# Discovering Cyclic Causal Models in Psychological Research

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### 1 Introduction

A fundamental task in various disciplines of science is to understand the mechanisms, that is, causal relations underlying the phenomena of interest. In psychology, for example, one of the core questions is how psychopathology comes about, with the network theory positing that mental disorder is produced by a system of direct causal interactions between symptoms (Borsboom & Cramer, 2013). In practice, empirical researchers often aim to gain insights into these causal relations by fitting statistical network models to observational data, an approach that can be characterized as a form of causal discovery (Spirtes, Glymour, Scheines, & Heckerman, 2000). However, it has been shown that network models are likely to perform poorly as causal discovery tools; relations in the network may not reflect the direct causal effects that researchers aim to discover, but can instead be produced by unwittingly conditioning on common effects or by failing to account for unobserved confounders (Dablander & Hinne, 2019; Ryan, Bringmann, & Schuurman, 2022).

In the field of causal discovery, using statistical independencies estimated from observational data to infer causal structures is known as *constraint-based* causal discovery (Spirtes & Glymour, 1991). Ryan et al. (2022) suggest that network models could be replaced by purposebuilt constraint-based causal discovery methods. However, the most popular and well-studied constraint-based methods assume that causal relationships are *acyclic*; if X causes Y, then Y does not cause X (Glymour, Zhang, & Spirtes, 2019). This is problematic since *cyclic* relationships

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or *feedback loops* are critical to the theoretical understanding of psychopathology (Borsboom, 2017). For example, Wittenborn, Rahmandad, Rick, and Hosseinichimeh (2016) suggest that several different causal feedback loops, such as *perceived stress* → *negative affect* → *rumination* → *perceived stress* play a key role in sustaining depression. Such theoretical expectations necessitate the use of *cyclic causal discovery* methods. Although some cyclic causal discovery algorithms have been developed (Mooij & Claassen, 2020), they have not been as well studied as their acyclic counterparts, which is in part due to practical difficulties in fitting and interpreting cyclic causal models. To our knowledge, little to no research has been done on the applicability of cyclic causal discovery methods in psychology, and much remains unknown about the performance of these methods. Therefore, in this paper, we aim to address the following question: how well do cyclic causal discovery methods perform in typical psychological research contexts? The goal of this study is twofold. First, we provide an accessible overview of different cyclic causal discovery methods. Second, we investigate how well each of these methods works by means of a simulation study.

# 2 Background

In this section, we introduce the basic concepts of graphical models, which are necessary to understand the causal discovery methods that we will study in the remainder of this paper.

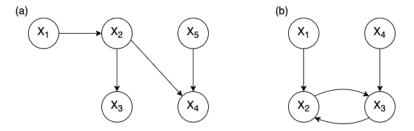
### 2.1 Graphical Models

A graph ( $\mathcal{G}$ ) is a diagram made up of a set of vertices ( $\mathcal{V}$ ) and edges ( $\mathcal{E}$ ), describing connections between vertices, denoted as  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ . A probabilistic graphical model uses a graph to express the conditional (in)dependencies between random variables, where the vertices represent random variables, and the edges encode conditional dependencies holding among the set of variables (Lauritzen, 1996).

In a *causal* graphical model, on the other hand, the edges describe *causal* relationships between variables; the edges are typically directed, with  $A \rightarrow B$  denoting that intervening on A results in a change in the probability distribution of B (Geiger & Pearl, 1990). Two example causal graphical models are shown in Figure 1. Figure 1a does not contain any cycles, whereas Figure 1b does, hence called a *directed acyclic graph* (DAG) and *directed cyclic graph* (DCG), respectively.

Causal graphical models also describe patterns of statistical independencies, which can be read off from the graph using Pearl's *d-separation criterion* (Geiger, Verma, & Pearl, 1990). For instance, in Figure 1a, we see a *chain* structure  $X_1 \rightarrow X_2 \rightarrow X_3$ , which implies that  $X_1$  and  $X_3$  are marginally dependent  $(X_1 \not\perp X_3)$ , but independent conditional on  $X_2$   $(X_1 \perp X_3 \mid X_2)$ . More formally, we would say  $X_1$  and  $X_3$  are *d-separated* by  $X_2$ . A *fork* structure  $X_3 \leftarrow X_2 \rightarrow X_4$  implies the same pattern of independencies;  $X_3$  and  $X_4$  are marginally dependent  $(X_3 \not\perp X_4)$ , but

Figure 1. Example causal graphical models.



Note. (a) is the example directed acyclic graph (DAG). (b) is the example directed cyclic graph (DCG).

independent conditional on  $X_2$  ( $X_3 \perp \!\!\! \perp X_4 \mid X_2$ ). That is,  $X_3$  and  $X_4$  are *d-connected* given an empty set, but *d-separated* by  $X_2$ . However, a *collider* structure  $X_2 \rightarrow X_4 \leftarrow X_5$  implies a contrasting pattern; here  $X_2$  and  $X_5$  are marginally independent ( $X_2 \perp \!\!\! \perp X_5$ ), but dependent conditional on  $X_4$  ( $X_2 \perp \!\!\! \perp X_5 \mid X_4$ ). This distinguishing characteristic of colliders is crucial when identifying the directions of causal relations, as will be shown later in section 2.4.

### 2.2 Acyclic vs. Cyclic Causal Graphs

The d-separation criterion described above applies to all acyclic graphs, but only applies to graphs with cycles under certain conditions. To understand these conditions, first we need to introduce some graph terminology. We can use kinship terminology to describe a graph structure as follows:

if 
$$\begin{cases} A \to B \\ A \leftarrow B \\ A \to \cdots \to B \text{ or } A = B \\ A \leftarrow \cdots \leftarrow B \text{ or } A = B \end{cases}$$
 in  $\mathcal{G}$  then  $A$  is a 
$$\begin{cases} \text{parent child} \\ \text{ancestor} \\ \text{descendant} \end{cases}$$
 of  $B$  and 
$$\begin{cases} A \in pa_{\mathcal{G}}(B) \\ A \in ch_{\mathcal{G}}(B) \\ A \in an_{\mathcal{G}}(B) \end{cases}$$
.

