# Conditional independences and causal relations implied by sets of equations

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### Abstract

Real-world complex systems are often modelled by sets of equations with exogenous random variables. What can we say about the probabilistic and causal aspects of variables that appear in these equations without explicitly solving for them? We prove that, under a solvability assumption, we can construct a *Markov ordering graph* that implies conditional independences and a *causal ordering graph* that encodes the effects of soft and perfect interventions by making use of Simon's causal ordering algorithm (Simon, 1953). Our results shed new light on discussions in causal discovery about the justification of using graphs to simultaneously represent conditional independences and causal relations in models with feedback.

# 1 Introduction

The discovery of causal relations is a fundamental objective in many scientific endeavours. The process of the scientific method usually involves a conjecture, such as a causal graph or a set of equations, that explains observed phenomena. In practice, such a graph structure can be learned automatically from conditional independences in observational data via the PC/FCI algorithms (Spirtes, Glymour, and Scheines, 2000; Zhang, 2008). The crucial assumption in *causal discovery* is that directed edges in this learned graph express causal relations between variables. However, an immediate concern is whether directed graphs actually can simultaneously encode the causal semantics and the conditional independence constraints of a system.<sup>1</sup> We explicitly define soft and perfect interventions on sets of equations and demonstrate that the effects of interventions and conditional independences cannot generally be unambiguously expressed in a single directed graph. In particular, we show that the output of the PC algorithm does not have a straightforward causal interpretation when it is applied to data generated by a simple dynamical model with feedback at equilibrium.

<sup>&</sup>lt;sup>1</sup>See, for example, (Dawid, 2010) and references therein for a discussion.

It is often said that the "gold standard" in causal discovery is controlled experimentation. Indeed, the main principle of the scientific method is to derive predictions from a conjecture, such as a causal graph or set of equations, that are then verified or rejected through experimentation. We show how, in practice, testable predictions can be derived automatically from sets of equations via the *causal ordering algorithm*, introduced by Simon (1953). We slightly adapt the algorithm to construct either a directed graph that we call the *Markov ordering* graph or a directed cluster graph that we call the causal ordering graph. We prove that the former implies conditional independences between variables which can be tested in observational data and the latter represents the effects of soft and certain perfect interventions which can be verified through experimentation. The technique of causal ordering is a useful and scalable tool in our search for and understanding of causal relations.

In this work, we also shed new light on differences between the causal ordering graph and the graph structure of Structural Causal Models (SCMs) (see Bongers, Forré, et al. (2020) and Pearl (2000)). Specifically, we demonstrate that the two graphical representations may model different sets of interventions. Furthermore, we show that a stronger Markov property can sometimes be obtained by applying causal ordering to the structural equations of an SCM. By explicitly defining interventions and by distinguishing between the Markov ordering graph and the causal ordering graph we gain new insights about the correct interpretation of results in Dash (2005) and Iwasaki and Simon (1994). Throughout this work, we discuss an example in Iwasaki and Simon (1994) to illustrate our ideas. This example highlights the contributions of this paper and provides an overview of its central concepts.

**Example 1.** Let us revisit a physical model of a filling bathtub in equilibrium that is presented in Iwasaki and Simon (1994). Consider a system where water flows from a faucet into a bathtub at a constant rate  $X_I$  and it flows out of the tub through a drain with diameter  $X_K$ . An ensemble of such bathtubs with different (unknown) faucets and drains can be modelled by the equations  $f_K$  and  $f_I$  below:

$$f_K: \qquad X_K = U_K,$$
  
$$f_I: \qquad X_I = U_I,$$

where  $U_K$  and  $U_I$  are random variables both taking value in  $\mathbb{R}_{>0}$ . When the faucet is turned on the water level  $X_D$  in the bathtub increases as long as the inflow  $X_I$  of the water exceeds the outflow  $X_O$  of water. The differential equation below defines the mechanism for changes in  $X_D$ , which is equal to zero when the bathtub system has reached equilibrium.

$$f_D: \quad \dot{X}_D = U_1(X_I - X_O) = 0,$$

where  $U_1$  is a constant or a random variable taking value in  $\mathbb{R}_{>0}$ . As the water level  $X_D$  increases, the pressure  $X_P$  that is exerted by the water increases as well. The mechanism for the change in pressure is defined in the differential equation below, which equals zero when the system is at rest.

$$f_P: \qquad X_P = U_2(g \, U_3 X_D - X_P) = 0,$$

where g is the gravitational constant and  $U_2, U_3$  are constants or random variables both taking value in  $\mathbb{R}_{>0}$ . The higher the pressure  $X_P$  or the bigger the size of the drain  $X_K$ , the faster the water flows through the drain. The equilibrium equation  $f_O$  below models the outflow rate  $X_O$  of the water.

$$f_O: \quad \dot{X}_O = U_4(U_5 X_K X_P - X_O) = 0,$$

where  $U_4, U_5$  are constants or random variables both taking value in  $\mathbb{R}_{>0}$ .

Graphical representations. A set of equations can be represented by a bipartite graph. In the case of the filling bathtub, the structure of equations  $f_K$  to  $f_O$  is represented by the bipartite graph in Figure 1(a). The set  $V = \{v_K, v_I, v_P, v_O, v_D\}$ consists of vertices that correspond to variables and the vertices in the set F = $\{f_K, f_I, f_P, f_O, f_D\}$  correspond to equations. There is an edge between a variable vertex  $v_i$  and an equation vertex  $f_j$  if the variable corresponding to *i* appears in the equation corresponding to j. A formal definition of a system of constraints and its associated bipartite graph will be provided in Section 1.3. The causal ordering algorithm, introduced by Simon (1953) and slightly reformulated by us in Section 2, takes a *self-contained* bipartite graph as input and returns a *causal* ordering graph. A causal ordering graph is a directed cluster graph which consists of variable vertices  $v_i$  and equation vertices  $f_j$  that are partitioned into clusters. Directed edges go from variable vertices to clusters. For the filling bathtub, the causal ordering graph is given in Figure 1(b). In Section 3 we will show how the Markov ordering graph can be constructed from a causal ordering graph. For the filling bathtub, the Markov ordering graph is given in Figure 1(c).

Markov property. The Markov ordering graph in Figure 1(c) encodes conditional independences between  $X_K$ ,  $X_I$ ,  $X_P$ ,  $X_O$ , and  $X_D$ . In particular, d-separations between variable vertices in the Markov ordering graph imply conditional independences between the corresponding variables, as we will prove in Theorem 2 in Section 3. In Figure 1(c), the variable vertices  $v_I$  and  $v_D$  are d-separated by  $v_O$ . It follows that the inflow rate  $X_I$  and the water level  $X_D$  are independent given the outflow rate  $X_O$ . In Section 4 we show how we can use a perfect matching for a bipartite graph to construct a directed graph that implies conditional independences between variables via  $\sigma$ -separations (see Forré and Mooij (2017)).

Soft interventions. The causal ordering graph in Figure 1(b) encodes the effects of soft interventions on equations. This type of intervention is often referred to as mechanism changes. We assume that the variables in each cluster can be solved from the equations in their cluster both before and after the intervention. A soft intervention has no effect on a variable if (a) the intervention target is in a different cluster and (b) there is no directed path from the intervention target to the cluster containing the variable, as we will prove in Theorem 4 in Section 5.1. Consider an experiment where the value of the gravitational constant g is altered (e.g. by moving the bathtub to the moon) resulting in an alteration of the equation  $f_P$ . This is a soft intervention on  $f_P$ . There is no directed path from  $f_P$  to clusters that contain the vertices  $\{v_K, v_I, v_P, v_O\}$  and  $f_P$  is not in a cluster with  $\{v_K, v_I, v_P, v_O\}$  in the causal ordering graph in Figure 1(b). Since the conditions of Theorem 4

are satisfied, the soft intervention on  $f_P$  has no effect on  $\{X_K, X_I, X_P, X_O\}$  but it generically does have an effect on  $X_D$ .

Perfect interventions. The causal ordering graph in Figure 1(b) also encodes the effects of perfect interventions on clusters. We will formally prove this in Proposition 2 in Section 5.2. Consider a perfect intervention on the cluster  $\{f_K, v_K\}$  (i.e. fixing the diameter  $X_K$  of the drain by altering the equation  $f_K$ ) in Figure 1(b). This intervention generically changes the solution for  $\{X_K, X_P, X_D\}$  because  $v_K$  is targeted by the intervention and there is a directed path from the cluster of  $v_K$  to the clusters of  $v_P$  and  $v_D$ . It has no effect on  $\{X_I, X_O\}$  because there is no directed path to the clusters of  $v_I$  and  $v_O$ .



Figure 1: Three graphical representations for the bathtub system. The bipartite graph in Figure 1(a) is a representation of the structure of equations  $F = \{f_K, f_I, f_P, f_O, f_D\}$ where the vertices  $V = \{v_K, v_I, v_P, v_O, v_D\}$  correspond to variables and there is an edge (v - f) if and only if the variable v appears in equation f. The outcome of the causal ordering algorithm is the directed cluster graph in Figure 1(b), in which rectangles represent a partition of the variable and equation vertices into clusters. The corresponding Markov ordering graph for the variable vertices is given in Figure 1(c).

# 1.1 Related work

Graphical models are a popular statistical tool to model probabilistic aspects of complex systems (Pearl, 2000). Formally, they represent a set of conditional independences between random variables that correspond to vertices which allows us to learn their graphical structure from data (Lauritzen, 1996). These models are often interpreted causally, so that directed edges between vertices are interpreted as causal relations between corresponding variables (Pearl, 2000). The strong assumptions that are necessary for this viewpoint in the context of Directed Acyclic Graphs (DAGs) have been the topic of debate (Dawid, 2010). This work contributes to this discussion by revisiting an example in Iwasaki and Simon (1994) for which we demonstrate that conditional independences and the effects of perfect interventions cannot be expressed in a single directed graph.

Our work slightly reformulates the causal ordering algorithm which was introduced by Simon (1953). Following (Dash and Druzdzel, 2008), we formally prove that the causal ordering graph that is constructed by the algorithm is unique. One of the novelties of this work is that we also prove that it encodes the effects of soft and certain perfect interventions and, moreover, we show how it can be used to construct a DAG that implies conditional independences via the d-separation criterion (see Pearl (2000)). There also exists a different, computationally more efficient, algorithm for causal ordering (Gonçalves and Porto, 2016; Nayak, 1995). We formally prove that this algorithm is equivalent to the one in Simon (1953). This alternative approach motivates an alternative representation of the system as a directed graph that may contain cycles. We prove that the *generalized directed global Markov property*, as formulated by Forré and Mooij (2017), holds for this graphical representation.

In Section 6 we will present a detailed discussion of how our work relates to that of Bongers, Forré, et al. (2020), Bongers and Mooij (2018), Dash (2005), and Iwasaki and Simon (1994). We show that the "causal graph" in Iwasaki and Simon (1994) coincides with the Markov ordering graph in our work. We take a closer look at the intricacies of (possible) causal implications of the Markov ordering graph and notice that it neither represents the effects of soft interventions nor does it have a straightforward interpretation in terms of perfect interventions. We therefore argue that the causal ordering graph, and not the Markov ordering graph, should be used to represent causal relations. This sheds some new light on the work of Dash (2005) on (causal) structure learning and *equilibration* in dynamical systems. We will also consider potential benefits (e.g. obtaining a stronger Markov property) of applying the technique of causal ordering to structural equations in a Structural Causal Model (SCM).

### **1.2** Preliminaries

Henceforth, variables will be denoted by capital letters and sets of variables will be denoted by boldfaced capital letters. The proofs of all propositions and theorems will be given in the supplementary material in Section 8. We first introduce necessary graphical background concepts.

### 1.2.1 Bipartite graphs

A bipartite graph is an ordered triple  $\mathcal{B} = \langle V, F, E \rangle$  where V and F are disjoint sets of vertices and E is a set of undirected edges (v - f) between vertices  $v \in V$  and  $f \in F$ . For a vertex  $x \in V \cup F$  we write  $\operatorname{adj}_{\mathcal{B}}(x) = \{y \in V \cup F : (x - y) \in E\}$  for its adjacencies, and for  $X \subseteq V \cup F$  we write  $\operatorname{adj}_{\mathcal{B}}(X) = \bigcup_{x \in X} \operatorname{adj}_{\mathcal{B}}(x)$  to denote the adjacencies of X in  $\mathcal{B}$ . A matching  $M \subseteq E$  for a bipartite graph  $\mathcal{B} = \langle V, F, E \rangle$ is a subset of edges that have no common endpoints. We say that two vertices xand y are matched when  $(x - y) \in M$ . We let M(x) denote the set of vertices to which x is matched. Note that if  $(x - y) \in M$  then  $M(x) = \{y\}$  and if x is not matched then  $M(x) = \emptyset$ . We let  $M(X) = \bigcup_{x \in X} M(x)$  denote the set of vertices to which the set of vertices  $X \subseteq V \cup F$  is matched. A matching is *perfect* if all vertices  $V \cup F$  are matched.

### 1.2.2 Directed graphs

A directed graph is an ordered pair  $\mathcal{G} = \langle V, E \rangle$  where V is a set of vertices and E is a set of directed edges  $(v \to w)$  between distinct vertices  $v, w \in V$ .<sup>2</sup> We say that a vertex v is a parent of w if  $(v \to w) \in E$  and write  $v \in \operatorname{pa}_{\mathcal{G}}(w)$ . Similarly we say that w is a child of v if  $(v \to w) \in E$  and write  $w \in \operatorname{ch}_{\mathcal{G}}(v)$ . A path is a sequence of distinct vertices and edges  $(v_1, e_1, v_2, e_2, \ldots, e_{n-1}, v_n)$  where for  $i = 1, \ldots, n-1$ either  $e_i = (v_i \to v_{i+1})$  or  $e_i = (v_i \leftarrow v_{i+1})$ . The path is called open if there is no  $v_i \in \{v_2, \ldots, v_{n-1}\}$  such that  $v_{i-1} \to v_i \leftarrow v_{i+1}$  (i.e. there is no collider on the path). A directed path  $(v \to \ldots \to w)$  from v to w is a path where all arrowheads point in the direction of w. We say that v is an ancestor of w if there is a directed path from v to w and write  $v \in \operatorname{an}_{\mathcal{G}}(w)$ . We say that w is a descendant of v if there is a directed path from v to w and write  $w \in \operatorname{de}_{\mathcal{G}}(v)$ .

Let  $\mathcal{G} = \langle V, E \rangle$  be a directed graph and consider the relation:

 $v \sim w \iff w \in \operatorname{an}_{\mathcal{G}}(v) \cap \operatorname{de}_{\mathcal{G}}(v) = \operatorname{sc}_{\mathcal{G}}(v).$ 

Since the relation is reflexive, symmetric, and transitive this is an equivalence relation. The equivalence classes  $sc_{\mathcal{G}}(v)$  are called the *strongly connected components* of  $\mathcal{G}$ . A directed graph without self-cycles is *acyclic* if all of its strongly connected components are singletons.

### 1.2.3 Interventions and marginalization on mixed graphs

A mixed graph is an ordered triple  $\mathcal{G} = \langle V, E, B \rangle$  where  $\langle V, E \rangle$  is a directed graph and B is a set of bi-directed edges between vertices in V. A perfect intervention do(I) on  $\mathcal{G}$  removes all edges with an arrowhead at one of the nodes  $i \in I \subseteq V$ . That is,  $\mathcal{G}_{do(I)} = \langle V, E', B' \rangle$  where  $E' = \{(x \to y) \in E : y \notin I\}$  and  $B' = \{(x \leftrightarrow y) \in B : x \notin I, y \notin I\}$ . Marginalizing out a set of nodes  $W \subseteq V$  from a mixed graph  $\mathcal{G} = \langle V, E, B \rangle$  results in a mixed graph  $\mathcal{G}_{mar(W)} = \langle V \setminus W, E_{mar(W)}, B_{mar(W)} \rangle$ where:

- (i)  $E_{\max(W)}$  consists of edges  $(x \to y)$  such that  $x, y \in V \setminus W$  and there exist  $w_1, \ldots, w_k \in W$  such that the path  $x \to w_1 \to \ldots \to w_k \to y$  is in  $\mathcal{G}$ .
- (ii)  $B_{\max(W)}$  consists of edges  $(x \leftrightarrow y)$  such that  $x, y \in V \setminus W$  and there exist  $w_1, \ldots, w_k \in W$  such that at least one of the following paths is in  $\mathcal{G}$ : (i)  $x \leftrightarrow y$ , or (ii)  $x \leftarrow w_1 \leftarrow \ldots \leftarrow w_i \rightarrow \ldots \rightarrow w_k \rightarrow y$ , or (iii)  $x \leftarrow w_1 \leftarrow \ldots \leftarrow w_i \leftrightarrow w_{i+1} \rightarrow \ldots \rightarrow w_k \rightarrow y$ .

The operations of marginalization and intervention commute (Forré and Mooij, 2017).

### 1.2.4 Graph separation and Markov properties

In the literature, several versions of Markov properties for graphical models and corresponding probability distributions have been put forward, see e.g. Forré and

 $<sup>^2\</sup>mathrm{We}$  do not allow for self-cycles in directed graphs.

