than the bias from utilizing the complete or learned graphs.



Figure 2: The 2-regular CG for a block of size 4



Figure 3: The 3-regular CG for a block of size 4

From Table 1 we see that causal effect estimates based on learned structure have the same or lower bias as com-

Block Size	Complete	Homogenous	Heterogenous
4	.009, 9.2e-5	.008, 8.1e-5	.009, 9.7e-5
8	.007, 6.6e-5	.006, 4.1e-5	.006, 4.5e-5
16	.006, 3.8e-5	.005, 1.9e-5	х
32	.007, 6.1e-5	.002, 7.6e-6	Х

Table 1: Bias and variance for estimating the PAOE.



Figure 4: Performance of structure learning algorithms as measured by precision and recall

pared with using the complete graph. Furthermore, the sparsity of the learned graph reduces variance of the estimates in most cases. This reduction in bias and variance is more easily achieved when we are able to exploit homogeneity in the network structure. In experiments with lower sample sizes, we see that the bias of effect estimates may increase (because the learning procedure may fail to recover the true graph) but that the variance of the estimates remains comparable to or lower than the estimates based on the complete graph.

## 6 CONCLUSION

We have developed a method for estimating causal effects under unit dependence induced by a network represented by a chain graph (CG) model [16], when there is uncertainty about network structure. Instead of estimating causal effects given a completely uninformative network where each pair of units is connected, as is typically done in the interference literature [40, 41], we estimated causal effects given a sparser network learned via a score-based model selection method based on the pseudolikelihood function [2]. We showed that this strategy can yield lower variance in estimates without sacrificing bias, if the underlying true network structure is recovered accurately. Our model selection method re-

lied on weak parametric assumptions, specifically that all Markov factors in the CG model corresponded to conditional Markov random fields in the exponential family. The approach here is a generalization of local score-based search algorithms for directed acyclic graph (DAG) models [4] to CG models. As a price of this generalization, our local search algorithms recompute a potentially larger part of the model score with every move through the model space. In addition, our approach only works for settings with partial interference, where units within a block exhibit dependence, but data on blocks is iid. The restriction to blocks of identical size may be relaxed by combining our heterogeneous procedure with a scheme of parameter sharing and hierarchical modeling across blocks that are of different sizes. In future work, we aim to extend our methods to full interference settings.

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# **Supplementary Material**

# CAUSAL CHAIN GRAPHS AND THEIR INTERPRETATION

Causal models associated with DAGs may be generalized to causal models associated with CGs. CGs may include directed edges, representing direct causation, and undirected edges, representing symmetric relationships between units in a network. A causal interpretation of CGs, understood as equilibria of dynamic models with feedback, was given in [17]. Under this interpretation, the distribution  $p(\mathbf{B} \mid pa_{\mathcal{G}}(\mathbf{B}))$  for each block  $\mathbf{B} \in \mathcal{B}(\mathcal{G})$  can be determined by a Gibbs sampler on the variables  $B \in \mathbf{B}$ . Here, each conditional distribution  $p(B \mid \mathbf{B} \setminus B, \mathrm{pa}_{\mathcal{G}}(\mathbf{B}))$  is produced by structural equations of the form  $f_B(\mathbf{B} \setminus B, \mathrm{pa}_G(\mathbf{B}), \epsilon_B)$ . Interventions on elements of **B** are defined by replacing the appropriate line in the Gibbs sampler program. For all disjoint sets Y and A, [17] showed that  $p(\mathbf{Y} \mid do(\mathbf{a}))$  is identified by a CG version of the g-formula (2).

If only interventions on entire blocks are of interest, i.e., we consider only treatment assignments **A** such that if  $\mathbf{B} \cap \mathbf{A} \neq \emptyset$  then  $\mathbf{B} \subseteq \mathbf{A}$ , then an alternative causal interpretation of a CG  $\mathcal{G}$  that does not rely on the Gibbs sampler machinery of [17] exists. Specifically, in such a case we consider a causal DAG model where each block **B** corresponds to a supervariable  $V_{\mathbf{B}}$  defined as a Cartesian product of variables in **B**, and a DAG causal model is defined on  $V_{\mathbf{B}}(\mathbf{A})$ , where **A** are values assigned to parents of  $V_{\mathbf{B}}$ .