For example, in Figure 1b,  $X_1 \in pa_{\mathcal{G}} X_2$ ,  $X_2 \in ch_{\mathcal{G}} X_1$ ,  $\{X_1, X_2, X_3, X_4\} \in an_{\mathcal{G}} \text{ and } X_3$ ,  $\{X_1, X_2, X_3\} \in de_{\mathcal{G}} X_1$ . With this in place, we can define the *causal Markov* condition; a graph  $\mathcal{G}$  is *causally Markov* with respect to a joint distribution  $\mathcal{P}$  over n random variables  $(X_1, X_2, ..., X_n)$  if it satisfies the *recursive factorization* property:

$$\mathcal{P}(X_1, X_2, ..., X_n) = \prod_{i=1}^{n} \mathcal{P}(X_i \mid pa_i^{\mathcal{G}}),$$

where  $pa_i^{\mathcal{G}}$  denotes the *parents* (i.e., direct cause) of node i in a graph  $\mathcal{G}$ . This states that a variable  $X_i$  is conditionally independent of its non-descendants (i.e., non-effect variables) given its parents. It allows us to read off a set of conditional independencies from a graph  $\mathcal{G}$  such that:

$$A \perp \!\!\! \perp_{\mathcal{G}} B \mid C \Longrightarrow X_A \perp \!\!\! \perp_{\mathcal{P}} X_B \mid X_C \text{ for all subsets of } A, B, \text{ and } C,$$

where  $\perp\!\!\!\perp_{\mathcal{G}}$  represents independence relations implied by a graph  $\mathcal{G}$  and  $\perp\!\!\!\perp_{\mathcal{P}}$  represents independence relations implied by a distribution  $\mathcal{P}$ .

If causal graphs are *acyclic* (i.e., DAG), then the *causal Markov* condition holds regardless of the functional forms of causal relations and the distributions of variables involved (Lauritzen, 1996). In addition, in DAGs, the *global Markov* condition also entails the *local Markov* condition stating that a variable is independent of its non-descendants given its parents (Lauritzen, 2000). The fact that one Markov property instantly implies the other comes in handy when reading off conditional independencies from a graph.

In contrast to the acyclic case, the situation is not so straightforward in *cyclic* graphs (i.e., DCG). In DCGs, the global Markov property does not always hold. Spirtes (1994), in fact, showed that it holds for DCGs when causal relations are *linear* and error terms are *independent*. Furthermore, the local Markov property may not hold, even when the global Markov property holds. For example, in Figure 1b, the global Markov property is preserved  $(X_1 \perp \!\!\!\perp_{\mathcal{G}} X_4 \mid \{X_2, X_3\}) \Longrightarrow X_1 \perp \!\!\!\perp X_4 \mid \{X_2, X_3\})$ , but the local Markov property is violated as  $X_2 \not\perp_{\mathcal{G}} X_4 \mid X_3$  (i.e.,  $X_2$  is *not* independent of its non-descendant  $X_4$  given its parent  $X_3$ ). This is because  $X_3$  is both a parent of  $X_2$  and a collider  $(X_2 \to X_3 \leftarrow X_4)$  at the same time.

#### 2.3 Structural Causal Model (SCM)

As a distribution  $\mathcal{P}$  may not obey the global Markov property when  $\mathcal{G}$  contains cycles, there has to be additional constraints imposed on  $\mathcal{P}$  such that it satisfies the property. To do that, first, we need to get the functional form of  $\mathcal{P}$ . We will use *structural causal models* (SCM) (Pearl, 2010), also known as (non-parametric) structural equation models (Bollen & Pearl, 2013), to specify distributions of causal models. A causal mechanism of variable  $X_i$  is described in SCM by:

$$X_i = f_i \, (\, pa_i^{\mathcal{G}}, \varepsilon_i \,),$$

where  $f_i$  refers to a deterministic function depending on the parents of  $X_i$  ( $pa_i^{\mathcal{G}}$ ), and  $\varepsilon_i$  is the error term for  $X_i$ . SCM can represent any form of causal graphical models, including linear/non-linear and acyclic/cyclic relationships. For example, assuming that the graph in Figure 1b conforms to a linear SCM with independent error terms, we can illustrate their relations by the linear structural equations as follows:

$$X_1 = \varepsilon_1,$$
  
 $X_2 = \beta_{21}X_1 + \beta_{23}X_3 + \varepsilon_2,$   
 $X_3 = \beta_{34}X_4 + \beta_{32}X_2 + \varepsilon_3,$   
 $X_4 = \varepsilon_4,$ 

where  $\varepsilon$  denotes a set of jointly independent error terms and  $\beta$  denotes a 4 by 4 coefficient matrix.

Here, we limit the scope of our study to cyclic causal graphs that represent *linear* causal relationships with jointly *independent* error terms, so for which the global Markov condition is satisfied. Additionally, we make use of one more assumption, known as *faithfulness*, which is required for constraint-based causal discovery. *Faithfulness* assumption is essentially the reverse of the global Markov condition, stating that statistical independencies map onto the structure of causal graphs such that:

$$X_A \perp \!\!\!\perp X_B \mid X_C \Longrightarrow A \perp \!\!\!\perp_G B \mid C.$$

Together with the global Markov property, faithfulness enables us to make inferences about causal relationships represented in graphs by testing for statistical independence among variables (Bongers, Forré, Peters, & Mooij, 2021).

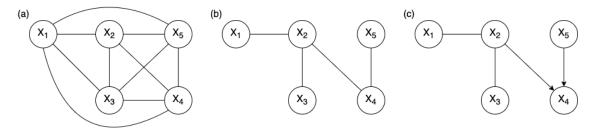
### 2.4 A Primer on Constraint-Based Causal Discovery

Under the aforementioned assumptions, constraint-based methods seek to recover the underlying causal structure using conditional independencies estimated from observational data. Constraint-based methods typically employ a two-step procedure; (1) first, establishing the *skeleton* – an undirected version of the underlying graph – and (2) second, attempting to assign directions to the edges. In general, constraint-based techniques are unable to uniquely identify the underlying causal graph, but instead return a set of causal graphs that imply the same statistical independence relations.