Mooij (2017), Lauritzen et al. (1990), and Pearl (2000). For Directed Acyclic Graphs (DAGs) and Acyclic Directed Mixed Graphs (ADMGs), the d-separation criterion is often used to relate conditional independences between variables in a model to the underlying (acyclic) graphical structure of the model (Pearl, 2000). For graphs that contain cycles, such a relation does not hold in general and for that purpose Forré and Mooij (2017) introduced the  $\sigma$ -separation criterion and the generalized directed global Markov property.

**Definition 1.** For a directed graph  $\mathcal{G} = \langle V, E \rangle$  we say that a path  $(v_1, \ldots, v_n)$  is  $\sigma$ -blocked by  $Z \subseteq V$  if

- (i)  $v_1 \in Z$  and/or  $v_n \in Z$ , or
- (ii) there is a vertex  $v_i \notin \operatorname{an}_{\mathcal{G}}(Z)$  on the path such that the adjacent edges both have an arrowhead at  $v_i$ , or
- (iii) there is a vertex  $v_i \in Z$  on the path such that:  $v_i \to v_{i+1}$  with  $v_{i+1} \notin \operatorname{sc}_{\mathcal{G}}(v_i)$ , or  $v_{i-1} \leftarrow v_i$  with  $v_{i-1} \notin \operatorname{sc}_{\mathcal{G}}(v_i)$ , or both.

The path is *d*-blocked by Z if it is  $\sigma$ -blocked or if there is a vertex  $v_i \in Z$  on the path such that at least one of the adjacent edges does not have an arrowhead at  $v_i$ . We say that  $X \subseteq V$  and  $Y \subseteq V$  are  $\sigma$ -separated by  $Z \subseteq V$  if every path in  $\mathcal{G}$  with one end-vertex in X and one end-vertex in Y is  $\sigma$ -blocked by Z, and write

$$X \stackrel{\sigma}{\perp}_{\mathcal{G}} Y \mid Z.$$

If every such path is d-blocked by Z then we say that X and Y are d-separated by Z, and write

$$X \stackrel{d}{\perp} Y \mid Z.$$

The d-separations or  $\sigma$ -separations in a probabilistic graphical model may imply conditional independences via the Markov properties in Definition 2 below.

**Definition 2.** For a directed graph  $\mathcal{G} = \langle V, E \rangle$  and a probability distribution  $\mathbb{P}_{\mathbf{X}}$ on a product  $\mathcal{X} = \bigotimes_{v \in V} \mathcal{X}_v$  of standard measurable spaces  $\mathcal{X}_v$ , we say that the pair  $(\mathcal{G}, \mathbb{P}_{\mathbf{X}})$  satisfies the *directed global Markov property* if for all subsets  $W, Y, Z \subseteq V$ :

$$W \stackrel{d}{\perp} Y | Z \implies X_W \underset{\mathbb{P}_X}{\perp} X_Y | X_Z.$$

The pair  $(\mathcal{G}, \mathbb{P}_{\mathbf{X}})$  satisfies the generalized directed global Markov property if for all subsets  $W, Y, Z \subseteq V$ :

$$W \stackrel{\sigma}{\underset{\mathcal{G}}{\sqcup}} Y | Z \implies X_W \underset{\mathbb{P}_X}{\amalg} X_Y | X_Z.$$

It has been shown that for acylic graphs the d-separation and  $\sigma$ -separation criteria are equivalent (Forré and Mooij, 2017). For acyclic structural causal models, which are also known as recursive structural equation models, the induced probability distribution on endogenous variables and the corresponding graph satisfy the directed global Markov property (Lauritzen et al., 1990). A more comprehensive account of Markov properties for structural causal models is provided by Bongers, Forré, et al. (2020).

# **1.3** System of constraints

We give a formal definition of sets of equations and a representation of their structure as a bipartite graph by introducing a mathematical object that we call a *system of constraints*.

**Definition 3.** A system of constraints is a tuple  $\langle \mathcal{X}, \mathcal{X}_W, \Phi, \mathcal{B} = \langle V, F, E \rangle \rangle$  where

- (i)  $\mathcal{X} = \bigotimes_{v \in V} \mathcal{X}_v$ , where each  $\mathcal{X}_v$  is a standard measurable space and the domain of a variable  $X_v$ ,
- (ii)  $\boldsymbol{X}_W = (X_w)_{w \in W}$  is a family of independent random variables taking value in  $\boldsymbol{\mathcal{X}}_W$  with  $W \subseteq V$  a set of indices corresponding to exogenous variables,<sup>3</sup>
- (iii)  $\mathbf{\Phi} = (\Phi_f)_{f \in F}$  is a family of constraints, each of which is a tuple  $\Phi_f = \langle \phi_f, c_f, V(f) \rangle$ , with:
  - (a)  $V(f) \subseteq V$
  - (b)  $c_f$  a constant taking value in a standard measurable space  $\mathcal{Y}$ ,
  - (c)  $\phi_f : \mathcal{X}_{V(f)} \to \mathcal{Y}$  a measurable function,
- (iv)  $\mathcal{B} = \langle V, F, E \rangle$  is a bipartite graph with:
  - (a) V a set of nodes corresponding to variables,
  - (b) F a set of nodes corresponding to constraints,
  - (c)  $E = \{(f v) : f \in F, v \in V(f)\}$  a set of edges.

Henceforth we will use the terms 'variables' and 'vertices corresponding to variables' interchangeably. We will also use the terms 'constraints', 'equations', and 'vertices corresponding to constraints' interchangeably. A constraint is formally defined as a triple consisting of a measurable function, a constant, and a subset of the variables. For the sake of convenience we will often write constraints as equations instead. Note that the notation for adjacencies in the associated bipartite graph is equivalent to the notation for the variables that belong to a constraint:  $V(f) = \operatorname{adj}_{\mathcal{B}}(f)$ . We will let  $\operatorname{adj}_{\mathcal{B}}(S_F) = V(S_F) = \bigcup_{f \in S_F} V(f)$  denote the adjacencies of the vertices  $f \in S_F \subseteq F$ .

# 2 Causal ordering

In this section, we adapt the causal ordering algorithm of Simon (1953), as it is described in Simon (1953), rephrase it in terms of *self-contained* bipartite graphs, and define the output of the algorithm as a *directed cluster graph*.<sup>4</sup> We then prove that Simon's causal ordering algorithm is well-defined and has a unique output.

**Definition 4.** A directed cluster graph is an ordered pair  $\langle \mathcal{V}, \mathcal{E} \rangle$ , where  $\mathcal{V}$  is a partition  $V^{(1)}, V^{(2)}, \ldots, V^{(n)}$  of a set of vertices V and  $\mathcal{E}$  is a set of edges  $v \to V^{(i)}$  with  $v \in V$  and  $V^{(i)} \in \mathcal{V}$ . For  $x \in V$  we let cl(x) denote the cluster in  $\mathcal{V}$  that contains x. We say that there is a directed path from  $x \in V$  to  $y \in V$  if either cl(x) = cl(y) or there is a sequence of clusters  $V_1 = cl(x), V_2, \ldots, V_{k-1}, V_k = cl(y)$  so that for all  $i \in \{1, \ldots, k-1\}$  there is a vertex  $z_i \in V_i$  such that  $(z_i \to V_{i+1}) \in \mathcal{E}$ .

<sup>&</sup>lt;sup>3</sup>This means that the nodes  $V \setminus W$  correspond to endogenous variables.

 $<sup>^{4}</sup>$ The notion of a directed cluster graph corresponds to the box representation of a collapsed graph in Richardson (1996), Chapter 4.

# 2.1 Self-contained bipartite graphs

The causal ordering algorithm in Simon (1953) is presented in terms of a *self-contained* set of equations and variables that appear in them. For bipartite graphs, the notion of *self-containedness* corresponds to the conditions in Definition 5.

**Definition 5.** Let  $\mathcal{B} = \langle V, F, E \rangle$  be a bipartite graph. A subset  $F' \subseteq F$  is said to be *self-contained* if

- (i)  $|F'| = |\operatorname{adj}_{\mathcal{B}}(F')|,$
- (ii)  $|F''| \leq |\operatorname{adj}_{\mathcal{B}}(F'')|$  for all  $F'' \subseteq F'$ .<sup>5</sup>

The bipartite graph  $\mathcal{B}$  is said to be *self-contained* if |F| = |V| and F is self-contained. A non-empty self-contained set  $F' \subseteq F$  is said to be a *minimal self-contained set*<sup>6</sup> if all its non-empty strict subsets are not self-contained.

Example 2. In Figure 2 a bipartite graph is shown with self-contained sets

$${f_1}, {f_1, f_2, f_3, f_4}, {f_1, f_2, f_3, f_4, f_5}$$

where  $\{f_1\}$  is a minimal self-contained set. Since the set  $\{f_1, f_2, f_3, f_4, f_5\}$  is self-contained and |V| = |F| = 5, we say that this bipartite graph is self-contained.  $\triangle$ 



Figure 2: A self-contained bipartite graph  $\mathcal{B} = \langle V, F, E \rangle$  with  $V = \{v_1, v_2, v_3, v_4, v_5\}$ and  $F = \{f_1, f_2, f_3, f_4, f_5\}$ . The sets  $\{f_1\}$ ,  $\{f_1, f_2, f_3, f_4\}$ , and  $\{f_1, f_2, f_3, f_4, f_5\}$  are self-contained, and  $\{f_1\}$  is the only minimal self-contained set.

Sets of equations that model systems in the real world often include both *endogenous* and *exogenous* variables. The distinction is that exogenous variables are assumed to be determined outside the system and function as inputs to the model, whereas the endogenous variables are part of the system. The following example illustrates that the associated bipartite graph for a set of equations with both endogenous and exogenous variables is usually not self-contained.

**Example 3.** Let  $V = \{v_1, v_2, w_1, w_2\}$  be an index set for endogenous and exogenous variables  $\mathbf{X} = (X_i)_{i \in V}$ ,  $W = \{w_1, w_2\}$  a subset that is an index set for exogenous variables only, and  $F = \{f_1, f_2\}$  an index set for equations:

$$\Phi_{f_1}: \qquad X_{v_1} - X_{w_1} = 0,$$
  
$$\Phi_{f_2}: \qquad X_{v_2} - X_{v_1} - X_{w_2} = 0.$$

<sup>&</sup>lt;sup>5</sup>This condition is also called the Hall Property (Hall, 1986).

<sup>&</sup>lt;sup>6</sup>In this case the Strong Hall Property holds, that is  $|F''| < |\operatorname{adj}_{\mathcal{B}}(F'')|$  for all  $\emptyset \subsetneq F'' \subsetneq F'$  (Hall, 1986).

The associated bipartite graph  $\mathcal{B} = \langle V, F, E \rangle$  is given in Figure 3(a). It has vertices V, correspond to both endogenous variables  $X_{v_1}, X_{v_2}$  and exogenous variables  $X_{w_1}, X_{w_2}$ . The vertices F correspond to constraints  $\Phi_{f_1}$  and  $\Phi_{f_2}$ . Edges between vertices  $v \in V$  and  $f \in F$  are present whenever  $v \in V(F)$  (i.e. when the variable  $X_v$  appears in the constraint  $\Phi_f$ ). Since  $|V| \neq |F|$ , the associated bipartite graph is not self-contained.  $\bigtriangleup$ 



Figure 3: The bipartite graph in Figure 3(a) is associated with the constraints in Example 3. Exogenous variables are indicated by dashed circles. The directed cluster graph that is obtained by applying Algorithm 1 is shown in Figure 3(b).

# 2.2 Causal ordering algorithm

The causal ordering algorithm, as formulated by Simon (1953), has as input a self-contained set of equations and as output it has an ordering on clusters of variables that appear in these equations. We reformulate the algorithm in terms of bipartite graphs and minimal self-contained sets. The input of the algorithm is then a self-contained bipartite graph and its output a directed cluster graph that we call the *causal ordering graph*.

The causal ordering algorithm can easily be adapted for systems of constraints with exogenous variables. The input is then a bipartite graph  $\mathcal{B} = \langle V, F, E \rangle$  and a set of vertices  $W \subseteq V$  (corresponding to exogenous variables) such that the subgraph  $\mathcal{B}'$  induced by  $(V \setminus W) \cup F$  is self-contained. The algorithm starts out by adding the exogenous vertices as singleton clusters to a cluster set  $\mathcal{V}$  during an initialization step. Subsequently, the algorithm searches for a minimal selfcontained set  $S_F \subseteq F$  in  $\mathcal{B}'$ . Together with the set of adjacent variable vertices  $S_V = \operatorname{adj}_{\mathcal{B}}(S_F)$  a cluster  $S_F \cup S_V$  is formed and added to  $\mathcal{V}$ . For each  $v \in V$ , an edge  $(v \to (S_F \cup S_V))$  is added to  $\mathcal{E}$  if  $v \notin S_V$  and  $v \in \operatorname{adj}_{\mathcal{B}}(S_F)$ . In other words, the cluster has an incoming edge from each variable vertex that is adjacent to the cluster but not in it. These steps are then repeated for the subgraph induced by the vertices  $(V \cup F) \setminus (S_V \cup S_F)$  that are not in the cluster, as long as this is not the null graph. The order in which the self-contained sets are obtained is represented by one of the topological orderings of the clusters in the causal ordering graph  $\operatorname{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ . See Algorithm 1 below for more details.

Theorem 1 shows that the output of causal ordering via minimal self-contained sets is well-defined and unique.

**Theorem 1.** The output of Algorithm 1 is well-defined and unique.

Algorithm 1: Causal ordering using minimal self-contained sets.

**Input:** a set of exogenous vertices W, a bipartite graph  $\mathcal{B} = \langle V, F, E \rangle$  such that the subgraph induced by  $(V \cup F) \setminus W$  is self-contained **Output:** directed cluster graph  $CO(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$  $\mathcal{E} \leftarrow \emptyset$ // initialization  $\mathcal{V} \leftarrow \{\{w\} : w \in W\}$ // initialization  $\mathcal{B}' \leftarrow \langle V', F', E' \rangle$  subgraph induced by  $(V \cup F) \setminus W$ // initialization while  $\mathcal{B}'$  is not the null graph do  $S_F \leftarrow$  a minimal self-contained set of F' $C \leftarrow S_F \cup \operatorname{adj}_{\mathcal{B}'}(S_F)$ // construct cluster  $\mathcal{V} \leftarrow \mathcal{V} \cup \{C\}$ // add cluster for  $v \in \operatorname{adj}_{\mathcal{B}}(S_F) \setminus \operatorname{adj}_{\mathcal{B}'}(S_F)$  do  $\[ \mathcal{E} \leftarrow \mathcal{E} \cup \{(v \to C)\}\]$ // add edges to cluster  $\mathcal{B}' \leftarrow \text{subgraph of } \mathcal{B}' \text{ induced by } (V' \cup F') \setminus C$ // remove cluster

The following example shows how the causal ordering algorithm works on the self-contained bipartite graph in Figure 2 and the bipartite graph in Figure 3(a).

**Example 4.** Consider the set of equations in Example 3 and its associated bipartite graph in Figure 3(a). The subgraph induced by the endogenous variables  $v_1, v_2$ and the constraints  $f_1, f_2$  is self-contained. We initialize Algorithm 1 with  $\mathcal{E}$  the empty set,  $\mathcal{V} = \{\{w_1\}, \{w_2\}\}$ , and  $\mathcal{B}'$  be the subgraph induced by  $\{v_1, v_2, f_1, f_2\}$ . We then first find the minimal self-contained set  $\{f_1\}$ . Its adjacencies are  $\{v_1\}$  in  $\mathcal{B}'$  and  $\{v_1, w_1\}$  in  $\mathcal{B}$ . We add  $\{v_1, f_1\}$  to  $\mathcal{V}$  and add the edge  $(w_1 \to \{v_1, f_1\})$  to  $\mathcal{E}$ . Finally, we add  $\{v_2, f_2\}$  to  $\mathcal{V}$  and the edges  $(v_1 \to \{v_2, f_2\})$  and  $(w_2 \to \{v_2, f_2\})$ to  $\mathcal{E}$ . The output of the causal ordering algorithm is the directed cluster graph in Figure 3(b). This reflects how one would solve the system of equations  $\Phi_{f_1}, \Phi_{f_2}$ with respect to  $X_{v_1}, X_{v_2}$  in terms of  $X_{w_1}, X_{w_2}$  by hand.

# 3 Markov ordering graph

First we consider (unique) solvability assumptions for systems of constraints. We will then prove that the constructed *Markov ordering graph* implies conditional independences between variables that appear in constraints. Finally, we apply our method to the model for the filling bathtub in Example 1.

# 3.1 Solvability for systems of constraints

We consider (unique) solutions of systems of constraints with exogenous random variables, and give a sufficient condition under which the output of the causal ordering algorithm can be interpreted as the order in which sets of (endogenous) variables can be solved in a set of equations (i.e. constraints).