If, for each block **B** in a CG  $\mathcal{G}$ , the graph  $(\mathcal{G}_{\mathrm{bd}_{\mathcal{G}}(\mathbf{B})})^a$  has a single clique, then this yields a classical causal model of a DAG, defined on  $\{V_{\mathbf{B}} | \mathbf{B} \in \mathcal{B}(\mathcal{G})\}$ . If not, we can still view the model as a classical causal model of a DAG, but with an extra restriction that the observed data distribution factorizes as (1). See also [23] for a perspective on interpreting chain graphs in an interference setting.

The model selection methodology introduced here does not depend on which causal interpretation for chain graphs one may choose, and all causal models described above lead to interventional distributions being identified by (2).

# **CONDITIONAL MRFs**

A CG model can be viewed as a set of conditional MRFs. A conditional MRF corresponds to a graph whose vertices can be partitioned into two disjoint sets: **W**, corresponding to non-random variables whose values are fixed; and **V**, corresponding to random variables. The only edges allowed in a conditional MRF are directed edges  $W \rightarrow V$  and undirected edges V - V'

for  $W \in \mathbf{W}$  and  $V, V' \in \mathbf{V}$ . A statistical model associated with a conditional MRF  $\mathcal{G}$  is a set of densities that factorize as:

$$p(\mathbf{V} \mid \mathbf{W}) = \frac{\prod_{\{\mathbf{C} \in \mathcal{C}((\mathcal{G}_{\mathrm{bd}_{\mathcal{G}}}(\mathbf{v}))^a): \mathbf{C} \not\subseteq \mathbf{W}\}} \phi_{\mathbf{C}}(\mathbf{C})}{Z(\mathbf{W})}$$

It is easy to see that the above factorization is analogous to the second level of CG factorization found in (1) where V is a block, and W are its parents.

# THE AUTO-G-COMPUTATION ALGORITHM

The auto-g-computation algorithm, introduced in [39], may be viewed as a generalization of the Monte Carlo sampling version of the g-computation algorithm for classical causal models (represented by DAGs) [42] to causal models of the sort we consider here, represented by CGs. We describe a version of this algorithm based on the pseudolikelihood estimator. An alternative based on the coding estimator [2] is less efficient, but leads to asymptotically normal estimators of the population average overall effect (PAOE).

Auto-g-computation generates samples from either the observed data distribution that factorizes as (1) according to a CG, or of functions of these distributions, such as counterfactual expectations identified using (4).

This is done by imposing a topological ordering on blocks in a CG, and generating samples for each block sequentially using Gibbs sampling. The parameters for Gibbs factors used in the sampler (which by the global Markov property for CGs take the form of  $p(X_i|X_{\mathrm{bd}_{\mathcal{G}}(X_i)})$ ) are learned via maximizing the pseudolikelihood function. For any block **X**, the Gibbs sampler draws samples from  $p(\mathbf{X} \mid \mathrm{bd}_{\mathcal{G}}(\mathbf{X}))$ , given a fixed set of samples drawn from all blocks with elements in  $\mathrm{pa}_{\mathcal{G}}(\mathbf{X})$  as follows:

Gibbs Sampler for X:

for 
$$t = 0$$
, let  $\mathbf{x}^{(0)}$  denote initial values ;  
for  $t = 1, ..., T$   
draw value of  $X_1^{(t)}$  from  $p(X_1 | \mathbf{x}_{\mathrm{bd}\mathcal{G}(X_1)}^{(t-1)}))$ ;  
draw value of  $X_2^{(t)}$  from  $p(X_2 | \mathbf{x}_{\mathrm{bd}\mathcal{G}(X_2)}^{(t-1)}))$ ;  
:  
draw value of  $X_m^{(t)}$  from  $p(X_m | \mathbf{x}_{\mathrm{bd}\mathcal{G}(X_m)}^{(t-1)}))$ ;