To develop an intuition for this, we examine how a constraint-based method works for the relatively simple DAG from Figure 1a. We start with a fully-connected graph, as shown in Figure 2a. In the first step, the *skeleton* is estimated by testing for conditional independence; if two variables are independent when conditioning on any subset of the remaining variables (e.g.,  $X_1 \perp\!\!\!\perp X_3 \mid X_2, X_1 \perp\!\!\!\perp X_4 \mid X_2, ...$ ), then the edge between the two variables is removed (see Figure 2b). In the second step, (some) edges are oriented by searching for *colliders* that induce distinctive patterns of independencies (e.g.,  $X_4$  is identified as a collider given  $X_2 \perp\!\!\!\perp X_5$  and  $X_2 \perp\!\!\!\perp X_5 \mid X_4$ , thus  $X_2 \rightarrow X_4 \leftarrow X_5$  is oriented; see Figure 2c).

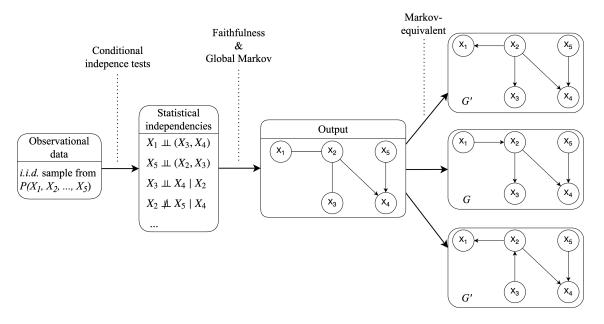
Note that the resulting graph in Figure 2c is not identical to the original true graph  $\mathcal{G}$ , as the two edges between  $X_1-X_2$  and  $X_2-X_3$  remain undirected. There are in fact three DAGs that are implied by the resulting graph, as shown in Figure 3. These DAGs are called *Markov equivalent*, meaning that they encode the same conditional independencies (i.e., the same d-separation relations hold), and we call such a set of equivalent graphs a *Markov equivalence class*, denoted by  $Equiv(\mathcal{G})$ . This illustrates a general difficulty in constraint-based approach; there are usually multiple graphs that are consistent with an observed set of statistical independencies. Here, we described the constraint-based approach procedure for DAGs, but the same principles are adapted for cyclic graphs, which will be the focus of the remainder of this paper. See Figure 3 for a summary of the constraint-based approach procedure.

Figure 2. Steps of a constraint-based method.



*Note.* (a) shows the fully-connected (undirected) graph for the example DAG from Figure 1a, which is the starting point. (b) shows the estimated *skeleton* – an undirected graph of the underlying causal structure – after the first step. (c) shows the resulting graph after the second step, which represents the *Markov equivalence class* of DAGs (i.e., a set of DAGs that entail the same set of conditional independencies).

Figure 3. Summary of the constraint-based causal discovery procedure.



*Note.* A constraint-based algorithm starts with performing a series of conditional independence tests on observational (*i.i.d.*: independent and identically distributed) data. Under the faithfulness and global Markov assumption, the algorithm estimates a graph structure based on the observed independence patterns. The output is a *partially directed* graph (as some edges remain undirected). It can represent multiple graphs that are *Markov equivalent*, meaning that they imply the same statistical independence relations. This equivalent set of graphs is called *Markov equivalence class*, and in this example, it consists of three different DAGs including the true DAG (*G*).

#### 3 Methods

In this paper, we compare the performance of three different constraint-based causal discovery algorithms for cyclic graphs using a simulation study: *cyclic causal discovery* (CCD) (Richardson, 1996b), *fast causal inference* (FCI) (Mooij & Claassen, 2020), and *cyclic causal inference* (CCI) (Strobl, 2019). Table 1 summarizes the set of assumptions made and the resulting output by each of the algorithms. In this section, we provide a detailed description of one of the considered algorithms, CCD, and illustrate how we conduct the simulation study. The other two algorithms, FCI and CCI, work in a similar way, except that they do not require the assumption of *no unobserved confounding* (i.e., causal sufficiency) needed by the CCD algorithm.<sup>1</sup> (See Appendices for the specifics of each of these three algorithms).

*Table 1.* Overview of algorithms.

	CCD	FCI	CCI
Causal Markov	$\checkmark$	$\checkmark$	✓
Faithfulness	✓	✓	$\checkmark$
Acyclicity	X	_a	X
Causal sufficiency	$\checkmark$	X	X
Linearity	$\checkmark$	✓	✓
Independent errors	$\checkmark$	✓	✓
Output	$PAG^b$	PAG	$PAAG^{c}$

*Note.* <sup>a</sup> FCI is originally designed assuming acyclicity, but in a recent research it has been proposed that it performs comparably well in the cyclic setting (Mooij & Claassen, 2020). <sup>b</sup> PAG stands for a partial ancestral graph. <sup>c</sup> PAAG stands for a partially-oriented MAAG (maximal almost ancestral graph).

### 3.1 CCD Algorithm

In what follows, we introduce the type of output generated by the CCD algorithm and trace the algorithm step-by-step using an example.

#### 3.1.1 Output Representation: Partial Ancestral Graph (PAG)

As was the case with DAGs shown in section 2.4, there typically exist multiple directed cyclic graphs (DCG) that imply the same statistical independencies, and so are statistically indistinguishable from one another. To represent a set of equivalent DCGs, a partial ancestral graph (PAG) is used. Due to the possibility of cyclic relations, the causal semantics of edges in PAGs are more complicated; directed edges denote causal ancestry (i.e.,  $A \rightarrow B$  means A is an ancestor of

<sup>&</sup>lt;sup>1</sup>The assumption that we have measured all common causes of variables involved.

*B*), and there are three different types of edge-endpoints available:  $\{\circ, >, -\}$ . Additionally, a solid underlining or dotted underlining can be added in a PAG. In the following definition that provides the semantics for PAGs (Richardson, 1996b), \* is used as a *meta-symbol* indicating one of the three possible edge-endpoints; A - \*B indicates any of the following edges: A - B, A - > B, or  $A - \circ B$ .