**Definition 6.** We say that a tuple of random variables  $X^* = (X_v^*)_{v \in V}$  taking value in  $\mathcal{X}$  is a solution to a system of constraints  $\langle \mathcal{X}, X_W, \Phi, \mathcal{B} \rangle$  if  $X_W^* = X_W$  almost surely and

$$\phi_f(\boldsymbol{X}_{V(f)}^*) = c_f, \quad \forall f \in F, \quad \mathbb{P}_{\boldsymbol{X}^*}\text{-a.s.}$$

We say that it is *uniquely* solvable if all its solutions are almost surely equal.

The system of constraints in the example below is not uniquely solvable and has solutions with different distributions. The example illustrates that the dependence or independence between solution components (i.e. endogenous variables) is not the same for all solutions.

**Example.** Consider a system of constraints  $\langle \mathcal{X}, \mathcal{X}_W, \Phi, \mathcal{B} \rangle$  with  $\mathcal{X} = \mathbb{R}^4$  and independent exogenous random variables  $\mathcal{X}_W = (X_w)_{w \in \{w_1, w_2\}}$  taking value in  $\mathbb{R}^2$ . Suppose that  $\Phi$  consists of the constraints

$$\Phi_{f_1} = \langle X_{V(f_1)} \mapsto X_{v_1} - X_{w_1}, 0, \{v_1, w_1\} \rangle,$$
  
$$\Phi_{f_2} = \langle X_{V(f_2)} \mapsto X_{v_2}^2 - |X_{w_2}|, 0, \{v_2, w_2\} \rangle.$$

This system of constraints has solutions with different distributions. One solution is given by the tuple  $(X_{v_1}^*, X_{v_2}^*, X_{w_1}^*, X_{w_2}^*) = (X_{w_1}^*, \sqrt{|X_{w_2}^*|}, X_{w_1}, X_{w_2})$  and another is given by  $(X_{v_1}', X_{v_2}', X_{w_1}', X_{w_2}') = (X_{w_1}', \operatorname{sgn}(X_{w_1}')\sqrt{|X_{w_2}'|}, X_{w_1}, X_{w_2})$ . Note that the solution components  $X_{v_1}^*$  and  $X_{v_2}^*$  are independent, whereas the solution components  $X_{v_1}'$  and  $X_{v_2}'$  may be dependent.  $\bigtriangleup$ 

In order to avoid underspecified systems of constraints we require that the system is *uniquely* solvable. In Definition 7 below we give a sufficient condition under which the solution can be obtained by solving clusters of variables from clusters of equations in the topological ordering of the causal ordering graph.

**Definition 7.** A system of constraints  $\mathcal{M} = \langle \mathcal{X}, \mathcal{X}_W, \Phi, \mathcal{B} \rangle$  is uniquely solvable w.r.t. constraints  $S_F \subseteq F$  and endogenous variables  $S_V \subseteq V(S_F) \setminus W$  if for all  $v \in S_V$  there exists a measurable function  $g_v : \mathcal{X}_{V(S_F) \setminus S_V} \to \mathcal{X}_v$  s.t. for all  $\mathcal{X}_{V(S_F)} \in \mathcal{X}_{V(S_F)}$ :

$$\phi_f(\boldsymbol{x}_{V(f)}) = c_f, \ \forall f \in S_F \iff x_v = g_v(\boldsymbol{x}_{V(S_F) \setminus S_V}), \ \forall v \in S_V.$$

We say that  $\mathcal{M}$  is uniquely solvable w.r.t. the causal ordering graph  $\operatorname{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ if it is uniquely solvable w.r.t.  $S \cap F$  and  $S \cap V$  for all  $S \in \mathcal{V}$  with  $S \cap W = \emptyset$ .

### 3.2 Directed global Markov property via causal ordering

The *Markov ordering graph* is constructed from a causal ordering graph by *declustering* and then marginalizing out the vertices that correspond to constraints.

**Definition 8.** Let  $\mathcal{G} = \langle \mathcal{V}, \mathcal{E} \rangle$  be a directed cluster graph. The *declustered* graph is given by  $D(\mathcal{G}) = \langle V, E \rangle$  with  $V = \bigcup_{S \in \mathcal{V}} S$  and  $(v \to w) \in E$  if and only if  $(v \to cl(w)) \in \mathcal{E}$ . For a system of constraints  $\mathcal{M} = \langle \mathcal{X}, \mathcal{X}_W, \Phi, \mathcal{B} = \langle V, F, E \rangle \rangle$ , where the subgraph of  $\mathcal{B}$  induced by  $(V \cup F) \setminus W$  is self-contained, we say that  $MO(\mathcal{B}) = D(CO(\mathcal{B}))_{mar(F)}$  is the *Markov ordering graph*.



Figure 4: The bipartite graph corresponding to the bathtub system in Section 3.3.

We assume that systems of constraints are uniquely solvable with respect to their causal ordering graph. Under this assumption Theorem 2 relates dseparations between vertices in the Markov ordering graph to conditional independences between the corresponding solution components of a uniquely solvable system of constraints.

**Theorem 2.** Let  $X^*$  be a solution of a system of constraints  $\mathcal{M} = \langle \mathcal{X}, X_W, \Phi, \mathcal{B} \rangle$ , where the subgraph of  $\mathcal{B} = \langle V, F, E \rangle$  induced by  $(V \cup F) \setminus W$  is self-contained. If  $\mathcal{M}$  is uniquely solvable with respect to the causal ordering graph  $CO(\mathcal{B})$  then the pair  $(MO(\mathcal{B}), \mathbb{P}_{X^*})$  satisfies the directed global Markov property.

# 3.3 Application to the filling bathtub

In Example 1 we informally described a model for a filling bathtub. The endogenous variables of the system are the diameter  $X_K$  of the drain, the rate  $X_I$  at which water flows from the faucet, the water pressure  $X_P$ , the rate  $X_O$  at which the water goes through the drain and the water level  $X_D$ . This model is formally represented by a system of constraints  $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$  where

- (i)  $\mathcal{X} = \mathbb{R}^{12}_{>0}$  is a product of standard measurable spaces corresponding to the domain of variables that are indexed by  $\{v_K, v_I, v_P, v_O, v_D, w_K, w_I, w_1, \dots, w_5\}$ ,
- (ii)  $\mathbf{X}_W = \{U_I, U_K, U_1, \dots, U_5\}$  is a family of independent exogenous random variables indexed by  $\{w_K, w_I, w_1, \dots, w_5\}$ ,
- (iii)  $\Phi$  is a family of constraints:

$$\begin{split} \Phi_{f_K} &= \langle X_{V(f_K)} \mapsto X_K - U_K, & 0, \quad V(f_K) = \{v_K, w_K\} \rangle, \\ \Phi_{f_I} &= \langle X_{V(f_I)} \mapsto X_I - U_I, & 0, \quad V(f_I) = \{v_I, w_I\} \rangle, \\ \Phi_{f_P} &= \langle X_{V(f_P)} \mapsto U_1(gU_2X_D - X_P), & 0, \quad V(f_P) = \{v_D, v_P, w_1, w_2\} \rangle, \\ \Phi_{f_O} &= \langle X_{V(f_O)} \mapsto U_3(U_4X_KX_P - X_O), & 0, \quad V(f_O) = \{v_K, v_P, v_O, w_3, w_4\} \rangle, \\ \Phi_{f_D} &= \langle X_{V(f_D)} \mapsto U_5(X_I - X_O), & 0, \quad V(f_D) = \{v_I, v_O, v_5\} \rangle, \end{split}$$

(iv) the associated bipartite graph  $\mathcal{B} = \langle V, F, E \rangle$  is as in Figure 4. The vertices  $F = \{f_K, f_I, f_P, f_O, f_D\}$  correspond to constraints and the vertices  $W = \{w_I, w_K, w_1, \ldots, w_5\}$  and  $V \setminus W = \{v_K, v_I, v_P, v_O, v_D\}$  correspond to endogenous and exogenous variable respectively. Note that the subgraph induced by the endogenous vertices  $V \setminus W$  is the self-contained bipartite graph presented in Figure 1(a).



Figure 5: The causal ordering graph for the system of a filling bathtub. The directed cluster graph is obtained by applying the causal ordering algorithm to the bipartite graph in Figure 4.

Solvability with respect to the causal ordering graph: Applying Algorithm 1 to the bipartite graph results in the causal ordering graph  $CO(\mathcal{B})$  in Figure 5. It is easy to verify that  $\mathcal{M}$  is uniquely solvable with respect to  $CO(\mathcal{B})$ :

- (i) For the cluster  $\{f_K, v_K\}$  we have that  $X_K U_K = 0 \iff X_K = U_K$ .
- (ii) For the cluster  $\{f_I, v_I\}$  we have that  $X_I U_I = 0 \iff X_I = U_I$ .
- (iii) For  $\{f_O, v_P\}$  we have that  $U_3(U_4X_KX_P X_O) = 0 \iff X_P = \frac{X_O}{U_4X_K}$ .
- (iv) For  $\{f_D, v_O\}$  we have that  $U_5(X_I X_O) \iff X_O = X_I$ .
- (v) For  $\{f_P, v_D\}$  we have that  $U_1(gU_2X_D X_P) \iff X_D = \frac{X_P}{aU_2}$ .

One way to verify unique solvability with respect to a directed cluster graph is to explicitly calculate its solutions, as we have done for the bathtub. In practice, we do not always need to manually check the assumption of unique solvability with respect to the causal ordering graph. For example, in linear systems of equations of the form AX = Y, we may use the fact that this assumption is satisfied when the matrix of coefficients A is invertible. More generally, global implicit function theorems give conditions under which (non-linear) systems of equations have a unique solution (Krantz and Parks, 2013).

**Markov ordering graph** By applying the causal ordering algorithm to the bipartite graph in Figure 4 we obtain the causal ordering graph in Figure 5. Application of declustering and marginalization of vertices in F, as in Definition 8 results in the Markov ordering graph in Figure 6(a). Since  $\mathcal{M}$  is uniquely solvable with respect to  $CO(\mathcal{B})$ , Theorem 2 tells us that the pair  $(MO(\mathcal{B}), \mathbb{P}_{X^*})$  satisfies the directed global Markov property, where  $X^*$  is a solution of  $\mathcal{M}$ .

**Encoded conditional independences:** Under the assumption of unique solvability with respect to the causal ordering graph, we can read off conditional independences between endogenous variables from the Markov ordering graph. More precisely, the d-separations in  $MO(\mathcal{B})$  between vertices in  $V \setminus W$  imply conditional



Figure 6: The Markov ordering graph for the system of a filling bathtub, obtained by applying Definition 8 to the causal ordering graph in Figure 5 is given in Figure 6(a). The d-separations in this graph imply conditional independences between corresponding endogenous variables. Most of these conditional independences cannot be read off from the graph for the SCM of the bathtub system in Figure 6(b), except for  $X_I \perp \!\!\!\perp X_K$ .

independences between the corresponding endogenous variables. For example:

$$\begin{array}{cccc} v_{K} \stackrel{d}{\underset{\mathrm{MO}(\mathcal{B})}{\perp}} v_{O} \implies X_{K} \perp \!\!\!\!\perp X_{O}, \\ \\ v_{K} \stackrel{d}{\underset{\mathrm{MO}(\mathcal{B})}{\perp}} v_{D} \mid v_{P} \implies X_{K} \perp \!\!\!\!\perp X_{D} \mid X_{P}, \\ \\ v_{I} \stackrel{d}{\underset{\mathrm{MO}(\mathcal{B})}{\perp}} v_{P} \mid v_{O} \implies X_{I} \perp \!\!\!\!\perp X_{P} \mid X_{O}, \\ \\ v_{O} \stackrel{d}{\underset{\mathrm{MO}(\mathcal{B})}{\perp}} v_{D} \mid v_{P} \implies X_{O} \perp \!\!\!\!\perp X_{D} \mid X_{P}. \end{array}$$

**Comparison to SCM representation:** The (random) differential equations that describe the system of a bathtub at equilibrium can also be mapped to an SCM with the following structural equations (see Bongers and Mooij (2018)):

$$X_K = U_K,$$
  

$$X_I = U_I,$$
  

$$X_P = gU_3 X_D,$$
  

$$X_O = U_5 X_K X_P,$$
  

$$X_D = X_D + U_1 (X_I - X_O).$$

The graph of this SCM is depicted in Figure 6(b). The graph contains both a cycle and a self-loop. There currently is no Markov property for such an SCM that would imply the conditional independence between the diameter  $X_K$  of the drain and the rate  $X_O$  at which water flows through the drain, for instance. Actually, most of the conditional independences implied by the Markov ordering graph cannot be read off from the graphical representation of the SCM via the d-separations, except for  $X_I \perp \!\!\perp X_K$ .

An important difference between SCMs and systems of constraints is that while the former require a particular one-to-one correspondence between endogenous variables and structural equations, the latter do not require a similar correspondence between endogenous variables and constraints. Interestingly, a one-to-one correspondence between variables and constraints is obtained automatically by the causal ordering algorithm. We will discuss several advantages of applying the technique of causal ordering to structural equations in Section 6.2.

# 4 Generalized dGMP via causal ordering

In this section we present an adaptation of an alternative, computationally less expensive, algorithm for causal ordering which uses perfect matchings instead of minimal self-contained sets, similar to the algorithms in Gonçalves and Porto (2016) and Nayak (1995). We provide a proof for the fact that causal ordering via minimal self-contained sets is equivalent to causal ordering via perfect matchings. We also present a novel result regarding the generalized directed global Markov property for solutions of systems of constraints and an *associated directed graph*.

# 4.1 Causal ordering via perfect matchings

The associated directed graph can be constructed from a matching M for a bipartite graph  $\mathcal{B}$  by orienting edges. The causal ordering graph is then constructed via the operations, that construct clusters and merge clusters, in Definition 9 below.

**Definition 9.** Let  $\mathcal{B} = \langle V, F, E \rangle$  be a bipartite graph and M a matching for  $\mathcal{B}$ .

- (i) Orient edges: For each  $(v f) \in E$  the edge set  $E_{\text{dir}}$  has an edge  $(v \leftarrow f)$ if  $(v - f) \in M$  and an edge  $(v \to f)$  if  $(v - f) \notin M$ . It has no additional edges. The associated directed graph is  $\mathcal{G}(\mathcal{B}, M) = \langle V \cup F, E_{\text{dir}} \rangle$ .
- (ii) Construct clusters: Let  $\mathcal{V}'$  be partition of vertices  $V \cup F$  into strongly connected components in  $\mathcal{G}(\mathcal{B}, M)$ . For each  $(x \to w) \in E_{\text{dir}}$  the edge set  $\mathcal{E}'$  has an edge  $(x \to \operatorname{cl}(w))$  if  $x \notin \operatorname{cl}(w)$ , where  $\operatorname{cl}(w) \in \mathcal{V}'$  is the strongly connected component of w in  $\mathcal{G}(\mathcal{B}, M)$ . It has no additional edges. The associated clustered graph is given by  $\operatorname{clust}(\mathcal{G}(\mathcal{B}, M)) = \langle \mathcal{V}', \mathcal{E}' \rangle$ .
- (iii) Merge clusters: Let  $\mathcal{V} = \{S \cup M(S) : S \in \mathcal{V}'\}$ . For each  $(x \to S) \in \mathcal{E}'$  with  $x \notin M(S)$  the edge set  $\mathcal{E}$  contains an edge  $(x \to S \cup M(S))$ . It has no additional edges. The associated clustered and merged graph is given by merge(clust( $\mathcal{G}(\mathcal{B}, M)$ )) =  $\langle \mathcal{V}, \mathcal{E} \rangle$ .

For causal ordering via perfect matchings we require a set of exogenous vertices W and a bipartite graph  $\mathcal{B} = \langle V, F, E \rangle$ , for which the subgraph  $\mathcal{B}'$  induced by the vertices  $(V \cup F) \setminus W$  is self-contained, as input. The output is a directed cluster graph. The details can be found in Algorithm 2. We see that the algorithm starts

out by finding a perfect matching<sup>7 8</sup> for  $\mathcal{B}'$ , which is then used to *orient edges* in the bipartite graph  $\mathcal{B}$ . The algorithm then proceeds by partitioning vertices in the resulting directed graph into strongly connected components to construct the associated clustered graph.<sup>9</sup> Finally, the merge operation is applied to construct the causal ordering graph.

Algorithm 2: Causal ordering via perfect matchings.

**Input:** a set of exogenous vertices W, a bipartite graph  $\mathcal{B} = \langle V, F, E \rangle$  such that the subgraph induced by  $(V \cup F) \setminus W$  is self-contained **Output:** directed cluster graph  $\langle \mathcal{V}, \mathcal{E} \rangle$  $\mathcal{B}' \leftarrow$  subgraph induced by  $(V \cup F) \setminus W$ // initialization  $M \leftarrow \text{perfect matching for } \mathcal{B}'$ // initialization  $E_{\mathrm{dir}} \leftarrow \emptyset$ // orient edges for  $(v - f) \in E$  do if  $(v-f) \in M$  then Add  $(v \leftarrow f)$  to  $E_{dir}$ else  $\mathcal{V}' \leftarrow$  strongly connected components of  $\langle V \cup F, E_{dir} \rangle$ // clustering  $\mathcal{E}' \gets \emptyset$ for  $(x \to w) \in E_{dir}$  do for  $S \in \mathcal{V}'$  do if  $w \in S$  and  $x \notin S$  then Add  $(x \to S)$  to  $\mathcal{E}'$  $\mathcal{V}, \mathcal{E} \leftarrow \emptyset$ // merge clusters for  $S \in \mathcal{V}'$  do Add  $S \cup M(S)$  to  $\mathcal{V}$ for  $(x \to S) \in \mathcal{E}'$  do if  $x \notin M(S)$  then Add  $(x \to S \cup M(S))$  to  $\mathcal{E}$ 

Theorem 3 below shows that causal ordering via perfect matchings is equivalent to causal ordering via minimal self-contained sets.