This method may be used to estimate the counterfactual expectation in (4) as follows. We first generate a set of samples  $\mathbf{L}^{(t)}$ , t = 1, ..., T. Then we generate a sample **A** directly using some  $\pi_i(\mathbf{A})$ , i = 1, 2. Finally, we use the above samples to generate a set of samples  $\mathbf{Y}^{(t)}$ , t = 1, ..., T using Gibbs factors  $p(Y_i | \mathbf{A}_{\mathbf{A} \cap \mathrm{bd}_{\mathcal{G}}}(Y_i), \mathrm{bd}_{\mathcal{G}}(Y_i) \setminus \mathbf{A})$ . Finally, we estimate

$$\frac{1}{m} \sum_{i=1}^{m} \mathbb{E}[Y_i(\mathbf{A})] = \frac{1}{m \cdot T} \sum_{i=1}^{m} \sum_{t=1}^{T} Y_i^{(t)}.$$

It is not difficult to show, (see [39] for details), that rerunning this procedure with different draws **A** from either  $\pi_1(\mathbf{A})$  or  $\pi_2(\mathbf{A})$ , and taking the difference of the resulting averages yields a valid estimate of the PAOE.

Fitting parameters of Gibbs factors using the pseudolikelihood function avoids the usual difficulties CGs inherit from Markov random fields, specifically, the intractability of the likelihood function due to the presence of normalizing functions. In addition, if the learned block structure is sparse, while the number of independent samples considered is small, this approach allows one to impose parameter sharing among Gibbs factors, which leads to reasonable estimates even in small samples. Taken to the extreme, this approach allows inferences to be made even from a *single sample* of a network, as discussed in detail in [39]. In this manuscript we only consider the setting where multiple independent samples from blocks are available.

# COMPUTATIONAL COMPLEXITY OF COMPUTING SCORES OF A CHAIN GRAPH MODEL

In blocks of a CG, the number of local terms that need to be computed corresponds to the number of vertices present in cliques containing the edge of interest in the augmented subgraph of the block and its parents. A term for  $V_j$  requires an  $O(|\operatorname{bd}_{\mathcal{G}}(V_j)|)$  computation to update, which in the worst case may be exponential in the number of vertices if the graph is not sparse. In search problems, restrictions can be made on the maximum size of the boundary set, sacrificing accuracy for tractability. For a block in a CG corresponding to a conditional MRF in the exponential family, and an edge that is present in a set of cliques spanning all vertices, we will have a local set of size O(d) in the worst case, with each local term requiring an O(clique size) computation. Thus, limiting the maximum clique size may speed up the computation of each local term, but in many cases we may be unable to avoid an O(d) number of such terms. In other words, our scoring method for CG models where blocks correspond to conditional MRFs in the exponential family may not scale to very large graphs, even if such graphs are sparse. Achieving such a scaling will entail making additional assumptions, such as Gaussianity, or nonexistence of higher order interaction terms in log-linear models. We contrast this with DAG models, where the local set is of constant size regardless of parametric assumptions made.

## FORWARD-BACKWARD SEARCH

Consistency of the score was sufficient to show consistency of a backwards greedy search involving only edge deletions starting from a complete conditional MRF. [4] showed that a property called *local consistency*, which follows from decomposability and consistency of the score, is sufficient to design a consistent forwardbackward greedy search in the space of (Markov equivalent) DAGs. The forward stepwise search considers additions, rather than deletions, of single edges to improve the score, which typically produces a more sparse starting model for the subsequent backwards search.