#### **Definition 1 (PAG)** $\Psi$ is a PAG for a directed cyclic graph G iff:

- 1. There is an edge between A and B in  $\Psi$  iff A and B are d-connected in  $\mathcal{G}$  given any subset of the remaining vertices.
- 2. If there is an edge A \*B in  $\Psi$ , then A is an ancestor of B in every graph in an equivalence class, Equiv(G).
- 3. If there is an edge A \* -> B in  $\Psi$ , then B is not an ancestor of A in every graph in  $Equiv(\mathcal{G})$ .
- 4. If there is a solid underlining  $A * *\underline{B} * *C$  in  $\Psi$ , then B is an ancestor of (at least one of) A or C in every graph in Equiv(G).
- 5. If there is a collider  $A \to B \leftarrow C$ , a dotted underlining is added  $A \to \underline{B} \leftarrow C$  iff B is *not* a descendant of a common child of A and C in every graph in Equiv(G).
- 6. Any edge-endpoint not marked in one of the above ways is left with a circle  $\circ *$ .

#### 3.1.2 Steps of CCD Algorithm

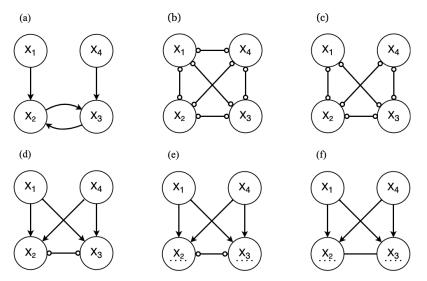
The CCD algorithm consists of 6 steps. We illustrate each step using the example DCG from Figure 4a.<sup>2</sup> The algorithm starts with a fully-connected PAG with circle endpoints, as shown in Figure 4b, and as it proceeds (some) circles will be replaced by either an arrow head or a tail.<sup>3</sup>

- **Step 1.** Estimate the *ancestral* skeleton an undirected version of a PAG based on conditional independencies. When two vertices A and B are d-separated given a set S, remove A\*-\*B and record  $S = \mathbf{Sepset}\langle A, B \rangle = \mathbf{Sepset}\langle B, A \rangle$ . Since  $X_1 \perp \!\!\! \perp X_4 \mid \emptyset$  in our example DCG,  $X_1 \leadsto X_4$  is removed and  $\mathbf{Sepset}\langle X_1, X_4 \rangle = \mathbf{Sepset}\langle X_4, X_1 \rangle = \emptyset$  is recorded, resulting in Figure 4c.
- **Step 2.** Search for collider structures. If  $B \notin \mathbf{Sepset}(A, C)$  in a triplet A \* \*B \* \*C, identify B as a collider and orient  $A \to B \leftarrow C$ . Given that  $X_2 \notin \mathbf{Sepset}(X_1, X_4)$  and  $X_3 \notin \mathbf{Sepset}(X_1, X_4)$  in our example,  $X_1 \leadsto X_2 \leadsto X_4$  and  $X_1 \leadsto X_3 \leadsto X_4$  are oriented respectively as  $X_1 \to X_2 \leftarrow X_4$  and  $X_1 \to X_3 \leftarrow X_4$ , resulting in Figure 4d.
- **Step 3.** Check for additional d-separating relations in each triplet  $\langle A, B, C \rangle$  such that: (i) A is not adjacent to B or C, (ii) B and C are adjacent, and (iii)  $B \notin \mathbf{Sepset}\langle A, C \rangle$ . If such triplets exist, orient B\*-\*C as  $B \leftarrow C$ . As no additional d-separating relations are found in our example, no further orientations are performed in step 3.

<sup>&</sup>lt;sup>2</sup>It is the same as the example DCG that we previously introduced in Figure 1b.

<sup>&</sup>lt;sup>3</sup>It is important to note, once again, that the algorithm aims to retrieve a PAG for the underlying cyclic graph, and the edges in a PAG represent *ancestral* relations that are common to all directed cyclic graphs (DCG) in an equivalence class.

Figure 4. Trace of CCD algorithm.



*Note.* (a) shows the true directed cyclic graph, G. (b) shows the fully-connected PAG for G, which is the starting point of the algorithm. (c) shows the *ancestral* skeleton (i.e., an undirected version of the PAG) estimated in step 1. (d) shows the state of the PAG after step 2, where some of the edges are oriented given the identified colliders. (e) shows the state of the PAG after step 4, where the *Supsets* are identified and the corresponding colliders are dotted-underlined. (f) shows the final state of the PAG after step 5, where an additional edge between  $X_2$  and  $X_3$  is oriented.

**Step 4.** Search for **Supsets**, which are d-separating sets including colliders. For each collider structure  $A \to B \leftarrow C$ , check if there is any set T including B that d-separates A and C. When such exists, record  $T = \mathbf{Supset}(A, B, C)$  and add a dotted-underlining  $A \to \underline{B} \leftarrow C$ . Since  $X_1 \perp \!\!\!\perp X_4 \mid \{X_2, X_3\}$  in our example,  $\mathbf{Supset}(X_1, X_2, X_4) = \mathbf{Supset}(X_1, X_3, X_4) = \{X_2, X_3\}$  is recorded and each of the colliders is dotted-underlined as  $X_1 \to \underline{X_2} \leftarrow X_4$  and  $X_1 \to \underline{X_3} \leftarrow X_4$ , resulting in Figure 4e.

**Step 5.** Search for quadruplets – four ordered vertices  $\langle A, B, C, D \rangle$  – where:

(i)  $A \to \underline{B} \leftarrow C$ , (ii)  $A \to D \leftarrow C$  or  $A \to \underline{D} \leftarrow C$ , and (iii) B and D are adjacent. If  $D \in \mathbf{Supset}\langle A, B, C \rangle$  in such quadruplets, orient B\*-\*D as B\*-D. Else, orient B\*-\*D as  $B \to D$ . In our example, there is such a quadruplet; (i)  $X_1 \to \underline{X_2} \leftarrow X_4$ , (ii)  $X_1 \to \underline{X_3} \leftarrow X_4$ , and (iii)  $X_2$  and  $X_3$  are adjacent. Since  $X_2 \in \mathbf{Supset}\langle X_1, X_3, X_4 \rangle$  and  $X_3 \in \mathbf{Supset}\langle X_1, X_2, X_4 \rangle$ ,  $X_2 \leadsto X_3$  is oriented as  $X_2 \multimap X_3$ , then  $X_2 \multimap X_3$  is subsequently oriented as  $X_2 - X_3$ , resulting in Figure 4f.