**Theorem 3.** The output of Algorithm 2 coincides with the output of Algorithm 1.

The following example illustrates that the output of causal ordering via perfect matchings does not depend on the choice of perfect matching and coincides with the output of Algorithm 1.

 $<sup>^7\</sup>mathrm{Note}$  that a bipartite graph has a perfect matching if and only if it is self-contained (Hall, 1986). See also Theorem 5 and Corollary 1 in Section 8.3 in the supplementary material.

<sup>&</sup>lt;sup>8</sup>The Hopcraft-Karp-Karzanov algorithm, which runs in  $\mathcal{O}(|E|\sqrt{|V \cup F|})$ , can be used to find a perfect matching (Hopcroft and Karp, 1973; Karzanov, 1973).

 $<sup>^{9}</sup>$ Tarjan's algorithm, which runs in linear time, can be used to find the strongly connected components in a directed graph (Tarjan, 1972).

**Example 5.** Consider the bipartite graph  $\mathcal{B}$  in Figure 7(a). The subgraph induced by the vertices  $V = \{v_1, \ldots, v_5\}$  and  $F = \{f_1, \ldots, f_5\}$  is the self-contained bipartite graph in Figure 2. We will follow the steps in both Algorithm 1 and 2 to construct the causal ordering graph.

For causal ordering with minimal self-contained sets we first add the exogenous variables to the cluster set  $\mathcal{V}$  as the singleton clusters  $\{w_1\}$ ,  $\{w_2\}$ ,  $\{w_3\}$ ,  $\{w_4\}$ ,  $\{w_5\}$ , and  $\{w_6\}$ . The only minimal self-contained set in the subgraph induced by the vertices  $V = \{v_1, \ldots, v_5\}$  and  $F = \{f_1, \ldots, f_5\}$  is  $\{f_1\}$ . Since  $f_1$  is adjacent to  $v_1$  we add  $C_1 = \{v_1, f_1\}$  to  $\mathcal{V}$ . Since  $f_1$  is adjacent to  $w_1$  in  $\mathcal{B}$  we add  $(w_1 \to C_1)$  to  $\mathcal{E}$ . The subgraph  $\mathcal{B}' = \langle V', F', E' \rangle$  induced by the remaining nodes  $V' = \{v_2, v_3, v_4, v_5\}$  and  $F' = \{f_2, f_3, f_4, f_5\}$  has  $\{f_2, f_3, f_4\}$  as its only minimal self-contained set. Since the set  $\{f_2, f_3, f_4\}$  is adjacent to  $\{v_2, v_3, v_4\}$  in  $\mathcal{B}'$ , we add  $C_2 = \{v_2, v_3, v_4, f_2, f_3, f_4\}$  to  $\mathcal{V}$ . Since  $v_1, w_2, w_3, w_4$ , and  $w_5$  are adjacent to  $\{f_2, f_3, f_4\}$  in  $\mathcal{B}$  but not part of  $C_2$ , we add the edges  $(v_1 \to C_2)$ ,  $(w_2 \to C_2)$ ,  $(w_3 \to C_2)$ ,  $(w_4 \to C_2)$ , and  $(w_5 \to C_2)$  to  $\mathcal{E}$ . The subgraph induced by the remaining nodes  $v_5$  and  $f_5$  has  $\{f_5\}$  as its minimal self-contained subset. We add  $C_3 = \{v_5, f_5\}$  to  $\mathcal{V}$  and the edges  $(v_4 \to C_3)$  and  $(w_6 \to C_3)$  to  $\mathcal{E}$ . The directed cluster graph  $\operatorname{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$  is given in Figure 7(e).

For causal ordering via perfect matchings, we consider the following two perfect matchings of the self-contained bipartite graph in Figure 2:

$$M_1 = \{ (v_1 - f_1), (v_2 - f_2), (v_3 - f_3), (v_4 - f_4), (v_5 - f_5) \}, M_2 = \{ (v_1 - f_1), (v_2 - f_4), (v_3 - f_2), (v_4 - f_3), (v_5 - f_5) \}.$$

We use these one-to-one correspondences between endogenous variable vertices and constraint vertices in the orientation step in Definition 9 to obtain the associated directed graphs  $\mathcal{G}(\mathcal{B}, M_1)$  and  $\mathcal{G}(\mathcal{B}, M_2)$  in Figures 7(b) and 7(c) respectively. Application of the clustering step in Definition 9 to either  $\mathcal{G}(\mathcal{B}, M_1)$  or  $\mathcal{G}(\mathcal{B}, M_2)$ results in the clustered graph  $\operatorname{clust}(\mathcal{G}(\mathcal{B}, M_2)) = \operatorname{clust}(\mathcal{G}(\mathcal{B}, M_1))$  in Figure 7(d). The final step is to merge clusters in this directed cluster graph. We find that the causal ordering graph merge( $\operatorname{clust}(\mathcal{G}(\mathcal{B}, M_1))) = \operatorname{merge}(\operatorname{clust}(\mathcal{G}(\mathcal{B}, M_2)))$  in Figure 7(e) does not depend on the choice of perfect matching. Note that the output of causal ordering with minimal self-contained sets coincides with the output of causal ordering via perfect matchings.

# 4.2 Generalized directed global Markov property

The main result of this section is stated in Proposition 1 below, which shows that, for systems that are uniquely solvable with respect to the causal ordering graph, the  $\sigma$ -separations between variable vertices in the directed graph  $\mathcal{G}(\mathcal{B}, M)_{\max(F)}$ imply conditional independences between the corresponding variables.

**Proposition 1.** Let  $X^*$  be a solution of a system of constraints  $\mathcal{M} = \langle \mathcal{X}, X_W, \Phi, \mathcal{B} \rangle$ , where the subgraph of  $\mathcal{B} = \langle V, F, E \rangle$  induced by  $(V \cup F) \setminus W$  has a perfect matching M. If for each strongly connected component S in  $\mathcal{G}(\mathcal{B}, M)$  with  $S \cap W = \emptyset$ , the system  $\mathcal{M}$  is uniquely solvable w.r.t.  $S_V = (S \cup M(S)) \cap V$  and  $S_F = (S \cup M(S)) \cap F$ 



(e) Causal ordering graph  $CO(\mathcal{B}) = merge(clust(\mathcal{G}(\mathcal{B}, M_1))) = merge(clust(\mathcal{G}(\mathcal{B}, M_2))).$ 

Figure 7: Causal ordering with two different perfect matchings  $M_1$  and  $M_2$  applied to the bipartite graph in Figure 7(a). The results of subsequently orienting edges, constructing clusters, and merging clusters as in Definition 9 are given in Figures 7(b) to 7(e).



Figure 8: The Markov ordering graph of the bipartite graph in Figure 7(a), after marginalization of exogenous vertices W, is given in Figure 8(a). The directed graphs in Figures 8(b) and 8(c) are obtained by marginalizig out the constraint vertices F and exogenous vertices W from the directed graphs  $\mathcal{G}(\mathcal{B}, M_1)$  and  $\mathcal{G}(\mathcal{B}, M_2)$  in Figures 7(b) and 7(c) respectively. Note that d-separations in the Markov ordering graph correspond to  $\sigma$ -separations in the associated directed graphs in Figures 7(b) and 7(c).

then the pair  $(\mathcal{G}(\mathcal{B}, M)_{\max(F)}, \mathbb{P}_{X^*})$  satisfies the generalized directed global Markov property.

**Example 6.** Consider a system of constraints  $\mathcal{M} = \langle \mathcal{X}, \mathcal{X}_W, \Phi, \mathcal{B} \rangle$  with  $W = \{w_1, \ldots, w_6\}, V \setminus W = \{v_1, \ldots, v_5\}, F = \{f_1, \ldots, f_5\}$ , and  $\mathcal{B} = \langle V, F, E \rangle$  as in Figure 7(a). Suppose that  $\mathcal{X} = \mathbb{R}^{11}$  and  $\Phi$  consists of constraints:

$$\begin{split} \Phi_{f_1}: & X_{v_1} - X_{w_1} = 0, \\ \Phi_{f_2}: & X_{v_2} - X_{v_1} + X_{v_3} + X_{w_2} - X_{w_3} = 0, \\ \Phi_{f_3}: & X_{w_4} - X_{v_3} + X_{v_4} = 0, \\ \Phi_{f_4}: & X_{w_5} + X_{v_2} - X_{v_4} = 0, \\ \Phi_{f_5}: & X_{w_6} - X_{v_4} + X_{v_5} = 0. \end{split}$$

It is easy to check that this linear system of equations can be uniquely solved in the order prescribed by the causal ordering graph  $\operatorname{CO}(\mathcal{B})$  in Figure 7(e). Therefore, according to Theorem 2 the d-separations among endogenous variables in the corresponding Markov ordering graph  $\operatorname{MO}(\mathcal{B})$  imply conditional independences between the corresponding endogenous variables. It follows that d-separations in the Markov ordering graph  $\operatorname{MO}(\mathcal{B})_{\max(W)}$  for the endogenous variables in Figure 8(a) imply conditional independences between the corresponding variables. For example, we see that  $v_1$  and  $v_5$  are d-separated by  $v_4$  and deduce that for a solution  $\mathbf{X}^*$  to the system of constraints it holds that  $X_{v_1}^* \perp X_{v_5}^* | X_{v_4}^*$ . Interestingly, d-separations in  $\operatorname{MO}(\mathcal{B})_{\max(W)}$  coincide with  $\sigma$ -separations in the associated directed graphs  $\mathcal{G}(\mathcal{B}, M_1)_{\max(F \cup W)}$  and  $\mathcal{G}(\mathcal{B}, M_2)_{\max(F \cup W)}$ . It follows from Proposition 1 that the  $\sigma$ -separations in  $\mathcal{G}(\mathcal{B}, M_1)_{\max(F \cup W)}$  and  $\mathcal{G}(\mathcal{B}, M_2)_{\max(F \cup W)}$ , which are given in Figures 8(b) and 8(c) respectively, imply conditional independences between the corresponding variables.

# 5 Causal implications for sets of equations

It is common to relate causation directly to the effects of manipulation (Pearl, 2000; Woodward, 2003), although there are many ways to model manipulations on sets of equations. In order to derive causal implications from systems of constraints, we explicitly define two types of manipulation. We consider the notions of both *soft* and *perfect* interventions.<sup>10</sup> We prove that the causal ordering graph represents the effects of both *soft interventions on equations* and *perfect interventions on clusters* in the causal ordering graph. We also show that these manipulations commute with causal ordering.

# 5.1 The effects of soft interventions

A *soft intervention*, also known as a "mechanism change", acts on a constraint. It replaces the targeted constraint by a constraint in which the same variables appear as in the original one. This type of intervention does not change the bipartite graph that represents the structure of the constraints.

**Definition 10.** Let  $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$  be a system of constraints,  $\Phi_f = \langle \phi_f, c_f, V(f) \rangle \in \Phi$  a constraint, c a constant taking value in a measurable space  $\mathcal{Y}$ , and  $\phi : \mathcal{X}_{V(f)} \to \mathcal{Y}$  a measurable function. A soft intervention  $\operatorname{si}(f, \phi, c)$  targeting  $\Phi_f$  results in the intervened system  $\mathcal{M}_{\operatorname{si}(f,\phi,c)} = \langle \mathcal{X}, \mathbf{X}_W, \Phi_{\operatorname{si}(f,\phi,c)}, \mathcal{B} \rangle$  where  $\Phi_{\operatorname{si}(f,\phi,c)} = (\Phi \setminus \{\Phi_f\}) \cup \{\Phi'_f\}$  with  $\Phi'_f = \langle \phi, c, V(f) \rangle$ .

Theorem 4 shows that, under the assumption of unique solvability w.r.t. the causal ordering graph, a soft intervention on a constraint has no effect on variables that cannot be reached by a directed path from that variable in the causal ordering graph, while it generically does have an effect on other variables.<sup>11</sup>

**Theorem 4.** Let  $\mathcal{M} = \langle \mathcal{X}, \mathcal{X}_W, \Phi, \mathcal{B} \rangle$  be a system of constraints such that the subgraph of  $\mathcal{B}$  induced by endogenous variables and constraints is self-contained. Suppose that  $\mathcal{M}$  is uniquely solvable w.r.t. the causal ordering graph  $\operatorname{CO}(\mathcal{B})$  and let  $\mathcal{X}^*$  be a solution. Assume that the intervened system  $\mathcal{M}_{\operatorname{si}(f,\phi,c)}$  is also uniquely solvable w.r.t.  $\operatorname{CO}(\mathcal{B})$  and let  $\mathcal{X}'$  be a solution. If there is no directed path from f to  $v \in V \setminus W$  in  $\operatorname{CO}(\mathcal{B})$  then  $X_v^* = X_v'$  almost surely. Conversely, if there is a directed path f to v in  $\operatorname{CO}(\mathcal{B})$  then  $X_v^*$  may have a different distribution than  $X_v'$ .

This shows that the effects of soft interventions can be read off from the causal ordering graph. We illustrate this idea on the bathtub system.

**Example 7.** Recall the system of constraints for the filling bathtub in Section 3.3. Think of an experiment where the gravitational constant g is changed so that it takes on a different value g' without altering the other equations that describe the bathtub system. Such an experiment is, at least in theory, feasible. For example, it can be accomplished by accelarating the bathtub system or by moving the bathtub system to another planet. We can model such an experiment by a soft intervention targeting  $f_P$  that replaces the constraint  $\Phi_{f_P}$  by

$$\langle X_{V(f_P)} \mapsto U_1(g'U_2X_D - X_P), 0, V(f_P) = \{v_D, v_P, w_1, w_2\} \rangle.$$

<sup>&</sup>lt;sup>10</sup>Our definitions in the context of systems of constraints may deviate from conventional defini-

tions of interventions on Structural Causal Models (also known as Structural Equation Models).  $^{11}$ Our results generalize Theorem 6.1 in Simon (1953), where a similar result is proven for linear systems of equations. The proof of our theorem is similar.

target	generic effect	non-effect
$f_K$	$X_K, X_P, X_D$	$X_I, X_O$
$J_I$ $f_P$	$\begin{array}{c} \boldsymbol{\Lambda}_{I},  \boldsymbol{\Lambda}_{P},  \boldsymbol{\Lambda}_{O},  \boldsymbol{\Lambda}_{D} \\ \boldsymbol{X}_{D} \end{array}$	$X_K$ $X_K, X_I, X_P, X_O$
$f_{O} f_{D}$	$X_P, X_D X_P, X_O, X_D$	$\begin{array}{l} X_K,  X_I,  X_O \\ X_K,  X_I \end{array}$

Table 1: The effects of soft interventions on constraints in the causal ordering graph for the bathtub system in Figure 5.

Which variables are and which are not affected by this soft intervention? We can read off the effects of this soft intervention from the causal ordering graph in Figure 5. There is no directed path from  $f_P$  to  $v_K, v_I, v_P$  or  $v_O$ . Therefore, perhaps surprisingly, Theorem 4 tells us that the soft intervention targeting  $f_P$ neither has an effect on the pressure  $X_P$  nor on the outflow rate  $X_O$ . Since there is a directed path from  $f_P$  to  $v_D$ , the water level  $X_D$  is generically different after the soft intervention on  $f_P$ . The effects and non-effects of soft interventions on other constraints can also be read off from the causal ordering graph and are presented in Table 1. Δ

#### 5.2The effects of perfect interventions

A *perfect* intervention acts on a variable and a constraint. It replaces the targeted constraint by a constraint that sets the targeted variable equal to a constant.<sup>12</sup>

**Definition 11.** Let  $\mathcal{M} = \langle \mathcal{X}, \mathcal{X}_W, \Phi, \mathcal{B} = \langle V, F, E \rangle$  be a system of constraints and let  $\xi_v \in \mathcal{X}_v$ . A perfect intervention  $do(f, v, \xi_v)$  targeting the variable  $v \in$  $V \setminus W$  and the constraint  $f \in F$  results in the intervened system  $\mathcal{M}_{\mathrm{do}(f,v,\xi_v)} =$  $\langle \boldsymbol{\mathcal{X}}, \boldsymbol{X}_W, \boldsymbol{\Phi}_{\mathrm{do}(f,v,\xi_v)}, \mathcal{B}_{\mathrm{do}(f,v)} \rangle$  where

- (i)  $\Phi_{\operatorname{do}(f,v,\xi_v)} = (\Phi \setminus \Phi_f) \cup \{\Phi'_f\}$  with  $\Phi'_f = \langle X_v \mapsto X_v, \xi_v, \{v\}\rangle$ , (ii)  $\mathcal{B}_{\operatorname{do}(f,v)} = \langle V, F, E' \rangle$  with  $E' = \{(i-j) \in E : i, j \neq f\} \cup \{(v-f)\}$ .