Consider a graph  $\mathcal{G}$  and another  $\mathcal{G}'$  that differs only by the addition of an edge  $V_i - V_j$  or  $V_i \rightarrow V_j$ . A score  $S(\mathbf{D}; \mathcal{G})$  is called locally consistent if:

- 1.  $V_i \not \perp_{\mathcal{G}_0} V_j \mid \mathrm{bd}_{\mathcal{G}}(V_i) \text{ or } V_j \not \perp_{\mathcal{G}_0} V_i \mid \mathrm{bd}_{\mathcal{G}}(V_j)$ then  $\lim_{n \to \infty} P(S(\mathbf{D}; \mathcal{G}') > S(\mathbf{D}; \mathcal{G})) \to 1$
- 2.  $V_i \perp \!\!\!\!\perp_{\mathcal{G}_0} V_j \mid \mathrm{bd}_{\mathcal{G}'}(V_i)$  and  $V_j \perp \!\!\!\!\perp_{\mathcal{G}_0} V_i \mid \mathrm{bd}_{\mathcal{G}}(V_j)$ then  $\lim_{n \to \infty} P(S(\mathbf{D}; \mathcal{G}') < S(\mathbf{D}; \mathcal{G})) \to 1$

Such a property requires a stronger notion of decomposability than is available in our general setting. In Section 4.2 we mention that if our model is an MRF that is multivariate normal, or corresponds to a log linear discrete model with only main effects and pairwise interactions, then it suffices to consider the following terms derived from the local set:  $\{s(V_i, bd_{\mathcal{G}}(V_i)), s(V_i, bd_{\mathcal{G}}(V_i))\}$  for an edge  $V_i - V_j$ , and  $\{s(V_j, bd_{\mathcal{G}}(V_j))\}$  for an edge  $V_i \to V_i$  (dropping implicit **D** and  $\mathcal{G}$  for brevity). This is the strong notion of decomposability we need for local consistency. Thus, in such settings one can follow the work in [4] to show that PBIC will be locally consistent and design a search procedure involving a forward phase followed by a backward phase. The advantage of such a procedure is that it is more scalable, even more so when the underlying true model is sparse.

## PROOFS

Let  $\mathcal{M}_0$  denote the true model and  $\mathcal{M}_1$ ,  $\mathcal{M}_2$  two candidate models. A scoring criterion  $S(\mathbf{D}; \mathcal{M})$  is said to be consistent if:

$$\lim_{n \to \infty} P_n(S(\mathbf{D}; \mathcal{M}_1) < S(\mathbf{D}; \mathcal{M}_2)) \to 1 \text{ when}$$
$$\mathcal{M}_1 \not\supseteq \mathcal{M}_0 \text{ and } \mathcal{M}_2 \supseteq \mathcal{M}_0 \text{ or } \qquad (*)$$

$$\mathcal{M}_1, \mathcal{M}_2 \supseteq \mathcal{M}_0 \text{ and } k_1 > k_2.$$
 (\*\*)

**Lemma 1** With dimension fixed and sample size increasing to infinity, the PBIC is a consistent score for curved exponential families whose natural parameter space  $\Theta$  forms a compact set.

*Proof.* To prove consistency we need to show that,

$$\lim_{n \to \infty} P_n(PBIC(\mathbf{D}; \mathcal{M}_1) < PBIC(\mathbf{D}; \mathcal{M}_2)) \to 1$$
(5)

when (\*) or (\*\*).

Note in all following steps, we assume **D** to be implicit in the calculation of the likelihoods and pseudolikelihoods.

To prove (5) holds under the scenario (\*), it is sufficient to show that the following is true for some  $\epsilon > 0$ 

$$\frac{1}{n}(\ln \mathcal{PL}_n(\hat{\theta}_2) - \ln \mathcal{PL}_n(\hat{\theta}_1)) > \epsilon$$
(6)

It was shown in [8] that for any  $\mathcal{M}_1$  outside of a neighbourhood N of  $\theta_0$ , and  $\mathcal{M}_2$  containing this neighbourhood, we can pick a  $\delta > 0$  such that:

$$\frac{1}{n}(\ln \mathcal{L}_n(\hat{\theta}_2) - \ln \mathcal{L}_n(\hat{\theta}_1)) > \delta$$
(7)

In order to extend this result to (6), we invoke a result from [22] stating that

$$\mathcal{PL}_n(\theta) \ge d\mathcal{L}_n(\theta) + \sum_{i=1}^d H_i(\widetilde{P}_n)$$
 (8)

where d is the dimensionality of the data, and  $H_i(\tilde{P}_n)$  is the Shannon entropy of the empirical distribution. It then follows that (6) holds when (7) is true.