**Step 6.** Search for quadruplets  $\langle A, B, C, D \rangle$ , where  $A \to \underline{B} \leftarrow C$  while D is adjacent to neither A nor C. If A and D are d-connected given **Supset** $\langle A, B, C \rangle \cup D$ , then orient  $B* \multimap D$  as  $B \to D$ . In our example, no such quadruplets exist; therefore Figure 4f remains the final PAG. As shown in Figure 5, the resulting PAG represents two different DCGs that entail the same conditional independencies.

Figure 5. Summary of CCD algorithm operation.

*Note.* Given the observed statistical independencies estimated from the observational data, CCD constructs a partial ancestral graph (PAG), which represents the *ancestral* features that are common to every directed cyclic graph (DCG) in a Markov equivalence class. In this example, the Markov equivalence class consists of two different DCGs, including the true graph *G*.

## 3.2 Simulation

To evaluate the performance of the considered algorithms, we conduct a simulation study. In this section, we discuss the simulation design, data generating process, and evaluation metrics in detail.

#### 3.2.1 Simulation Design

We test each algorithm under different conditions by varying the number of variables (rows of Figure 6) and the number of edges – the density (columns of Figure 6). We also evaluate the effect of an unobserved confounder by adding a latent variable ( $L_1$  in Figure 6). Lastly, we vary the sample size across the range we often encounter in psychological research;  $n \in \{150, 500, 1000\}$  for every simulated cyclic model (Constantin & Cramer, 2022). Thus, it leads to a  $2 \times 2 \times 2 \times 3$  design; number of variables  $\times$  density  $\times$  latent confounder (presence/absence)  $\times$  sample size.

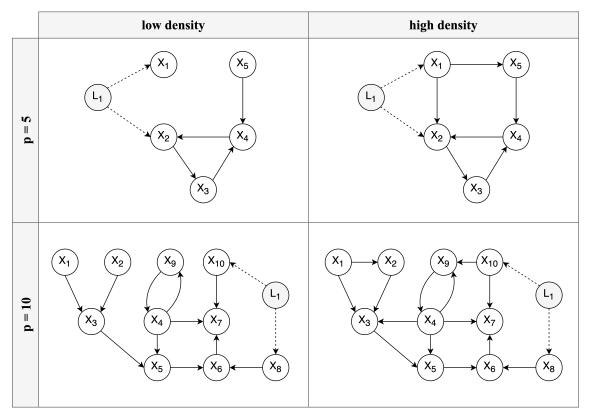


Figure 6. Simulation settings.

*Note.* We vary the number of variables:  $p \in \{5, 10\}$ , the density: high / low, the influence of a latent confounder  $(L_1)$ : absence / presence, and the sample size:  $n \in \{150, 500, 1000\}$ , which results in a  $2 \times 2 \times 2 \times 3$  simulation design.

#### 3.2.2 Data Generation

As illustrated above, we simulate data from different cyclic models, all of which are characterized by *linear* relations and *independent Gaussian* error terms. These types of models are not only often used in psychological research, but also satisfy the global Markov property – the necessary condition for constraint-based causal discovery – as shown in section 2.2.

To generate data, we first define a coefficient matrix **B** and sample the error terms ( $\varepsilon$ ) from independent Gaussian distributions. After drawing the values of  $\varepsilon$ , we generate observations of **X** by solving the following equation:

$$\mathbf{X} = (\mathbf{I} - \mathbf{B})^{-1} \boldsymbol{\varepsilon},$$

where **I** denotes the identity matrix and  $\varepsilon$  denotes a set of jointly independent Gaussian error terms. Note that this data generation scheme is possible provided that (**I**-**B**) is invertible, which is the case when the eigenvalues of **B** are smaller than one,  $|\lambda| < 1$  (Eberhardt, Hoyer, & Scheines, 2010). While this is guaranteed if **B** defines an acyclic model, for cyclic models, this does not always hold. Therefore, we check if this condition is satisfied for every cyclic model when specifying **B**.

*Table 2.* Confusion matrix for the three types of edge-endpoints.

#### **Estimated endpoint**

		Arrow head (>)	Arrow tail (-)	Null
True endpoint	Arrow head (>)	a	b	c
	Arrow tail (–)	d	e	f
	Null	g	h	i

*Note.* The true endpoints are presented in rows, and the estimated endpoints are presented in columns. There are in total four possible edge-endpoints that can occur in an output: arrow head, arrow tail, null (no endpoint), and circle. The circle endpoints (o), however, are not counted toward the calculation of *precision* and *recall* but are used for calculating the *uncertainty rate*.

#### 3.2.3 Evaluation Metrics

We assess the performance of each algorithm using both *local* and *global* evaluation metrics; at a local level, we look at the individual edge-endpoints and at a global level, we look at the graph structure as a whole. As the local metrics, we utilize *precision*, *recall*, and *uncertainty rate*.

$$Precision = \frac{True \ Positive}{True \ Positive + False \ Positive}$$

$$Recall = \frac{True \ Positive}{True \ Positive + False \ Negative}$$

$$Uncertainty \ rate = \frac{Number \ of \ circle \ endpoints \ (\circ)}{Total \ number \ of \ edge-endpoints}$$

Precision reflects the prediction accuracy (i.e., out of all predicted cases, how many are correct), and recall reflects the retrieval rate (i.e., out of all true cases, how many are retrieved). There are in total four possibilities for each edge-endpoint in a resulting graph: no edge-endpoint (null), arrow head (>), arrow tail (-), and circle ( $\circ$ ). Given that circle endpoints imply an algorithm is unsure of the direction, the uncertainty rate is defined as a proportion of the circle endpoints occurred in an output. For the other endpoints, we calculate precision and recall. For example, for the arrow head, they are computed as:  $precision = \frac{a}{a+d+g}$ ;  $recall = \frac{a}{a+b+c}$  (see Table 2).