Perfect interventions on a set of variable-constraint pairs  $\{(f_1, v_1), \ldots, (f_n, v_n)\}$ in a system of constraints are denoted by  $do(S_F, S_V, \boldsymbol{\xi}_{S_V})$  where  $S_F = \langle f_1, \ldots, f_n \rangle$ and  $S_V = \langle v_1, \ldots, v_n \rangle$  are tuples. For a bipartite graph  $\mathcal{B}$  so that the subgraph induced by  $(V \cup F) \setminus W$  is self-contained, Lemma 1 shows that  $\operatorname{CO}(\mathcal{B}_{\operatorname{do}(S_F \cup S_V)})$ is well-defined if  $S = (S_F \cup S_V)$  is a cluster in  $CO(\mathcal{B})$  with  $S \cap W = \emptyset$ .

 $<sup>^{12}\</sup>mathrm{In}$  an SCM, each variable is associated with a single structural equation. Pearl (2000) defines perfect interventions on a variable as an operation that replaces its corresponding structural equation by an equation that sets the variable equal to a constant. This notion of a perfect intervention is not possible in general for a system of constraints since there is no imposed one-to-one correspondence between equations and variables.

**Lemma 1.** Let  $\mathcal{B} = \langle V, F, E \rangle$  be a bipartite graph and  $W \subseteq V$ , so that the subgraph of  $\mathcal{B}$  induced by  $V \cup F$  is self-contained. Consider an intervention  $\operatorname{do}(S_V, S_F)$  on a cluster  $S = S_V \cup S_F$  with  $S \cap W = \emptyset$  in the causal ordering graph  $\operatorname{CO}(\mathcal{B})$ . The subgraph of  $\mathcal{B}_{\operatorname{do}(S_V, S_F)}$  induced by  $(V \cup F) \setminus W$  is self-contained.

Proposition 2 shows how the causal ordering graph can be used to read off the effects of *perfect interventions on clusters* under the assumption of unique solvability with respect to the causal ordering graph.

**Proposition 2.** Let  $\mathcal{M} = \langle \mathcal{X}, \mathcal{X}_W, \Phi, \mathcal{B} = \langle V, F, E \rangle \rangle$  such that the subgraph of  $\mathcal{B}$  induced by  $(V \cup F) \setminus W$  is self-contained. Assume that it is uniquely solvable w.r.t.  $\operatorname{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$  and let  $\mathbf{X}^*$  be a solution of  $\mathcal{M}$ . Let  $S_F \subseteq F$  and  $S_V \subseteq V \setminus W$  be such that  $(S_F \cup S_V) \in \mathcal{V}$ . Assume that the intervened system  $\mathcal{M}_{\operatorname{do}(S_F,S_V,\boldsymbol{\xi}_{S_V})}$  is uniquely solvable w.r.t.  $\operatorname{CO}(\mathcal{B}_{\operatorname{do}(S_F,S_V)})$  and let  $\mathbf{X}'$  be a solution of  $\mathcal{M}_{\operatorname{do}(S_F,S_V,\boldsymbol{\xi}_{S_V})}$ . If there is no directed path from any  $x \in S_V$  to  $v \in V$  in  $\operatorname{CO}(\mathcal{B})$  then  $X_v^* = X_v'$  almost surely. Conversely, if there is  $x \in S_V$  such that there is a directed path x to v in  $\operatorname{CO}(\mathcal{B})$  then  $X_v^*$  may have a different distribution than  $X_v'$ .

One way to determine whether a perfect intervention has an effect on a certain variable is to explicitly solve the system of constraints before and after the intervention and check which solution components are altered. Under a solvability assumption we can establish the effects of a perfect intervention without solving the equations. Example 8 illustrates this notion of perfect intervention on the system of constraints for the filling bathtub that we first introduced in Example 1 and shows how the effects and non-effects of perfect interventions on clusters can be read off from the causal ordering graph.

**Example 8.** Recall the system of constraints  $\mathcal{M}$  for the filling bathtub in Section 3.3. Consider the perfect interventions  $do(f_P, v_D, \xi_D)$ ,  $do(f_D, v_O, \xi_O)$ , and  $do(f_D, v_D, \xi_D)$ . These interventions model experiments that can, at least in principle, be conducted in practice:

- (i) The intervention  $do(f_P, v_D, \xi_D)$  replaces the constraint  $f_P$  by a constraint that sets the water level  $X_D$  equal to a constant. This could correspond to an experimental set-up where the constant g in the constraint  $\Phi_{f_P}$  is controlled by accelerating and decelerating the bathtub system precisely in such a way that the water level  $X_D$  is forced to take on a constant value  $\xi_D$ .
- (ii) The interventions  $do(f_D, v_O, \xi_O)$  and  $do(f_D, v_D, \xi_D)$ , may correspond to an experiment where a hose is added to the system that can remove or add water precisely in such a way that either the outflow rate  $X_O$  or the water level  $X_D$  is kept at a constant level.

By explicit calculation we obtain the (unique) solutions in Table 2 for the observed and intervened bathtub systems. By comparing with the solutions in the observed column we read off that the perfect intervention  $do(f_P, v_D, \xi_D)$  does not change the solution for the variables  $X_K, X_I, X_P, X_O$ , but it generically does change the solution for  $X_D$ . We further find that  $do(f_D, v_D, \xi_D)$  and  $do(f_D, v_O, \xi_D)$  affect the solution for the variables  $X_P, X_O, X_D$  but not of  $X_K$  and  $X_I$ .

Table 2: Solutions for system of constraints describing the bathtub system in Section 3.3 without interventions (i.e. the observed system) and after perfect interventions  $do(f_P, v_D, \xi_D)$ ,  $do(f_D, v_O, \xi_O)$ , and  $do(f_D, v_D, \xi_D)$ .

	observed	$\operatorname{do}(f_P, v_D, \xi_D)$	$\operatorname{do}(f_D, v_O, \xi_O)$	$\operatorname{do}(f_D, v_D, \xi_D)$
$X_K^*$	$X_{U_K}$	$X_{U_K}$	$X_{U_K}$	$X_{U_K}$
$X_I^*$	$X_{U_{I_{-}}}$	$X_{U_{I_{-}}}$	$X_{U_I}$	$X_{U_I}$
$X_P^*$	$\frac{X_{U_I}}{(X_{C_4}X_{U_K})}$	$\frac{X_{U_I}}{(X_{C_4}X_{U_K})}$	$\frac{\xi_O}{(X_{C_4}X_{U_K})}$	$gX_{C_2}\xi_D$
$X_O^*$	$X_{U_I}$	$X_{U_I}$	ξο	$X_{C_4} X_{U_K} g X_{C_2} \xi_D$
$X_D^*$	$\frac{X_{U_I}}{(X_{C_4}X_{U_K}gX_{C_2})}$	$\xi_D$	$\frac{\xi_O}{(X_{C_4}X_{U_K}gX_{C_2})}$	$\xi_D$

Table 3: The effects of perfect interventions on variables and constraints in the causal ordering graph for the bathtub system in Figure 5 obtained by Proposition 2.

target	generic effect	non-effect
$f_K, v_K$	$X_K, X_P, X_D$	$X_I, X_O$
$f_I, v_I$	$X_I, X_P, X_O, X_D$	$X_K$
$f_P, v_D$	$X_D$	$X_K, X_I, X_P, X_O$
$f_O, v_P$	$X_P, X_D$	$X_K, X_I, X_O$
$f_D, v_O$	$X_P, X_O, X_D$	$X_K, X_I$
$f_P, f_D, f_O, v_P, v_D, v_O$	$X_P, X_O, X_D$	$X_K, X_I$

The causal ordering graph  $CO(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$  for the bathtub system is given in Figure 5. It has clusters  $\mathcal{V} = \{\{f_K, v_K\}, \{f_I, v_I\}, \{f_P, v_D\}, \{f_O, v_P\}, \{f_D, v_O\}\}\}$ . Under the assumption that the (intervened) system is uniquely solvable w.r.t. its causal ordering graph, we can apply Proposition 2 and read off the effects and noneffects of perfect interventions on clusters, which are presented in Table 3. This illustrates the fact that we can establish the generic effects and non-effects of the perfect interventions  $do(f_P, v_D, \xi_D)$  and  $do(f_D, v_O, \xi_O)$ , which act on clusters in the causal ordering graph, without explicitly solving the system of equations. We will discuss differences between causal implications of the causal ordering graph and the graph of the SCM in Figure 6(b) in Section 6.

# 5.3 Interventions commute with causal ordering

We define an operation of "perfect intervention" directly on causal ordering graphs. Roughly speaking, a perfect intervention on a cluster in a directed cluster graph removes all incoming edges to that cluster and separates all variable vertices and constraint vertices in the targeted cluster into separate clusters in a specified way.

**Definition 12.** Let  $\mathcal{B} = \langle V, F, E \rangle$  be a bipartite graph and W a set of exogenous variables such that the subgraph of  $\mathcal{B}$  induced by  $(V \cup F) \setminus W$  is self-contained. Let  $CO(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$  be the corresponding causal ordering graph and consider  $S \in \mathcal{V}$ 

with  $S \cap W = \emptyset$ . Let  $S_F = \langle f_i : i = 1, ..., n \rangle$  and  $S_V = \langle v_i : i = 1, ..., n \rangle$  with  $n = |S \cap V| = |S \cap F|$  be tuples consisting of all the vertices in  $S \cap F$  and  $S \cap V$  respectively. A *perfect intervention on a cluster* do $(S_F, S_V)$  results in the directed cluster graph  $CO(\mathcal{B})_{do(S_F, S_V)} = \langle \mathcal{V}', \mathcal{E}' \rangle$  where

- (i)  $\mathcal{V}' = (\mathcal{V} \setminus \{S\}) \cup \{\{v_i, f_i\} : i = 1, \dots, n\},\$
- (ii)  $\mathcal{E}' = \{ (x \to T) \in \mathcal{E} : T \neq S \}.$

A soft intervention on a system of constraints has no effect on the graphical structure of the constraints and the variables that appear in them. Since the bipartite graph of the system is thus the same before and after soft interventions, it trivially follows that soft interventions commute with causal ordering. The following proposition shows that perfect interventions on clusters also commute with causal ordering.

**Proposition 3.** Let  $\mathcal{B} = \langle V, F, E \rangle$  be a bipartite graph and W a set of exogenous variables such that the subgraph of  $\mathcal{B}$  induced by  $(V \cup F) \setminus W$  is self contained. Let  $CO(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$  be the corresponding causal ordering graph. Let  $S_F \subseteq F$  and  $S_V \subseteq V \setminus W$  be such that  $(S_F \cup S_V) \in \mathcal{V}$ . Then:

$$\mathrm{CO}(\mathcal{B}_{\mathrm{do}(S_F,S_V)}) = \mathrm{CO}(\mathcal{B})_{\mathrm{do}(S_F,S_V)}.$$

The bipartite graph in Figure 9(a) has the causal ordering graph depicted in Figure 9(b). The perfect intervention  $do(S_F, S_V)$  with  $S_F = \langle f_2, f_3 \rangle$  and  $S_V = \{v_2, v_3\}$  on this causal ordering graph results in the directed cluster graph in Figure 9(c). Since perfect interventions on clusters commute with causal ordering this graph can also be obtained by applying the causal ordering graph to the intervened bipartite graph in Figure 9(c). Proposition 3 shows that perfect interventions on the graphical level can be used to draw conclusions about dependencies and causal implications of the underlying intervened system of constraints.

# 6 Discussion

In this section we give a detailed account of how our work relates to some of the existing literature on causal ordering and causal modelling.

# 6.1 "The causal graph": A misnomer?

Our work extends the work of Simon (1953) who introduced the causal ordering algorithm. In this work, we extensively discussed the example of a bathtub that first appeared in Iwasaki and Simon (1994), in which the authors refer to the Markov ordering graph as "the causal graph" and claim that this graph represents the effects of "manipulations". We note that the Markov ordering graph in the previous section does not have clear causal implications, contrary to claims in the literature. In this work we have formalized soft and perfect interventions, which are two common types of manipulation. This allows us to show that the Markov ordering graph, unlike the causal ordering graph, neither represents the effects of soft interventions nor does it have a straightforward interpretation in terms of



Figure 9: The intervention  $do(S_F, S_V)$  with ordered sets  $S_F = \langle f_2, f_3 \rangle$  and  $S_V = \langle v_2, v_3 \rangle$  commutes with causal ordering. Application of causal ordering and the intervention to the bipartite graph in Figure 9(a) results in the causal ordering graph in Figure 9(b) and the intervened bipartite graph in Figure 9(c) respectively. The directed cluster graph in Figure 9(d) can be obtained either by applying causal ordering to the intervened bipartite graph or by intervening on the causal ordering graph.

perfect interventions. Iwasaki and Simon (1994) do not clarify what the correct causal interpretation of the Markov ordering graph should be and therefore we believe that the term "causal graph" is a misnomer.

**Markov ordering.** To support this claim, we consider the bathtub system in Iwasaki and Simon (1994) that we presented in Example 1. The structure of the equations and the endogenous variables that appear in them can be represented by the bipartite graph in Figure 10(a). The corresponding Markov ordering graph in Figure 10(c) corresponds to the graph that Iwasaki and Simon (1994) call the "causal graph" for the bathtub system. Note that Iwasaki and Simon (1994) do not make a distinction between variable vertices and equation vertices like we do. Their "causal graph" therefore has vertices K, I, P, O, D instead of  $v_K, v_I, v_P, v_O, v_D$ . An aspect that is not discussed at all by Iwasaki and Simon (1994), is that the Markov ordering graph represents conditional independences between components of solutions of equations.

**Soft interventions.** Table 1 shows that a soft intervention on  $f_D$  has a generic effect on the solution for the variables  $v_P, v_O$ , and  $v_D$ . This soft intervention cannot be read off from the Markov ordering graph in Figure 10(c) because there is no vertex  $f_D$  in the graph. Since Iwasaki and Simon (1994) make no distinction between variable vertices and equation vertices, a manipulation on D should perhaps be interpreted as a soft intervention on the vertex D in the graph in Figure 10(c) instead. However, the graphical structure would lead us to erroneously conclude that the soft intervention on D only has an effect on the variable D. We conclude that the Markov ordering graph does not represent the effects of soft interventions on equations in general.

**Perfect interventions.** In Example 8 we calculated that the perfect intervention do $(f_D, v_D, \xi_D)$  had an effect on the solution of the variables  $v_P, v_O$  and  $v_D$ . If we would interpret this manipulation as a perfect intervention on D in the Markov ordering graph in Figure 10(c) then we would mistakenly find that this intervention only affects the variable D. Since Iwasaki and Simon (1994) do not make a distinction between variable vertices and equation vertices we could also interpret a manipulation on D as the perfect interventions do $(f_P, v_D, \xi_D)$  or do $(f_D, v_O, \xi_O)$ . From Table 2 we see that these perfect interventions would change the solution of the variables  $\{v_D\}$  and  $\{v_P, v_O, v_D\}$  respectively. Only the perfect intervention do $(f_P, v_D, \xi_D)$  which targets the cluster containing  $v_D$  corresponds to a perfect intervention on D in the Markov ordering graph in Figure 10(c). Since it is not clear from the graph what type of experiment a perfect intervention on one of its vertices should correspond to, we conclude that the Markov ordering graph cannot be used to read off the effects of perfect interventions.

**Causal ordering graph.** The causal ordering graph for the bathtub system is given in Figure 1(b). We proved that the causal ordering graph, contrary to the Markov ordering graph, represents the effects of soft interventions on equations and perfect interventions on clusters (see Theorem 2 and Proposition 2). To derive causal implications from sets of equations we therefore propose to use the notion of the causal ordering graph instead. The distinction between variable vertices and equations vertices is also made by Simon (1953) who shows how, for linear systems of equations, the principles of causal ordering can be used to qualitatively assess the effects of soft interventions on equations. A different, but closely related, notion of the causal ordering graph is used by Hautier and Barre (2004) in the context of control systems modelling.

# 6.2 Relation to other causal models

The results in this work apply to self-contained sets of equations and are easily applicable to other modelling frameworks, such as the popular framework provided by SCMs (Bongers, Forré, et al., 2020; Pearl, 2000). There are clear benefits of applying causal ordering to constraints implied by structural equations in SCMs. In particular, causal ordering may lead to a stronger Markov property or a representation of effects of a different set of (perfect) interventions. Even though the causal ordering graph itself may not allow us to read off the (non)-effects of arbitrary perfect interventions, these can still be derived by intervening on the bipartite graph and then applying the causal ordering algorithm. The corresponding Markov ordering graph generally gives the strongest Markov property for a causal model formulated in terms of a set of equations.