Showing that (5) holds under the scenario (\*\*) is equivalent to showing that the following difference is  $O_p(1/n)$ :

$$\frac{1}{n} \left| \ln \mathcal{PL}_n(\hat{\theta}_1) - \ln \mathcal{PL}_n(\hat{\theta}_2) \right| \tag{9}$$

Consider the difference between the full log-likelihoods:

$$\frac{1}{n} |\ln \mathcal{L}_n(\hat{\theta}_1) - \ln \mathcal{L}_n(\hat{\theta}_2)|.$$
(10)

We first closely follow the proof in [8] to show that the quantity in (10) is  $O_p(1/n)$ . Consider data drawn from a curved exponential family density  $p(\mathbf{X}; \theta) = h(\mathbf{X})\exp(\theta T(\mathbf{X}) - Z(\theta))$ , where  $\theta \in \mathbb{R}^k$  is a set of canonical parameters in the natural parameter space  $\Theta$ ,  $T(\mathbf{X})$  is a set of sufficient statistics, and  $Z(\theta)$  is a normalizing function. For a particular choice of a model  $\mathcal{M}$  in this setting, the BIC can be written as  $\ln \mathcal{L}_n(\mathbf{D}; \hat{\theta}) - \frac{k}{2}\ln(n)$  or equivalently,

$$\sup_{\theta \in \mathcal{M} \cap \Theta} \sum_{i=1}^{n} \theta T(\mathbf{X}_i) - Z(\theta) - \frac{k}{2} \ln(n), \qquad (11)$$

Note that for simplicity of notation and without loss of generality, we set  $h(\mathbf{X}) = 1$ . Now consider  $\mathbf{T}_n = \frac{1}{n} \sum_{i=1}^{n} T(\mathbf{X}_i)$ , the sample average of the sufficient statistics. We can then express (11) as

$$n \sup_{\theta \in \mathcal{M} \cap \Theta} \theta \mathbf{T}_n - Z(\theta) - \frac{k}{2} \ln(n).$$
 (12)

Define the quantities  $S_{n,i}$  and  $U_n$  as,

$$S_{n,i} \equiv \sup_{\theta_i \in \mathcal{M}_i \cap \Theta} \theta_i \mathbf{T}_n - Z(\theta_i) = \theta_{n,i} \mathbf{T}_n - Z(\theta_{n,i}),$$
$$U_n \equiv \theta_0 \mathbf{T}_n - Z(\theta_0),$$

where  $\hat{\theta}_{n,i}$  is the MLE. We now show that  $S_{n,i} - U_n$  and by extension each term in (10) is  $O_p(1/n)$ . Since  $\theta_0$  lies in both model spaces under scenario (\*\*),

$$S_{n,i} - U_n = (\hat{\theta}_{n,i} - \theta_0) \mathbf{T}_n - Z(\hat{\theta}_{n,i}) + Z(\theta_0) \ge 0.$$
(13)

Considering the Taylor expansion of Z about  $\theta_0$ , we have that  $Z(\hat{\theta}_{n,i}) - Z(\theta_0) = (\hat{\theta}_{n,i} - \theta_0)\nabla Z(\theta_0) + O_p(1/n)$ , where the  $O_p(1/n)$  term comes from the efficiency of MLE [11]. Plugging this into (13) we get,

$$S_{n,i} - U_n = (\mathbf{T}_n - \nabla Z(\theta_0))(\hat{\theta}_{n,i} - \theta_0) + O_p(1/n).$$
 (14)

By the Central Limit Theorem,  $\mathbf{T}_n - \nabla Z(\theta_0)$  is  $O_p(1/\sqrt{n})$  and by the efficiency of MLE,  $\hat{\theta}_{n,i} - \theta_0$  is also  $O_p(1/\sqrt{n})$ . Thus,  $S_{n,i} - U_n$  is  $O_p(1/n)$ , and we have our result.