As the global metric, we use *structural Hamming distance* (SHD) (de Jongh & Druzdzel, 2009). SHD quantifies the level of differences between two graphs by counting the number of edge insertions, deletions, and direction changes required to move from one graph (estimated graph  $\hat{\mathcal{G}}$ ) to the other (true graph  $\mathcal{G}$ ). It can be formulated as: SHD = A + D + C, where A, D, and C represent, respectively, the number of added edges, deleted edges, and direction changes. Thus, the smaller the SHD value is, the more similar  $\hat{\mathcal{G}}$  is to  $\mathcal{G}$ , indicating that an algorithm recovers the true graph well.

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# **Appendix A** CCD Details

#### **Algorithm 1** Cyclic Causal Discovery (CCD)

**Input:** A conditional independent oracle for a distribution  $\mathcal{P}$ , satisfying global directed Markov property and faithfulness conditions with respect to a directed graph  $\mathcal{G}$  with vertex set  $\mathcal{V}$ .

**Output:** A PAG  $\Psi$  for the Markov equivalence class Equiv( $\mathcal{G}$ ).

- 1: Step 1. Form a complete graph  $(\Psi)$  with the edge  $\infty$  between every pair of vertices in  $\mathcal{V}$ .
- 2: n = 0
- 3: repeat
- 4: repeat
- 5: Select an ordered pair of variables X and Y that are adjacent in  $\Psi$  such that the number of vertices in  $\mathbf{Adjacent}(\Psi, X) \setminus \{Y\} \ge n$ , and select a subset S of  $\mathbf{Adjacent}(\Psi, X) \setminus \{Y\}$  with n vertices.
  - If  $X \perp \!\!\! \perp Y \mid S$ , then delete the edge  $X \leadsto Y$  and record S in **Sepset** $\langle X, Y \rangle$  and **Sepset** $\langle X, Y \rangle$ .
- 6: **until** all pairs of adjacent variables X and Y such that the number of vertices in  $Adjacent(\Psi, X) \setminus \{Y\} \ge n$  and all sets S such that the number of vertices in S = n have been tested.

```
n = n + 1:
```

- 7: **until** for all ordered pairs of adjacent vertices *X* and *Y*, **Adjacent**( $\Psi$ , *X*)\{*Y*} < *n*.
- 8: **Step 2.** For each triple of vertices A, B, C such that each of the pair of A, B and the pair B, C are adjacent in  $\Psi$  but the pair A, C are not adjacent in  $\Psi$ , then:
- 9: (i) orient A \* \*B \* \*C as  $A \to B \leftarrow C$  iff  $B \notin \mathbf{Sepset}(A, B)$ .
- 10: (ii) orient A \* \*B \* \*C as A \* \*B \* \*C iff  $B \in \mathbf{Sepset}(A, B)$ .
- 11: **Step 3.** For each triple of vertices A, X, Y in  $\Psi$  such that (a) A is not adjacent to X or Y, (b) X and Y are adjacent, (c)  $X \notin \mathbf{Sepset}(A, Y)$ , then orient X \* \* Y as  $X \leftarrow Y$  if  $A \not\perp\!\!\!\perp X \mid \mathbf{Sepset}(A, Y)$ .
- 12: **Step 4.** For each vertex V in  $\Psi$  form the following set:  $X \in \mathbf{Local}(\Psi, V)$  or there is a vertex Y such that  $X \to Y \leftarrow V$  in  $\Psi$ .
- 13: m = 0
- 14: repeat
- 15: repeat
- 16: Select an ordered triple  $\langle A, B, C \rangle$  such that  $A \to B \leftarrow C$ , A and C are not adjacent, and Local( $\Psi, A$ )\ $\{B, C\}$  has  $\geq m$  vertices.

Select a set  $T \subseteq \mathbf{Local}(\Psi, A) \setminus \{B, C\}$  with m vertices. If  $A \perp \!\!\! \perp C \mid T \cup \{B\}$ , then orient  $A \to B \leftarrow C$  as  $A \to \underline{B} \leftarrow C$  and record  $T \cup \{B\}$  in  $\mathbf{Supset}(A, B, V)$ .

- 17: **until** for all triples such that  $A \to B \leftarrow C$  (not  $A \to \underline{B} \leftarrow C$ ), A and C are not adjacent, **Local**( $\Psi, A$ )\{B} has  $\geq m$  vertices, every subset T with m vertices has been considered.
- 18: m = m + 1;

- 19: **until** all ordered triples  $\langle A, B, C \rangle$  such that  $A \to B \leftarrow C$ , A and C are not adjacent, are such that **Local**( $\Psi, A$ )\{B} have < m vertices.
- 20: Step 5. If there is a quadruple A, B, C, D in  $\Psi$  of distinct vertices such that:
- 21: (i)  $A \rightarrow B \leftarrow C$ ,
- 22: (ii)  $A \to D \leftarrow C$  or  $A \to D \leftarrow C$ ,
- 23: (iii) B and D are adjacent,
- 24: then orient B \* \* D ad  $B \to D$  in  $\Psi$  if  $D \notin \mathbf{Subset}(A, B, C)$ . Else orient B \* \* D as B \* D in  $\Psi$ .
- 25: **Step 6.** For each quadruple A, B, C, D in  $\Psi$  of distinct vertices such that:
- 26: (i) D is not adjacent to both A and C,
- 27: (ii)  $A \rightarrow B \leftarrow C$ ,
- 28: if  $A \not\perp D \mid \mathbf{Supset}(A, B, C) \cup \{D\}$ , then orient B \* \* D as  $B \to D$  in  $\Psi$ .

# **Appendix B** FCI Details

### **Algorithm 2** Fast Causal Inference (FCI)

**Input:** A conditional independent oracle for a distribution  $\mathcal{P}$ , satisfying global directed Markov property and faithfulness conditions with respect to a directed graph  $\mathcal{G}$  with vertex set  $\mathcal{V}$ .