**Structural Causal Models.** In an SCM, each endogenous variable is on the left-hand side of exactly one structural equation and perfect interventions always act on a structural equation and its corresponding variable. In comparison, a system of constraints consists of symmetric equations and the asymmetric relations between variables are learned automatically by the causal ordering algorithm.

![](_page_27_Figure_0.jpeg)

Figure 10: The bipartite graph for the bathtub system without exogenous variable is given in Figure 10(a). The intervened bipartite graph is given in Figure 10(b). The Markov ordering graphs for the observed and intervened bathtub system are given in Figures 10(c) and 10(e) respectively. Figure 10(d) shows the graph that we obtain by intervening on the Markov ordering graph. Note that this does not correspond with the Markov ordering graph of the intervened bathtub system.

Consider, for example, the following structural equations:

$$X_1 = U_1$$
$$X_2 = aX_1 + U_2$$

where  $X_1, X_2$  are endogenous variables,  $U_1, U_2$  are exogenous random variables, and *a* is a constant. The ordering  $X_1 \to X_2$  can also be obtained by causal ordering of the following set of equations:

$$X_1 - U_1 = 0,$$
  
$$X_2 - aX_1 - U_2 = 0.$$

Note that any set of structural equations implies a self-contained set of equations.<sup>13</sup> We can thus always apply the causal ordering algorithm to structural equations. Interestingly, since the output of the causal ordering algorithm is unique (see Theorem 1), the structure that is provided by the structural equations is actually redundant if the structural equations contain no cycles. If cycles are present it is not clear exactly what the assumed SCM structure (or equivalently the perfect matching) adds.

 $<sup>^{13}</sup>$ In a set of structural equations each variable is matched to a single equation. Since the set of equations has a perfect matching it is self-contained by Hall's marriage theorem (see Theorem 5 in Section 8).

**SCM for the bathtub.** Recall that at equilibrium, the bathtub system can be described by the following structural equations:

$$\begin{aligned} X_{K} &= U_{K}, & X_{O} &= U_{5}X_{K}X_{P}, \\ X_{I} &= U_{I}, & X_{D} &= X_{D} + U_{1}(X_{I} - X_{O}), \\ X_{P} &= gU_{3}X_{D}. \end{aligned}$$

The graph of this SCM is depicted in Figure 6(b), and the descendants and nondescendants of vertices in this graph are given in Table 4. Can we use this table to read off generic causal effects of perfect interventions targeting  $\{f_K, v_K\}, \{f_I, v_I\}, \{f_P, v_P\}, \{f_O, v_O\}, \text{ and } \{f_D, v_D\}$ ? The graph of the SCM contains cycles and does not have a (unique) solution under each perfect intervention.<sup>14</sup> Therefore, the graph of this SCM does not have a straightforward causal interpretation (Bongers, Forré, et al., 2020). More precisely, the presence or absence of directed paths between vertices may not directly correspond to the presence or absence of causal relations.<sup>15</sup> For the bathtub system, the advantages of causal ordering on the structural equations of the SCM are:

- (i) There currently is no Markov property for the graph of the SCM in Figure 6(b) that implies all the conditional independences that are implied by the d-separations in the Markov ordering graph in Figure 6(a).
- (ii) The graph of the SCM and the causal ordering graph represent different intervention targets. In the graph of the SCM, we have intervention targets of the form  $\{f_i, v_i\}$  with  $i \in \{K, I, P, O, D\}$ , while the causal ordering graph represents perfect interventions on clusters  $\{f_K, v_K\}, \{f_I, v_I\}, \{f_P, v_D\}, \{f_O, v_P\},$  and  $\{f_D, v_O\}$ .
- (iii) The causal ordering graph of the bathtub has a straightforward causal interpretation because the bathtub system has a unique solution under interventions on clusters in the causal ordering graph.<sup>16</sup> In contrast, the graph of the SCM for the bathtub system does not have a straightforward causal interpretation and the bathtub system does not have a solution under each perfect intervention on the SCM. Note that Table 4 shows that  $v_O$  is a descendant of  $v_K$  in the graph of the SCM while the solution for the outflow rate  $X_O$  does not change after the perfect intervention do( $f_K, v_K$ ), a fact that can be read off from the causal ordering graph in Figure 1(b).

<sup>&</sup>lt;sup>14</sup>Note that the perfect interventions on the SCM  $\{f_K, v_K\}$ ,  $\{f_I, v_I\}$ ,  $\{f_P, v_P\}$ ,  $\{f_O, v_O\}$ ,  $\{f_D, v_D\}$  are a subset of the perfect interventions on the set of equations. Furthermore, there is no unique solution if one fixes the outflow rate of the system  $X_O$  to a value that is not equal to  $X_I$  via a change in the equation  $f_O$ . This reflects the draining or overflowing of the bathtub in this type of experiment.

 $<sup>^{15}</sup>$ Instead, we could check the conditions of Proposition 7.1.1. in Bongers, Forré, et al. (2020) to test for the presence of generic causal effects. The causal effects of interventions that are implied by the SCM are presented in Table 5 in the supplementary material.

<sup>&</sup>lt;sup>16</sup>Because directed cluster graphs are acyclic by construction, it is often easy to verify that the system is uniquely solvable with respect to an intervened causal ordering graph. The existence of a directed path from a cluster targeted by an intervention to a certain variable implies that the intervention generically changes the solution of that variable.

**Other frameworks.** Since the causal ordering algorithm can be applied to any self-contained set of equations, the results that we developed here are generally applicable to sets of equations in other modelling frameworks. For example, the recently introduced Causal Constraint Models (CCMs) do not yet have a graphical representation for the independence structure between the variables (Blom, Bongers, and Mooij, 2019). The causal ordering algorithm can be directly applied to a self-contained set of active constraints to obtain a Markov ordering graph.

Table 4: The descendants and non-descendants of intervention targets in the graph of the SCM for the bathtub system in Figure 6(b).

target	descendants	non-descendants
$f_K, v_K$	$v_K, v_P, v_O, v_D$	$v_I$
$f_I, v_I$	$v_I, v_P, v_O, v_D$	$v_K$
$f_P, v_P$	$v_P, v_O, v_D$	$v_K, v_I$
$f_O, v_O$	$v_P, v_O, v_D$	$v_K, v_I$
$f_D, v_D$	$v_P, v_O, v_D$	$v_K, v_I$

# 6.3 Equilibration in dynamical models

Dynamical models in terms of first order differential equations can be *equilibrated* to a set of equations by equating each time-derivative to zero, as in Mooij, Janzing, and Schölkopf (2013). They can be *equilibrated to a causal ordering graph* by applying the causal ordering algorithm to the resulting set of equilibrium equations. They can also be *equilibrated to a Markov ordering graph* by subsequently applying Definition 8 to this causal ordering graph. The bathtub system provides an example of what Dash (2005) calls a "violation of the Equilibration Manipulation Commutability property".<sup>17</sup> Following Iwasaki and Simon (1994), and quite confusingly, the Markov ordering graph is referred to as the "causal graph" by Dash (2005).<sup>18</sup> Consequently, the "equilibration" operator in Dash (2005) should be interpreted as equilibration to the Markov ordering graph.

Markov ordering graph for the bathtub. The bathtub system shows that the directed edges in the Markov ordering graph cannot be directly interpreted as causal relations. Consider the perfect intervention  $do(f_D, v_D)$  for which the Markov ordering graphs  $MO(\mathcal{B})_{do(D)}$  and  $MO(\mathcal{B}_{do(f_D, v_D)})$  are wildly different, as can be seen by comparing Figures 10(d) and 10(e) respectively. Clearly, equilibration to the Markov ordering graph does not commute with the perfect intervention

 $<sup>^{17}</sup>$ We argue that this is confusing terminology. As shown by Bongers and Mooij (2018), equilibration to an SCM does commute with manipulation (perfect interventions). In his "equilibration" operator, Dash (2005) considers equilibration to the Markov ordering graph (not to an SCM). Therefore, a better name would have been Equilibration-Markov ordering Commutability.

 $<sup>^{18}</sup>$  For the bathtub, we argued in Section 6.1 that this is a misnomer, as in general there is no straightforward one-to-one correspondence between the Markov ordering graph and the causal semantics of the system.

 $do(f_D, v_D)$ . We shed some new light on the commutability of interventions and equilibration to the Markov ordering graph by considering the following novel insights:

- (i) Interventions on the dynamics of the bathtub system target pairs of equations and variables:  $\{f_K, v_K\}, \{f_I, v_I\}, \{f_P, v_P\}, \{f_O, v_O\}, \text{ or } \{f_D, v_D\}.$
- (ii) The causal ordering graph of the bathtub systems has intervention targets (i.e. clusters in the causal ordering graph):  $\{f_K, v_K\}$ ,  $\{f_I, v_I\}$ ,  $\{f_P, v_D\}$ ,  $\{f_O, v_P\}$ , and  $\{f_D, v_O\}$ .
- (iii) By Proposition 3 we know that application of the causal ordering algorithm to a set of equations commutes with perfect interventions on clusters in the resulting causal ordering graph.

This tells us that equilibration to the causal ordering graph commutes with all perfect interventions that are both represented by the dynamical model and by the causal ordering graph.<sup>19</sup> For the bathtub system, equilibration to the causal ordering graph thus commutes with perfect interventions targeting  $\{f_K, v_K\}$  and  $\{f_I, v_I\}$ , or combinations thereof. Consequently, equilibration of a dynamical model to the Markov ordering graph also commutes with these interventions. That is, the graph that we obtain by performing interventions  $do(v_K)$  and  $do(v_I)$  on the Markov ordering graph in Figure 6(a) coincides with the graph that we obtain by applying interventions  $do(v_K, f_K, \xi_K)$  and  $do(v_I, f_I, \xi_I)$  to the dynamical causal model and then constructing the Markov ordering graph.

# 6.4 Structure learning

We have shown that, under a solvability assumption, d-separations in the Markov ordering graph (or  $\sigma$ -separations in the directed graph associated with a particular perfect matching) imply conditional independences between variables in a system of constraints (see Theorem 2 and Proposition 1). Constraint-based causal discovery algorithms relate conditional independences in data to graphs under the Markov and faithfulness assumptions. Roughly speaking, the equivalence class of the Markov ordering graph (or the directed graph associated with a particular perfect matching) can be learned from data under the assumption that all conditional independences in the data are implied by the graph. The bathtub system in Example 1 is used by Dash (2005), who simulates data from the dynamical model until it reaches equilibrium, and then applies the PC-algorithm to learn the graphical structure of the system. It is no surprise that the learned structure is the Markov ordering graph in Figure 10(c). The usual assumption is then that the Markov ordering graph equals the causal graph, where directed edges express direct causal relations between variables. In this work we have shown that this learned Markov ordering graph does not have a straightforward causal interpretation.

<sup>&</sup>lt;sup>19</sup>Bongers and Mooij (2018) prove that equilibrating a dynamical causal model to the graph of an SCM commutes with perfect interventions. By applying the causal ordering algorithm to structural equations, we find that equilibrating a dynamical causal model to a causal ordering graph commutes with interventions that are modelled by both the SCM and the causal ordering graph.

# 7 Conclusion and future work

In this work, we slightly reformulated Simon's causal ordering algorithm and demonstrated that it is a convenient and scalable tool to study causal and probabilistic aspects of models consisting of equations. In particular, we showed how the technique of causal ordering can be used to construct either a *Markov ordering* graph or a causal ordering graph from a set of equations without calculating explicit solutions. One of the novelties of this paper is that we proved that the Markov ordering graph implies conditional independences between variables whereas the causal ordering graph encodes the effects of soft and perfect interventions.

To model causal relations between variables in sets of equations unambiguously, we generalized existing notions of perfect interventions. The main idea is that a perfect intervention on a set of equations targets variables and specified equations, whereas a perfect intervention on a Structural Causal Model (SCM) targets variables and their associated structural equations. We considered a simple dynamical model with feedback and demonstrated that, contrary to claims in the literature, the Markov ordering graph does not generally have a straightforward causal interpretation in terms of soft or perfect interventions. We showed that the causal ordering graph does encode the effects of soft and certain perfect interventions. The main take-away is that we need to make a distinction between graphical representations of the probabilistic and causal aspects of models with feedback. By making this distinction, we clarified the correct interpretation of existing results in the literature. Additionally, we shed new light on discussions in causal discovery about the justification of using a single graph to simultaneously represent causal relations and conditional independences. We believe that the phenomenon where conditional independences and causal semantics must be represented by different graphs manifests itself in certain (biological) models with feedback. In future work we plan to investigate these occurrences further.

The causal ordering algorithm can currently only be applied to self-contained sets of equations. Particularly for non-linear sets of equations, this is a limiting assumption since there might be more equations than variables required to specify a unique solution. An interesting direction for future research is to develop extensions of the causal ordering algorithm for non self-contained sets of equations.

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# 8 Supplementary material

This section is for the most part devoted to the proofs of the theorems and propositions that were presented in Sections 2, 3, 4, and 5. In section 8.8 we discuss the directed edges in SCM representations of the bathtub system in Example 1 that were mentioned in Section 6.2.

### 8.1 Proof of Theorem 1

# Theorem 1. The output of Algorithm 1 is well-defined and unique.

Lemma 2 below shows that the minimal self-contained sets in a self-contained bipartite graph are disjoint. Lemma 3 shows that the induced subgraph after one iteration of Algorithm 1, with a self-contained bipartite graph as input, is self-contained. The minimal self-contained sets in the graph which are not used in the iteration are minimal self-contained sets of the induced subgraph. This shows that the output of Algorithm 1 is well-defined. We then use Lemma 2 and 3 to prove Lemma 4 which states that the output of Algorithm 1, with a self-contained bipartite graph as input, is unique. This implies that the output of Algorithm 1, which has an initialization that is uniquely determined by the specification of exogenous variables W, must also be unique.

**Lemma 2.** Let  $\mathcal{B} = \langle V, F, E \rangle$  be a self-contained bipartite graph. Let  $\mathcal{S}_F$  be the set of minimal self-contained sets in  $\mathcal{B}$ . The sets in  $\mathcal{S}_F$  are pairwise disjoint, and, likewise, the sets of adjacent nodes

$$\mathcal{S}_V = \{ \operatorname{adj}_{\mathcal{B}}(S) : S \in \mathcal{S}_F \},\$$

of the minimal self-contained sets in  $\mathcal{S}_F$  are pairwise disjoint.

*Proof.* Let  $S_1 \subseteq F$  and  $S_2 \subseteq F$  be non-empty distinct minimal self-contained sets in  $\mathcal{S}_F$ . For the sake of contradiction, assume that  $S_1 \cap S_2 \neq \emptyset$ . Since  $S_1$  is minimal self-contained, we know that  $S_1 \cap S_2 \subset S_1$  is not self-contained. Hence, by Definition 5, we have that

$$|S_1 \cap S_2| < |\operatorname{adj}_{\mathcal{B}}(S_1 \cap S_2)|.$$

$$\tag{1}$$

Consider the following equations:

$$|\mathrm{adj}_{\mathcal{B}}(S_1)| + |\mathrm{adj}_{\mathcal{B}}(S_2)| - |S_1 \cap S_2| = |S_1| + |S_2| - |S_1 \cap S_2|$$
(2)

$$= |S_1 \cup S_2|$$

$$\leq |\operatorname{adj}_{\mathcal{B}}(S_1 \cup S_2)| \qquad (3)$$

$$= |\operatorname{adj}_{\mathcal{B}}(S_1) \cup \operatorname{adj}_{\mathcal{B}}(S_2)| = |\operatorname{adj}_{\mathcal{B}}(S_1)| + |\operatorname{adj}_{\mathcal{B}}(S_2)| - |\operatorname{adj}_{\mathcal{B}}(S_1) \cap \operatorname{adj}_{\mathcal{B}}(S_2)|$$

$$\leq |\operatorname{adj}_{\mathcal{B}}(S_1)| + |\operatorname{adj}_{\mathcal{B}}(S_2)| - |\operatorname{adj}_{\mathcal{B}}(S_1 \cap S_2)|, \qquad (4)$$

where equality (2) holds by condition (i) of Definition 5, since  $\mathcal{B}$  is self-contained inequality (3) holds by condition (ii) of Definition 5, and inequality (4) holds because  $\operatorname{adj}_{\mathcal{B}}(S_1 \cap S_2) \subseteq \operatorname{adj}_{\mathcal{B}}(S_1) \cap \operatorname{adj}_{\mathcal{B}}(S_2)$ . It follows that

$$|S_1 \cap S_2| \ge |\operatorname{adj}_{\mathcal{B}}(S_1) \cap \operatorname{adj}_{\mathcal{B}}(S_2)| \ge |\operatorname{adj}_{\mathcal{B}}(S_1 \cap S_2)| \ge 0.$$

This is in contradiction with equation (1), and hence  $S_1 \cap S_2 = \emptyset$ . This implies that  $|S_1 \cap S_2| = 0$  and therefore by the inequalities above we have that  $|\operatorname{adj}_{\mathcal{B}}(S_1) \cap \operatorname{adj}_{\mathcal{B}}(S_2)| = 0$ . Thus  $\operatorname{adj}_{\mathcal{B}}(S_1) \cap \operatorname{adj}_{\mathcal{B}}(S_2) = \emptyset$ .