In order to extend this result to (9), we once again invoke the result from [22] that

$$\mathcal{PL}_n(\theta) \ge d\mathcal{L}_n(\theta) + \sum_{i=1}^d H_i(\widetilde{P}_n)$$
 (15)

where  $H_i(\tilde{P}_n)$  is the Shannon entropy of the empirical distribution. We see that as long  $d \ll n$  (which in our setting we assume to be true), (10) being  $O_p(1/n)$  implies that (9) is as well.

**Lemma 2** Let  $\mathcal{G}$  and  $\mathcal{G}'$  be graphs which differ by a single edge between  $V_i$  and  $V_j$ . For conditional MRFs in the exponential family, the local score difference between  $\mathcal{G}$  and  $\mathcal{G}'$  is given by:  $\sum_{V \in \text{loc}(V_i, V_j; \mathcal{G}) \cap \mathbf{B}_{\text{loc}}} \{s_V(\mathbf{D}; \mathcal{G}) - s_V(\mathbf{D}; \mathcal{G}')\}$ , where  $s_V(.)$  denotes the component of the score for V.

*Proof.* A conditional MRF corresponding to  $p(\mathbf{B} | pa_{\mathcal{G}}(\mathbf{B}))$  for a block **B** in a CG  $\mathcal{G}$  in the (conditional) exponential family has a probability distribution of the general form:

$$p(\mathbf{B} \mid \mathrm{pa}_{\mathcal{G}}(\mathbf{B}); \psi) =$$
(16)  
$$\exp\left(\sum_{\{\mathbf{C} \in \mathcal{C}((\mathcal{G}_{\mathrm{bd}_{\mathcal{G}}(\mathbf{B})})^{\alpha}): \mathbf{C} \not\subseteq \mathrm{pa}_{\mathcal{G}}(\mathbf{B})\}} \psi_{\mathbf{C}} T(\mathbf{C}) - Z(\psi, \mathrm{pa}_{\mathcal{G}}(\mathbf{B}))\right)$$

where

$$\left\{\psi_{\mathbf{C}}: \mathbf{C} \in \mathcal{C}((\mathcal{G}_{\mathrm{bd}_{\mathcal{G}}(\mathbf{B})})^{a}), \mathbf{C} \not\subseteq \mathrm{pa}_{\mathcal{G}}(\mathbf{B})
ight\}$$

is a set of canonical parameters associated with potential functions  $\phi_{\rm C}$  in the CG factorization,

$$\{T(\mathbf{C}): \mathbf{C} \in \mathcal{C}((\mathcal{G}_{\mathrm{bd}_{\mathcal{G}}(\mathbf{B})})^{a}), \mathbf{C} \not\subseteq \mathrm{pa}_{\mathcal{G}}(\mathbf{B})\}$$

is a set of sufficient statistics for  $\psi_{\mathbf{C}}$ , and  $Z(\theta, \operatorname{pa}_{\mathcal{G}}(\mathbf{B}))$  is a normalizing function.

Assume V is in a clique C that contains the edge  $V_i - V_j$ in  $\mathcal{G}$ , and let  $\mathcal{G}^-$  be the edge subgraph of  $\mathcal{G}$  with that edge removed. Then  $p(V \mid \mathrm{bd}_{\mathcal{G}}(V))$  will only be a function of clique parameters  $\psi_{\mathbf{S}}$ , where  $\mathbf{S} \subseteq \mathcal{C}((\mathcal{G}_{\mathrm{bd}_{\mathcal{G}}(\mathbf{B})})^a) : \mathbf{C} \not\subseteq$  $\mathrm{pa}_{\mathcal{G}}(\mathbf{B})$  and  $V \in \mathbf{S}$ . All others terms in the factorization cancel by definition of conditioning. As a consequence,  $p(V \mid \mathrm{bd}_{\mathcal{G}}(V))$  will be a function of  $\psi_{\mathbf{C}}$ .