**Output:** A PAG  $\hat{\mathcal{G}}'$  for the Markov equivalence class of MAGs (Equiv( $\mathcal{G}$ )).

- 1: Step 1. Form the complete undirected graph Q on the vertex set V.
- 2: n = 0
- 3: repeat
- 4: repeat
- Select an ordered pair of variables X and Y that are adjacent in Q such that the number of vertices in  $\mathbf{Adjacent}(Q, X) \setminus \{Y\} \ge n$ , and select a subset S of  $\mathbf{Adjacent}(Q, X) \setminus \{Y\}$  with n vertices.
  - If  $X \perp \!\!\! \perp Y \mid S$ , then delete the edge  $X \multimap Y$  and record S in **Sepset** $\langle X, Y \rangle$  and **Sepset** $\langle X, Y \rangle$ .
- 6: **until** all pairs of adjacent variables X and Y such that the number of vertices in  $\mathbf{Adjacent}(Q, X) \setminus \{Y\} \ge n$  and all sets S such that the number of vertices in S = n have been tested.

$$n = n + 1;$$

- 7: **until** for all ordered pairs of adjacent vertices *X* and *Y*, **Adjacent**(Q, X)\{Y} < n.
- 8: **Step 2.** Let Q' be the undirected graph resulting from step 1. For each triplet  $\langle A, B, C \rangle$  such that each of the pair of A, B and the pair B, C are adjacent in Q' but the pair A, C are not adjacent in Q', then:
- 9: (i) orient A \* \*B \* \*C as  $A \to B \leftarrow C$  iff  $B \notin \mathbf{Sepset}(A, B)$ .
- 10: (ii) orient A \* \*B \* \*C as A \* \*B \* \*C iff  $B \in \mathbf{Sepset}(A, B)$ .

- 11: **Step 3.** For each pair of variables A and B adjacent in Q', if A and B are d-separated given any subset S of **Possible-d-sepset** $(A, B) \setminus \{A, B\}$  or any subset S of **Possible-d-sepset** $(B, A) \setminus \{A, B\}$  in Q', then remove the edge between A and B, and record S in **Sepset**(A, B) and **Sepset**(B, A).
- 12: **Step 4.** Reorient an edge between any pair of variables X and Y ( $X \leadsto Y$ ) following the orientation rules below.

```
13: repeat
        if there is a directed path from A to B, and an edge A * - * B then
14:
15:
             orient A * - * B as A * \rightarrow B,
        else if B is a collider along \langle A, B, C \rangle, B is adjacent to D, and D \in \mathbf{Sepset} \langle A, C \rangle then
16:
17:
             orient B * - * D as B \leftarrow *D,
        else if U is a definite discriminating path between A and B for M in the path \prod, and P
18:
    and R are adjacent to M on U, and P - M - R is a triangle then
19:
            if M \in \mathbf{Sepset}(A, B) then M is marked as non-collider on subpath P * - *M * - *R
            else P * - *M * - *R is oriented as P * \to M \leftarrow *R.
20:
            end if
21:
        else if P* \rightarrow M* - *R then
22:
            orient as P* \to M \to R.
23:
        end if
24:
25: until no more edges can be oriented.
```

# **Appendix C** CCI Details

#### Algorithm 3 Cyclic Causal Inference (CCI)

**Input:** A conditional independent oracle for a distribution  $\mathcal{P}$ , satisfying global directed Markov property and faithfulness conditions w.r.t. a directed graph  $\mathcal{G}$  with vertex set  $\mathcal{V}$ . ( $\mathcal{V} = \mathbf{O} \cup \mathbf{L} \cup \mathbf{S}$ ), where  $\mathbf{O}$ ,  $\mathbf{L}$ , and  $\mathbf{S}$  refer to the sets of observable, latent, and selection variables, respectively.

**Output:** A PAAG  $(\hat{\mathcal{G}}')$  for the Markov equivalence class of MAAGs (Equiv $(\mathcal{G})$ ).

- 1: Step 1. Run FCI's skeleton discovery procedure.
- 2: Step 2. Run FCI's collider structure (v-structure) orientation procedure.
- 3: Step 3. For any triplet  $\langle O_i, O_k, O_j \rangle$ , such that we have  $O_k \hookrightarrow *O_i$ , if  $O_i \perp\!\!\!\perp_{\mathcal{G}} O_j \mid \mathbf{Sepset} \langle O_i, O_j \rangle \cup \mathbf{S}$ , where  $\mathbf{Sepset} \langle O_i, O_j \rangle$  is a separating set discovered in step 1,  $O_k \notin \mathbf{Sepset} \langle O_i, O_j \rangle$ ,  $O_i \perp\!\!\!\perp_{\mathcal{G}} O_k \mid \mathbf{Sepset} \langle O_i, O_j \rangle \cup \mathbf{S}$  and  $O_j \perp\!\!\!\perp_{\mathcal{G}} O_k \mid \mathbf{Sepset} \langle O_i, O_j \rangle \cup \mathbf{S}$ , then orient  $O_k \hookrightarrow *O_i$  as  $O_k \leftarrow *O_i$ .
- 4: Step 4. Find additional non-minimal d-separating sets.
- 5: m = 0
- 6: repeat
- 7: repeat
- 8: Select an ordered triplet  $\langle O_i, O_j, O_k \rangle$  with the collider structure  $O_i * \to O_j \leftarrow *O_k$  such that  $|\mathbf{PD\text{-}Sep}(O_i)| \ge m$

9: repeat

10: Select a subset

 $\mathbf{W} \subseteq \mathbf{PD\text{-}Sep}(O_i) \setminus \{\mathbf{Sepset}(O_i, O_k) \cup \{O_j, O_k\}\}\$  with m vertices

 $T = W \cup Sepset(O_i, O_k) \cup O_i$ 

if  $O_i$  and  $O_k$  are d-separated given  $T \cup S$ , then record the set T in **Supset** $\langle O_i, O_j, O_k \rangle$ 