**Lemma 3.** Let  $\mathcal{B} = \langle V, F, E \rangle$  be a self-contained bipartite graph. Suppose that F has minimal self-contained sets  $\mathcal{S}_F$ . Let  $\mathcal{B}'$  be the subgraph of  $\mathcal{B}$  induced by

$$V' := V \setminus \operatorname{adj}_{\mathcal{B}}(S), \quad and \quad F' := F \setminus S,$$

with  $S \in S_F$ . Then the following two properties hold:

- (i)  $\mathcal{B}'$  is self-contained, and
- (ii) the sets in  $\mathcal{S}_F \setminus \{S\}$  are minimal self-contained in  $\mathcal{B}'$ .

*Proof.* Let  $S \in S_F$  be a minimal self-contained subset in  $\mathcal{B}$ . Since  $\mathcal{B}$  and S are self-contained we have that |V| = |F| and  $|S| = |\operatorname{adj}_{\mathcal{B}}(S)|$  respectively. Therefore

$$|V'| = |V \setminus \operatorname{adj}_{\mathcal{B}}(S)| = |V| - |\operatorname{adj}_{\mathcal{B}}(S)| = |F| - |S| = |F \setminus S| = |F'|.$$

This shows that condition (i) of Definition 5 is satisfied for  $\mathcal{B}'$ . Assume, for the sake of contradiction, that F' does not satisfy condition (ii) of Definition 5 in the induced subgraph  $\mathcal{B}'$ . Then there exists  $S' \subseteq F'$  such that  $|S'| > |\operatorname{adj}_{\mathcal{B}'}(S')|$ . Consider the following equations:

$$\begin{aligned} |S \cup S'| &= |S| + |S'| \\ &> |\operatorname{adj}_{\mathcal{B}}(S)| + |\operatorname{adj}_{\mathcal{B}'}(S')| \\ &= |\operatorname{adj}_{\mathcal{B}}(S)| + |\operatorname{adj}_{\mathcal{B}}(S')| - |\operatorname{adj}_{\mathcal{B}}(S) \cap \operatorname{adj}_{\mathcal{B}}(S')| \\ &= |\operatorname{adj}_{\mathcal{B}}(S) \cup \operatorname{adj}_{\mathcal{B}}(S')| \\ &= |\operatorname{adj}_{\mathcal{B}}(S \cup S')| \\ &> |S \cup S'|. \end{aligned}$$

where the last inequality holds because  $\mathcal{B}$  is self-contained by assumption. This is a contradiction, and we conclude that both conditions of Definition 5 are satisfied for  $\mathcal{B}'$ . This shows that  $\mathcal{B}'$  is self-contained.

Let  $S_1 \in S_F$  and  $S_2 \in S_F$  be two distinct minimal self-contained sets in  $\mathcal{B}$ . Suppose that  $\mathcal{B}_1$  is a subgraph of  $\mathcal{B}$  induced by  $V \setminus \operatorname{adj}_{\mathcal{B}}(S_1)$  and  $F \setminus S_1$ . By Lemma 2 we know that  $S_1 \cap S_2 = \emptyset$  and  $\operatorname{adj}_{\mathcal{B}}(S_1) \cap \operatorname{adj}_{\mathcal{B}}(S_2) = \emptyset$ . It follows that for all  $S' \subseteq S_2$  we have that  $\operatorname{adj}_{\mathcal{B}}(S') = \operatorname{adj}_{\mathcal{B}_1}(S')$ . We find that

$$|S_2| = |\operatorname{adj}_{\mathcal{B}}(S_2)| = |\operatorname{adj}_{\mathcal{B}_1}(S_2)|,$$
  
$$|S'| \le |\operatorname{adj}_{\mathcal{B}}(S')| = |\operatorname{adj}_{\mathcal{B}_1}(S')|,$$

for all  $S' \subseteq S_2$ . This shows that  $S_2$  satisfies the conditions of Definition 5 in the bipartite graph  $\mathcal{B}_1$ . Since  $S_2$  has no non-empty strict subsets that are self-contained in  $\mathcal{B}$  we have that  $S_2$  has no non-empty strict subsets that are self-contained in  $\mathcal{B}_1$ . We conclude that  $S_2$  is a minimal self-contained subset in  $\mathcal{B}_1$ . This shows that the sets  $\mathcal{S}_F \setminus \{S\}$  are minimal self-contained in  $\mathcal{B}'$ .

**Lemma 4.** Let  $\mathcal{B} = \langle V, F, E \rangle$  be a self-contained bipartite graph. The output  $CO(\mathcal{B})$  of Algorithm 1 is unique.

*Proof.* Suppose  $\mathcal{G}_1 = \langle \mathcal{V}_1, \mathcal{E}_2 \rangle$  and  $\mathcal{G}_2 = \langle \mathcal{V}_2, \mathcal{E}_2 \rangle$  are directed cluster graphs that are obtained by running Algorithm 1. Let  $A = (1, 2, \ldots, |\mathcal{V}_1|)$  be an ordered set that indicates the order in which clusters  $S^{(a)}$  (with  $a \in A$ ) are added to  $\mathcal{V}_1$  in the first run of the algorithm. Similarly,  $B = (1, 2, \ldots, |\mathcal{V}_2|)$  is an ordered set that indicates the order in which clusters  $T^{(b)}$  (with  $b \in B$ ) are added to  $\mathcal{V}_2$  in the second run of the algorithm. With a slight abuse of notation we define  $\mathcal{B} \setminus (S^{(k)})_{k < i}$  as the subgraph of  $\mathcal{B}$  induced by the nodes  $(S^{(k)})_{k \geq i}$ . Similarly,  $\mathcal{B} \setminus (T^{(k)})_{k < i}$  denotes the subgraph of  $\mathcal{B}$  induced by the nodes  $(T^{(k)})_{k \geq i}$ .

Intermediate result: We will prove that for  $i \in (1, 2, ..., |\mathcal{V}_1|)$  there exists  $b_i \in B$  such that  $S^{(i)} = T^{(b_i)}$  by induction.

Base case: The algorithm adds the cluster  $S^{(1)}$  to  $\mathcal{V}_1$  in the first step of the first run. Therefore, we know that the set of nodes  $F \cap S^{(1)}$  must be minimal self-contained in  $\mathcal{B}$ . Let  $1 \leq k \leq |\mathcal{V}_2|$  be arbitrary. By Lemma 3 it follows that  $F \cap S^{(1)}$  is minimal self-contained in  $\mathcal{B} \setminus (T^{(j)})_{j < k}$  provided  $S^{(1)} \neq T^{(j)}$  for all j < k. Since  $\mathcal{B}$  is finite, the minimal self-contained set  $S^{(1)}$  must be chosen eventually, and hence there exists  $b_1 \in B$  such that  $S^{(1)} = T^{(b_1)}$ .

Induction hypothesis: Let  $1 \leq i < |\mathcal{V}_1|$  be arbitrary and assume that for all  $j \leq i$  there exists  $b_j \in B$  such that  $S^{(j)} = T^{(b_j)}$ . We want to show that there exists  $b_{i+1} \in B$  such that  $S^{(i+1)} = T^{(b_{i+1})}$ .

Induction step: Let  $B' = B \setminus (b_1, \ldots, b_i) = (b'_1, \ldots, b'_{|\mathcal{V}_2|-i})$  be an ordered set such that  $b'_i \prec b'_{i+1}$  for all  $j = 1, \ldots, |\mathcal{V}_2| - (i+1)$ .

(i) In the second run of the algorithm, the cluster  $T^{(b'_1)}$  is added to  $\mathcal{V}_2$  right after the clusters  $T^{(b_j)}$  with  $b_j \prec b'_1$  are added to  $\mathcal{V}_2$  and removed from the graph. Therefore, the set  $F \cap T^{(b'_1)}$  is minimal self-contained in  $\mathcal{B} \setminus (T^{(b_j)})_{j \leq i, b_j \prec b'_1}$ . In the first run of the algorithm, the clusters  $S^{(1)} = T^{(b_1)}, \ldots, S^{(i)} = T^{(b_i)}$ are subsequently added to  $\mathcal{V}_1$  and removed from the graph. Therefore, by Lemma 2 and Lemma 3, we have that  $F \cap T^{(b'_1)}$  is minimal self-contained in  $\mathcal{B}' = \mathcal{B} \setminus (T^{(b_j)})_{j \leq i} = \mathcal{B} \setminus (S^{(k)})_{k \leq i}$ . Hence, both  $F \cap T^{(b'_1)}$  and  $F \cap S^{(i+1)}$ are minimal self-contained in  $\mathcal{B}'$ . Therefore, by Lemma 2 and Lemma 3, either  $T^{(b'_1)} = S^{(i+1)}$  (in which case we are done) or  $F \cap S^{(i+1)}$  is minimal self-contained in  $\mathcal{B}' \setminus T^{(b'_1)}$ .

(ii) Let  $k \leq |\mathcal{V}_2| - i$  be arbitrary. By iteration of the argument in the previous step we find that  $F \cap T^{(b'_k)}$  is minimal self-contained in  $(\mathcal{B} \setminus (T^{(b_j)})_{j \leq i, b_j \prec b'_k}) \setminus (T^{(b'_j)})_{j < k}$  and hence in  $\mathcal{B}' \setminus (T^{(b'_j)})_{j < k}$ , so that either  $T^{(b'_k)} = S^{(i+1)}$  or  $F \cap S^{(i+1)}$  is minimal self-contained in  $\mathcal{B}' \setminus (T^{(b'_j)})_{j \leq k}$ . Since the graph is finite, there exists  $m \in 1, \ldots, |\mathcal{V}_2| - i$  such that  $T^{(b'_m)} = S^{(i+1)}$ . By definition of B' there exists  $b_{i+1} \in B$  such that  $S^{(i+1)} = T^{(b_{i+1})}$ .

This proves that the clusters in  $\mathcal{V}_1$  are also clusters in  $\mathcal{V}_2$ . By symmetry we find that the clusters  $S^{(a)}$  in  $\mathcal{V}_1$  and the clusters  $T^{(b)}$  in  $\mathcal{V}_2$  coincide. Since  $\mathcal{V}_1 = \mathcal{V}_2$  it follows immediately from the construction of edges in the algorithm that  $\mathcal{E}_1 = \mathcal{E}_2$  and hence  $\mathcal{G}_1 = \mathcal{G}_2$ .

# 8.2 Proof of Theorem 2

**Theorem 2.** Let  $X^*$  be a solution of a system of constraints  $\mathcal{M} = \langle \mathcal{X}, X_W, \Phi, \mathcal{B} \rangle$ , where the subgraph of  $\mathcal{B} = \langle V, F, E \rangle$  induced by  $(V \cup F) \setminus W$  is self-contained. If  $\mathcal{M}$  is uniquely solvable with respect to the causal ordering graph  $CO(\mathcal{B})$  then the pair  $(MO(\mathcal{B}), \mathbb{P}_{X^*})$  satisfies the directed global Markov property.

Let  $v \in V \setminus W$  be arbitrary and define  $S_V = \operatorname{cl}(v) \cap V$  and  $S_F = \operatorname{cl}(v) \cap F$ . First, we will show that  $V(S_F) \setminus S_V = \operatorname{pa}_{\operatorname{MO}(\mathcal{B})}(v)$ . Let  $x \in \operatorname{adj}_{\mathcal{B}}(S_F) \setminus S_V$  be an arbitrary vertex that is adjacent to  $S_F$  but not in  $S_V$ . The following equivalences hold:

$$\begin{aligned} x \in V(S_F) \setminus S_V &\iff x \in \operatorname{adj}_{\mathcal{B}}(S_F) \setminus S_V & \text{(by Definition 3)} \\ &\iff (x \to \operatorname{cl}(v)) \text{ in } \operatorname{CO}(\mathcal{B}) & \text{(by definition of Algorithm 1)} \\ &\iff (x \to v) \text{ in } D(\operatorname{CO}(\mathcal{B})) & \text{(by Definition 8)} \\ &\iff (x \to v) \text{ in } D(\operatorname{CO}(\mathcal{B}))_{\max(F)} \\ &\iff (x \to v) \text{ in } \operatorname{MO}(\mathcal{B}) & \text{(by Definition 8)} \\ &\iff x \in \operatorname{pa}_{\operatorname{MO}(\mathcal{B})}(v). \end{aligned}$$

By assumption, the system of constraints is uniquely solvable with respect to  $\operatorname{CO}(\mathcal{B})$ . Note that  $S_V \subseteq V(S_F)$ . Hence, there exists a measurable function  $g_i : \mathcal{X}_{\operatorname{pa}_{\operatorname{MO}(\mathcal{B})}(v)} \to \mathcal{X}_i$  for all  $i \in S_V$  s.t. for all  $\mathbf{x}_{V(S_F)} \in \mathcal{X}_{V(S_F)}$ :

$$\forall f \in S_F, \ \phi_f(\boldsymbol{x}_{V(f)}) = c_f \iff \forall i \in S_V, \ x_i = g_i(\boldsymbol{x}_{\mathrm{pa}_{\mathrm{MO}(\mathcal{B})}(v)}).$$

Let  $X^*$  be a solution to the system of constraints. Since  $v \in V \setminus W$  was chosen arbitrarily it follows that

$$X_v^* = g_v(\boldsymbol{X}_{\mathrm{pa}_{\mathrm{MO}(\mathcal{B})}(v)}^*),$$

for all  $v \in V \setminus W$  almost surely. The directed global Markov property was already shown to hold for pairs  $(\mathcal{G}, \mathbb{P}_{\mathbf{X}})$  where  $\mathcal{G}$  is a DAG and  $\mathbf{X}$  is a solution to a set of structural equations with functional dependences corresponding to the DAG (Lauritzen, 1996; Pearl, 2000). Because the Markov ordering graph MO( $\mathcal{B}$ ) is acyclic by construction this finishes the proof.

# 8.3 Proof of Theorem 3

**Theorem 3.** The output of Algorithm 2 coincides with the output of Algorithm 1.

The following result gives a necessary and sufficient condition for the existence of a perfect matching for a bipartite graph and can be found in (Hall, 1986).

**Theorem 5** (Hall's Marriage Theorem). Let  $\mathcal{B} = \langle V, F, E \rangle$  be a bipartite graph with |V| = |F|. Then  $\mathcal{B}$  has a perfect matching if and only if  $|F'| \leq |\operatorname{adj}_{\mathcal{B}}(F)|$  for all  $F' \subseteq F$ .

From Hall's Marriage Theorem it trivially follows that a bipartite graph has a perfect matching if and only if it is self-contained.

**Corollary 1.** Let  $\mathcal{B} = \langle V, F, E \rangle$  be a bipartite graph. Then  $\mathcal{B}$  has a perfect matching if and only if  $\mathcal{B}$  is self-contained.

*Proof.* If  $\mathcal{B}$  has a perfect matching then |V| = |F|. By Definition 5 we know that if  $\mathcal{B}$  is self-contained then |V| = |F|. Hence, the statement follows from Definition 5 and Theorem 5.

The following technical lemma is used to prove Lemma 6, which shows that the output of Algorithm 1 coincides with that of Algorithm 2 in the case that the input of the algorithm is a self-contained bipartite graph and  $W = \emptyset$ .

**Lemma 5.** Let M be a perfect matching for a self-contained bipartite graph  $\mathcal{B} = \langle V, F, E \rangle$ . Let  $S_V^{(1)}, \ldots, S_V^{(n)}$  be a topological ordering of the strongly connected components in  $\mathcal{G}(\mathcal{B}, M)_{\max(F)}$ . Let  $\mathcal{B}^{(i)}$  be the subgraph of  $\mathcal{B}$  induced by  $\bigcup_{j=i}^n (S_V^{(j)} \cup M(S_V^{(j)}))$ . Then  $\mathcal{B}^{(i)}$  is self-contained and  $M(S_V^{(i)})$  is a minimal self-contained set in  $\mathcal{B}^{(i)}$ .

*Proof.* We use the notation  $\mathcal{G}^{(k)} := \mathcal{G}(\mathcal{B}^{(k)}, M^{(k)})$  and  $S_F^{(k)} := M^{(k)}(S_V^{(k)})$ , where  $M^{(1)} = M$  (we will define  $M^{(i)}$  with i > 1 later). First we show that  $S_F^{(1)}$  is self-contained in  $\mathcal{B}^{(1)}$ . We proceed by proving that  $S_F^{(1)}$  is minimal self-contained in  $\mathcal{B}^{(1)}$  and that  $\mathcal{B}^{(2)}$  is a self-contained bipartite graph. Finally, we consider how these arguments can be iterated to prove the lemma.