However, after  $V_i - V_j$  is removed, **C** will no longer be a clique in  $\mathcal{G}^-$ , by definition, but will instead decompose into two cliques, say  $\mathbf{C}_1$  and  $\mathbf{C}_2$ . By following the above reasoning,  $p(V \mid \mathrm{bd}_{\mathcal{G}^-}(V))$  will be a function of all clique parameters { $\psi_{\mathbf{S}} : \mathbf{S} \subseteq \mathcal{C}((\mathcal{G}_{\mathrm{bd}_{\mathcal{G}}}(\mathbf{B}))^a), \mathbf{C} \not\subseteq$  $\mathrm{pa}_{\mathcal{G}}(\mathbf{B}), V \in \mathbf{S}$ }, which will include  $\psi_{\mathbf{C}_1}$  and  $\psi_{\mathbf{C}_2}$ . Since the parameterization for  $p(V \mid \mathrm{bd}_{\mathcal{G}^-}(V))$  is thus different in models for  $\mathcal{G}$  and  $\mathcal{G}^-$ , the contribution to the score associated with this term will also be different.

Assume V is not in a clique that contains the edge  $V_i - V_j$ in  $\mathcal{G}$ , and let  $\mathcal{G}^-$  be the edge subgraph of  $\mathcal{G}$  with that edge removed, as before. Then  $p(V \mid \mathrm{bd}_{\mathcal{G}}(V))$  will only be a function of clique parameters  $\psi_{\mathbf{S}}$ , where **S** contains V, all others will cancel by definition of conditioning.

Note that since no such **S** contains the edge  $V_i - V_j$  in  $\mathcal{G}$ , the set of cliques **S** in  $\mathcal{G}$  is the same as the set of cliques **S** in  $\mathcal{G}^-$ . Moreover, since  $\mathcal{G}^-$  is an edge subgraph of  $\mathcal{G}$ , no new cliques are introduced. As a result,  $p(V | \operatorname{bd}_{\mathcal{G}^-}(V))$  will be parameterized by the same set of  $\psi_{\mathbf{S}}$  in the model for  $\mathcal{G}^-$  as it was in the model for  $\mathcal{G}$ .

Our conclusion then follows because, by properties of the exponential family, the sufficient statistics for a clique parameter  $\psi_{\mathbf{S}}$  are functions of only **S**. Since draws from  $p(\mathbf{S})$  are fixed, the estimates for  $\psi_{\mathbf{S}}$  will coincide if the data is evaluated under the model for  $\mathcal{G}$ , and the model for  $\mathcal{G}^-$ . Furthermore, the number of parameters in  $p(V \mid \mathrm{bd}_{\mathcal{G}}(V))$  and  $p(V \mid \mathrm{bd}_{\mathcal{G}^-}(V))$  is the same. This implies the score contribution for  $p(V \mid \mathrm{bd}_{\mathcal{G}^-}(V))$  in  $\mathcal{G}$  will equal the score contribution of  $p(V \mid \mathrm{bd}_{\mathcal{G}^-}(V))$ in  $\mathcal{G}^-$ . The only terms remaining in the score difference between  $\mathcal{G}$  and  $\mathcal{G}'$  are then local scores for  $V \in$  $\mathrm{loc}(V_i, V_j; \mathcal{G})$ .

This implies the conclusion. 
$$\Box$$

**Lemma 3** If the generating distribution is Markov to a CG satisfying tier symmetry and the causal ordering assumption, then the search space of GREEDY NET-WORK SEARCH consists of graphs belonging to their own equivalence classes of size 1.