11: **until** all subsets

 $\mathbf{W} \subseteq \mathbf{PD\text{-}Sep}(O_i) \setminus \{\mathbf{Sepset}(O_i, O_k) \cup \{O_j, O_k\}\}\$  have been considered or a d-separating set of  $O_i$  and  $O_k$  has been recorded in  $\mathbf{Supset}(O_i, O_j, O_k)$ ;

- 12: **until** all triplets  $\langle O_i, O_j, O_k \rangle$  with the collider structure  $O_i * \to O_j \leftarrow *O_k$  and  $|\mathbf{PD\text{-Sep}}(O_i)| \ge m$  have been selected;
- 13: **until** all ordered triplets  $\langle O_i, O_j, O_k \rangle$  with the collider structure  $O_i * \rightarrow O_j \leftarrow *O_k$  have  $|\mathbf{PD\text{-}Sep}(O_i)| < m$ ;
- 14: Step 5. Find all quadruples of vertices  $\langle O_i, O_j, O_k, O_l \rangle$  such that  $O_i$  and  $O_k$  are non-adjacent,  $O_i * \to O_l \leftarrow *O_k$ , and  $O_i \perp \!\!\! \perp_{\mathcal{G}} O_k \mid \mathbf{W} \cup \mathbf{S}$  with  $O_j \in \mathbf{W}$  and  $\mathbf{W} \subseteq \mathbf{O} \setminus \{O_i, O_k\}$ . If  $O_l \notin \mathbf{W} = \mathbf{Sepset} \langle O_i, O_k \rangle$  as discovered in step 2, then orient  $O_j * \multimap O_l$  as  $O_j * \to O_l$ . If we also have  $O_i * \to O_j \leftarrow *O_k$  and  $O_l \in \mathbf{W} = \mathbf{Supset} \langle O_i, O_j, O_k \rangle$  as discovered in step 4, then orient  $O_i * \multimap O_l$  as  $O_j * \multimap O_l$ .
- 15: *Step 6.* For any two vertices  $O_i$  and  $O_k$ , if we have  $O_i \perp \!\!\! \perp_{\mathcal{G}} O_k \mid \mathbf{W} \cup \mathbf{S}$  for some  $\mathbf{W} \subseteq \mathbf{O} \setminus \{O_i, O_k\}$  discovered in step 1 or step 4 with  $O_j \in \mathbf{W}$  but we have  $O_i \perp \!\!\! \perp_{\mathcal{G}} O_k \mid O_l \cup \mathbf{W} \cup \mathbf{S}$ , then orient  $O_l \sim *O_j$  as  $O_l \leftarrow *O_j$ .
- 16: **Step 7.** Execute orientation rules until no more endpoints can be oriented. The orientation rules are as follows:
  - (i) If we have  $O_i * \to O_j \sim *O_k$  with  $O_i$  and  $O_k$  non-adjacent, then orient  $O_j \sim *O_k$  as  $O_j *O_k$ . Furthermore, if  $O_i * \to O_j$  is not potentially 2-triangulated w.r.t.  $O_k$ , then orient  $O_j \sim O_k$  as  $O_j \to O_k$ .
  - (ii) If we have  $O_i *O_j \sim *O_k$  with  $O_i$  and  $O_k$  non-adjacent, and  $O_j \sim O_k$  is not potentially 2-triangulated w.r.t.  $O_i$ , then orient  $O_j \sim *O_k$  as  $O_j *O_k$ .
  - (iii) Suppose we have  $O_i^* \to O_j O_k$  with  $O_i$  and  $O_k$  non-adjacent, and  $O_i^* \to O_j$  is potentially 2-triangulated w.r.t.  $O_k$ . If  $O_i^* \to O_j$  can be potentially 2-triangulated w.r.t.  $O_k$  using only one vertex  $O_l$  in the triangle involve  $\{O_i, O_j, O_l\}$ , then orient  $O_i^* \to O_l$  as  $O_i^* \to O_l$  as  $O_j^* \to O_l$  and/or  $O_j^* \to O_l$  as  $O_j^* \to O_l$ . Next, if there exists only one potentially undirected path  $\prod_{O_l,O_k}$  between  $O_l$  and  $O_k$ , then substitute all circle endpoints on  $\prod_{O_l,O_k}$  with tail endpoints (-).
  - (iv) If  $O_i * \to O_j *O_k$ , there exists a path  $\prod = \langle O_k, ..., O_i \rangle$  with at least  $n \ge 3$  vertices such that we have  $O_h *O_{h+1}$  for all  $1 \le i \le n-1$ , and we have  $O_1 \multimap *O_n$ , then orient  $O_1 \multimap *O_n$  as  $O_1 *O_n$ .
  - (v) If we have the sequence of vertices  $\langle O_1, ..., O_n \rangle$  such that  $O_i *O_{i+1}$  with  $1 \le i \le n-1$ , and we have  $O_1 \multimap *O_n$ , then orient  $O_1 \multimap *O_n$  as  $O_1 *O_n$ .
  - (vi) If we have  $O_k * \multimap O_i$ , there exists a non-potentially 2-triangulated path  $\prod = \langle O_i, O_j, O_l, ..., O_k \rangle$  such that  $O_k * \multimap O_i$  is not potentially 2-triangulated w.r.t.  $O_j$ , and  $O_i * * O_i * * O_k$  is an unshielded non-v-structure, then orient  $O_k * \multimap O_i$  as  $O_k * \multimap O_i$ .
  - (vii) Suppose we have  $O_i endsymbol{\sim} O_k, O_i *O_k * -O_l$ , a non-potentially 2-triangulated path  $\prod_1$  from  $O_i$  to  $O_j$ , and a non-potentially 2-triangulated path  $\prod_2$  from  $O_i$  to  $O_l$ . Let  $O_m$  be a vertex adjacent to  $O_i$  on  $\prod_1$ , and let  $O_n$  be the vertex adjacent to  $O_i$  on  $\prod_2$ . If further  $O_m * *O_i * *O_n$  is an unshielded non-v-structure and  $O_i \sim *O_k$  is not potentially 2-triangulated w.r.t. both  $O_n$  and  $O_m$ , then orient  $O_i \sim *O_k$  as  $O_i *O_k$ .