*Proof.* Under the restrictions listed above, the only changes allowed are edge deletions or additions of the form  $L_i - L_j$ ,  $A_i - A_j$ ,  $Y_i - Y_j$ ,  $L_i \rightarrow A_j$ ,  $L_i \rightarrow Y_j$ ,  $A_i \rightarrow Y_j$ .

Consider an edge deletion  $V_i - V_j$  in  $\mathcal{G}$ , giving rise to a graph  $\mathcal{G}'$ . Notice that boundaries of  $V_i$  and  $V_j$  have changed. Thus by the local Markov property on chain graphs,  $\mathcal{G}$  and  $\mathcal{G}'$  must imply different conditional independences. Concretely,  $\mathcal{G}$  implies:

$$V_i \perp \!\!\!\!\perp \mathbf{V} \setminus \operatorname{cl}_{\mathcal{G}}(V_i) \mid \operatorname{bd}_{\mathcal{G}}(V_i)$$
$$V_j \perp \!\!\!\!\perp \mathbf{V} \setminus \operatorname{cl}_{\mathcal{G}}(V_j) \mid \operatorname{bd}_{\mathcal{G}}(V_j)$$

while G' implies:

$$V_i \perp\!\!\!\!\perp \mathbf{V} \setminus (\operatorname{cl}_{\mathcal{G}}(V_i) \setminus V_j) \mid \operatorname{bd}_{\mathcal{G}}(V_i) \setminus V_j$$
$$V_j \perp\!\!\!\!\perp \mathbf{V} \setminus (\operatorname{cl}_{\mathcal{G}}(V_j) \setminus V_i) \mid \operatorname{bd}_{\mathcal{G}}(V_j) \setminus V_i$$

We can similarly show that an edge deletion  $V_i \rightarrow V_j$ also implies different conditional independences in  $\mathcal{G}$  and  $\mathcal{G}'$ . Thus, in general, an edge deletion or addition in our search space gives rise to graphs that are not Markov equivalent and hence, reside in their own equivalence classes of size 1.

**Theorem 1** If the generating distribution is in the exponential family (with compact natural parameter space  $\Theta$ )

and is Markov and faithful to a CG satisfying tier symmetry and causal ordering, then GREEDY NETWORK SEARCH is consistent.

*Proof.* The algorithm begins with a complete conditional MRF that contains the true underlying distribution. We are guaranteed that the truth is contained in every state through the entirety of the algorithm by the following argument. Consider the first edge deletion performed by GNS to a conditional MRF that does not contain the true model. It follows from consistency of the PBIC that any such deletion would decrease the score. Choosing such an edge deletion would contradict the greediness of the algorithm.

Now assume the algorithm stops at a sub optimal conditional MRF  $\mathcal{G}$  that contains the truth but has more parameters than the true model  $\mathcal{G}^*$ . We know there exists a series of single edge deletions in  $\mathcal{E}_N$  that takes us from  $\mathcal{G}$  to  $\mathcal{G}^*$ . By Lemma 3, each of these edge deletions yield graphs in separate equivalence classes. It follows then from the consistency of the PBIC that each of these edge deletions strictly increases the score (each edge deletion yields a smaller model containing the truth) and thus, a local optimum found by greedily maximizing the PBIC corresponds to finding the global optimum  $\mathcal{G}^*$ .

**Corollary 1.1** *The* HETEROGENOUS *procedure is consistent.* 

*Proof.* By consistency of GNS, each conditional MRF returned for  $\mathbf{L}$ ,  $\mathbf{A}$ , and  $\mathbf{Y}$  corresponds to the true model. The union of these will then produce the true CG on  $\mathbf{V}$ .

**Corollary 1.2** When the true network ties are homogenous, HOMOGENOUS network search is consistent.

*Proof.* Each of the homogenous procedures described above can be decomposed into a series of single edge deletions that we have shown to be consistent.  $\Box$