By definition of a perfect matching and the fact that  $\mathcal{B}^{(1)} = \mathcal{B}$  is self-contained, we know that:

$$|S_V^{(1)}| = |S_F^{(1)}| \le |\mathrm{adj}_{\mathcal{B}^{(1)}}(S_F^{(1)})|.$$

By definition of topological ordering and the orientation step in Definition 9 we know that:

$$\operatorname{adj}_{\mathcal{B}^{(1)}}(S_F^{(1)}) \subseteq S_V^{(1)}$$

Together, these two inequalities show that  $|S_F^{(1)}| = |\operatorname{adj}_{\mathcal{B}^{(1)}}(S_F^{(1)})|$ . Because  $\mathcal{B}^{(1)}$  is self-contained, the set  $S_F^{(1)}$  satisfies both conditions of Definition 5. We conclude that  $S_F^{(1)}$  is self-contained in  $\mathcal{B}^{(1)}$ .

Assume, for the sake of contradiction, that  $S_F^{(1)}$  is not *minimal* self-contained. Then there exists a non-empty strict subset  $F' \subset S_F^{(1)}$  that is self-contained in  $\mathcal{B}^{(1)}$ . First note that, by Definition 5, we have that  $|F'| = |\operatorname{adj}_{\mathcal{B}^{(1)}}(F')|$  and  $|S_V^{(1)}| = |S_F^{(1)}|$  so that  $S_V^{(1)} \setminus \operatorname{adj}_{\mathcal{B}^{(1)}}(F') \neq \emptyset$  and  $\operatorname{adj}_{\mathcal{B}^{(1)}}(F') \neq \emptyset$ . Furthermore, by Definition 9 (orientation step), we must have that:

$$\operatorname{pa}_{\mathcal{G}^{(1)}}(\operatorname{adj}_{\mathcal{B}^{(1)}}(F')) = M^{(1)}(\operatorname{adj}_{\mathcal{B}^{(1)}}(F')) = F'.$$

Therefore there is no directed edge from any vertex in  $F \setminus F'$  to any vertex in  $\operatorname{adj}_{\mathcal{B}^{(1)}}(F')$ . Clearly, there can be no edge in  $\mathcal{G}^{(1)}$  between any vertex  $v \in S_V^{(1)} \setminus \operatorname{adj}_{\mathcal{B}^{(1)}}(F')$  and any vertex  $f' \in F'$  and hence

$$\operatorname{pa}_{\mathcal{G}^{(1)}}(S_V^{(1)} \setminus \operatorname{adj}_{\mathcal{B}^{(1)}}(F')) = M^{(1)}(S_V^{(1)} \setminus \operatorname{adj}_{\mathcal{B}^{(1)}}(F')) = F \setminus F'.$$

Therefore, there can be no directed path from any  $v \in S_V^{(1)} \setminus \operatorname{adj}_{\mathcal{B}^{(1)}}(F')$  to any  $f \in F'$  in  $\mathcal{G}^{(1)}$ . This contradicts the assumption that  $S_V^{(1)}$  is a strongly connected component in  $\mathcal{G}_{\operatorname{mar}(F)}^{(1)}$ . We conclude that  $S_F^{(1)}$  is minimal self-contained in  $\mathcal{B}^{(1)}$ .

Clearly, the set  $M^{(2)} := \{(i-j) \in M^{(1)} : i, j \notin S_V^{(1)} \cup S_F^{(1)}\}$  is a perfect matching for  $\mathcal{B}^{(2)}$ . By Corollary 1 we therefore know that  $\mathcal{B}^{(2)}$  is self-contained. Since  $S_V^{(2)}, \ldots, S_V^{(n)}$  is a topological ordering for the strongly connected components in  $\mathcal{G}_{\max(F)}^{(2)}$  the above argument can be repeated to show that  $S_F^{(2)}$  is minimal self-contained in  $\mathcal{B}^{(2)}$ . For arbitrary  $i \in \{1, \ldots, n\}$  this entire argument can be iterated to show that  $S_F^{(i)}$  is minimal self-contained in the self-contained bipartite graph  $\mathcal{B}^{(i)}$ .

**Lemma 6.** Let M be an arbitrary perfect matching for a self-contained bipartite graph  $\mathcal{B} = \langle V, F, E \rangle$ . The directed cluster graph  $\mathcal{G}_1 = \langle \mathcal{V}_1, \mathcal{E}_1 \rangle$  that is obtained by application of Definition 9 coincides with the output  $\mathcal{G}_2 = \langle \mathcal{V}_2, \mathcal{E}_2 \rangle$  of Algorithm 1.

*Proof.* Let  $S^{(1)}, \ldots, S^{(n)}$  be a topological ordering of the strongly connected components in  $\mathcal{G}(M, \mathcal{B})_{\max(F)}$ . By Definition 9 the cluster set  $\mathcal{V}_1$  consists of clusters  $S^{(i)} \cup M(S^{(i)})$  with  $i \in \{1, \ldots, n\}$ . By Lemma 5, Algorithm 1 can be run in such a way that the clusters  $S^{(i)} \cup M(S^{(i)})$  are added to  $\mathcal{V}_2$  in the order specified by the topological ordering. By Theorem 1 the output of Algorithm 1 is unique and therefore  $\mathcal{V}_1 = \mathcal{V}_2$ . By Definition 9 the following equivalences hold for  $C \in \mathcal{V}_1 = \mathcal{V}_2$  and  $v \in V \setminus C$ :

$$\begin{aligned} (v \to C) \in \mathcal{E}_1 &\iff \exists w \in C \text{ s.t. } (v \to w) \text{ in } \mathcal{G}(M, \mathcal{B}) \\ &\iff \exists w \in C \text{ s.t. } (v - w) \in E \text{ and } (v - w) \notin M \\ &\iff v \in \operatorname{adj}_{\mathcal{B}}(C \cap F) \setminus M(C \cap F) \\ &\iff v \in \operatorname{adj}_{\mathcal{B}}(C \cap F) \setminus (C \cap V) \\ &\iff (v \to C) \in \mathcal{E}_2. \end{aligned}$$

Let  $C \in \mathcal{V}_1 = \mathcal{V}_2$  and  $f \in F \cap (\operatorname{adj}_{\mathcal{B}}(C) \setminus C)$ . By definition of Algorithm 1 we know that  $(f \to C) \notin \mathcal{E}_2$ . Note that  $M(C \cap F) = C \cap V$ . By Definition 9 there

is no edge  $(f \to v)$  with  $v \in C \cap V$  in  $\mathcal{G}(\mathcal{B}, M)$  and hence by Definition we know that  $(f \to C) \notin \mathcal{E}_2$ . By construction, edges  $(x \to C)$  with  $x \in C$  are neither in  $\mathcal{E}_1$ nor in  $\mathcal{E}_2$ . We conclude that  $\mathcal{E}_1 = \mathcal{E}_2$  and consequently  $\mathcal{G}_1$  coincides with  $\mathcal{G}_2$ .  $\Box$ 

Lemma 6 shows that the output of Algorithm 1 coincides with the output of Algorithm 2 if the input is a self-contained bipartite graph. Otherwise, both Algorithm 1 and 2 have an initialization that is determined by the specification of exogenous variables. The exogenous variables are placed into separate clusters and there are directed edges from each exogenous variable to the clusters of its adjacencies for both algorithms. The output of the two algorithms coincides for any valid input.

# 8.4 **Proof of Proposition 1**

**Proposition 1.** Let  $\mathbf{X}^*$  be a solution of a system of constraints  $\mathcal{M} = \langle \mathbf{\mathcal{X}}, \mathbf{X}_W, \mathbf{\Phi}, \mathcal{B} \rangle$ , where the subgraph of  $\mathcal{B} = \langle V, F, E \rangle$  induced by  $(V \cup F) \setminus W$  has a perfect matching M. If for each strongly connected component S in  $\mathcal{G}(\mathcal{B}, M)$  with  $S \cap W = \emptyset$ , the system  $\mathcal{M}$  is uniquely solvable w.r.t.  $S_V = (S \cup M(S)) \cap V$  and  $S_F = (S \cup M(S)) \cap F$ then the pair  $(\mathcal{G}(\mathcal{B}, M)_{\max(F)}, \mathbb{P}_{\mathbf{X}^*})$  satisfies the generalized directed global Markov property.

The proof of this proposition relies on results by Forré and Mooij (2017), who define the notion of an *acyclic augmentation* for a class of graphical models that they call *HEDGes*. They define the *augmentation* of a HEDG as a directed graph where hyperedges are represented by vertices with additional edges. The acyclic augmentation of a HEDG is obtained by *acyclification* of the edge set of it augmentation (Forré and Mooij, 2017).

**Definition 13.** Let  $\mathcal{G} = \langle V, E \rangle$  be a directed graph. The *acyclification* of E, denoted by  $E^{acy}$ , has edges  $(i \to j) \in E^{acy}$  if and only if  $i \notin sc_{\mathcal{G}}(j)$  and there exists  $k \in sc_{\mathcal{G}}(j)$  such that  $(i \to k) \in E$ .

Lemma 7 shows that the clustering operation in Definition 9 on directed graphs, followed by the declustering operation in Definition 8, results in the same directed graph as the one that is obtained by applying the acyclification operation to its edge set.

**Lemma 7.** Let  $\mathcal{G} = \langle V, E \rangle$  be a directed graph. It holds that  $\mathcal{G}^{acy} = \langle V, E^{acy} \rangle = D(clust(\mathcal{G}))).$ 

*Proof.* This follows from Definitions 8, 9, and 13.

The following proposition shows that  $\sigma$ -separations in a directed graph coincide with *d*-separations in the graph that is obtained by clustering and subsequently declustering that directed graph.

**Proposition 4.** Let  $\mathcal{G} = \langle V, E \rangle$  be a directed graph with nodes V and  $\mathcal{G}^{acy} = \langle V, E^{acy} \rangle$ . Then for all subsets  $A, B, C \subseteq V$ :

$$A \stackrel{\sigma}{\underset{\mathcal{G}}{\perp}} B | C \implies A \stackrel{d}{\underset{\mathcal{G}^{\operatorname{acy}}}{\perp}} B | C \iff A \stackrel{d}{\underset{D(\operatorname{clust}(\mathcal{G}))}{\perp}} B | C.$$

*Proof.* The proof of the first implication follows from Corollary 2.8.4 and Lemma 2.7.7 in Forré and Mooij (2017). The second equivalence follows directly from Lemma 7.  $\hfill \square$ 

We now have all ingredients to finish the proof of Proposition 1. First note that, since the subgraph of  $\mathcal{B} = \langle V, F, E \rangle$  induced by  $(V \cup F) \setminus W$  has a perfect matching,  $\operatorname{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$  is well-defined by Corollary 1. Let  $S_V^{(1)}, \ldots, S_V^{(n)}$  be the strongly connected components in  $\mathcal{G}_{\operatorname{dir}}$ , where  $\mathcal{G}_{\operatorname{dir}} := \mathcal{G}(\mathcal{B}, M)_{\operatorname{mar}(F)}$ . By Lemma 5 and the definition of Algorithm 1 we know that  $\mathcal{V}$  consists of the clusters  $S_V^{(i)} \cup M(S_V^{(i)})$ with  $i = 1, \ldots, n$ . Therefore,  $\mathcal{M}$  is uniquely solvable with respect to  $\operatorname{CO}(\mathcal{B})$ . By Theorem 2 we have that for subsets  $A, B, C \subseteq V$ :

$$A \stackrel{d}{\underset{\mathrm{MO}(\mathcal{B})}{\perp}} B \mid C \implies \mathbf{X}_A \underset{\mathbb{P}_{\mathbf{X}}}{\perp} \mathbf{X}_B \mid \mathbf{X}_C.$$
(5)

By Proposition 4 we have that:

$$A \stackrel{\sigma}{\underset{\mathcal{G}_{\mathrm{dir}}}{\perp}} B | C \implies A \stackrel{d}{\underset{\mathcal{G}_{\mathrm{dir}}}{\perp}} B | C \iff A \stackrel{d}{\underset{D(\mathrm{clust}(\mathcal{G}_{\mathrm{dir}}))}{\perp}} B | C.$$
(6)

The desired result follows from implications (5) and (6) when  $D(\text{clust}(\mathcal{G}_{\text{dir}})) = \text{MO}(\mathcal{B})$ . Consider the cluster set  $\mathcal{V}_{\text{mar}(F)} = \{S \cap V : S \in \mathcal{V}\}$  and note that edges in  $\text{CO}(\mathcal{B})$  go from vertices in V to clusters in  $\mathcal{V}$ . By Definition 8 and 9 we have that:

$$D(\langle \mathcal{V}_{\operatorname{mar}(F)}, \mathcal{E} \rangle) = D(\langle \mathcal{V}, \mathcal{E} \rangle)_{\operatorname{mar}(F)}$$
 and  $\operatorname{clust}(\mathcal{G}_{\operatorname{dir}}) = \langle \mathcal{V}_{\operatorname{mar}(F)}, \mathcal{E} \rangle$ ,

respectively. It follows that

$$D(\operatorname{clust}(\mathcal{G}_{\operatorname{dir}})) = D(\operatorname{CO}(\mathcal{B}))_{\operatorname{mar}(F)} = \operatorname{MO}(\mathcal{B}).$$

This finishes the proof.

### 8.5 Proof of Theorem 4

**Theorem 4.** Let  $\mathcal{M} = \langle \mathcal{X}, \mathcal{X}_W, \Phi, \mathcal{B} \rangle$  be a system of constraints such that the subgraph of  $\mathcal{B}$  induced by endogenous variables and constraints is self-contained. Suppose that  $\mathcal{M}$  is uniquely solvable w.r.t. the causal ordering graph  $\operatorname{CO}(\mathcal{B})$  and let  $\mathcal{X}^*$  be a solution. Assume that the intervened system  $\mathcal{M}_{\operatorname{si}(f,\phi,c)}$  is also uniquely solvable w.r.t.  $\operatorname{CO}(\mathcal{B})$  and let  $\mathcal{X}'$  be a solution. If there is no directed path from f to  $v \in V \setminus W$  in  $\operatorname{CO}(\mathcal{B})$  then  $X_v^* = X_v'$  almost surely. Conversely, if there is a directed path f to v in  $\operatorname{CO}(\mathcal{B})$  then  $X_v^*$  may have a different distribution than  $X_v'$ .

The directed cluster graph  $CO(\mathcal{B})$  is acyclic by construction and therefore there exists a topological ordering of its clusters. When there is no directed path from f to v in  $CO(\mathcal{B})$  then there exists a topological ordering  $V^{(1)}, \ldots, V^{(n)}$  of the clusters such that cl(v) comes before cl(f). By the assumption of unique solvability w.r.t.  $CO(\mathcal{B})$  we know that the solution component for any variable  $v \in V^{(i)}$  can be solved from the constraints in  $V^{(i)}$  after plugging in the solution components  $\bigcup_{j=1}^{i-1} V^{(j)}$ . By the assumption of unique solvability, the solution components  $X_v^*$  and  $X_v'$  are equal almost surely.

By assumption, the variables in cl(f) can be solved from the constraints in cl(f). Hence, a soft intervention on a constraint in cl(f) will generically change the distribution of the solution components  $\mathbf{X}^*_{cl(f)\cap V}$  that correspond to the variable vertices in cl(f). Suppose that there exists a sequence of clusters  $V_1 = cl(f), V_2, \ldots, V_{k-1}, V_k = cl(v)$  such that for all  $V_i \in \{V_1, \ldots, V_{k-1}\}$  there is a vertex  $z_i \in V_i$  such that  $(z_i \to V_{i+1})$  in  $CO(\mathcal{B})$ . By the assumption of unique solvability w.r.t.  $CO(\mathcal{B})$  the solution components for the variables in  $V_2, \ldots, V_k$  generically depend on the distribution of the solution components  $\mathbf{X}^*_{cl(f)\cap V}$  that correspond to the variable vertices in cl(f). It follows that the solution  $\mathbf{X}^*_v$  is generically different from that of  $\mathbf{X}'_v$ , if there is a directed path from f to v in  $CO(\mathcal{B})$ .

# 8.6 Proof of Lemma 1 and Proposition 2

**Lemma 1.** Let  $\mathcal{B} = \langle V, F, E \rangle$  be a bipartite graph and  $W \subseteq V$ , so that the subgraph of  $\mathcal{B}$  induced by  $V \cup F$  is self-contained. Consider an intervention  $\operatorname{do}(S_V, S_F)$  on a cluster  $S = S_V \cup S_F$  with  $S \cap W = \emptyset$  in the causal ordering graph  $\operatorname{CO}(\mathcal{B})$ . The subgraph of  $\mathcal{B}_{\operatorname{do}(S_V, S_F)}$  induced by  $(V \cup F) \setminus W$  is self-contained.

*Proof.* By definition of Algorithm 2 we know that the subgraph of  $\mathcal{B}$  induced by  $(V \cup F) \setminus W$  has a perfect matching M such that  $M(S_F) = S_V$ . By definition of a perfect intervention on the bipartite graph we know that M is also a perfect matching for the subgraph of  $\mathcal{B}_{\operatorname{do}(S_V,S_F)}$  induced by  $(V \cup F) \setminus W$ . The result follows from Corollary 1.

**Proposition 2.** Let  $\mathcal{M} = \langle \mathcal{X}, \mathcal{X}_W, \Phi, \mathcal{B} = \langle V, F, E \rangle \rangle$  such that the subgraph of  $\mathcal{B}$  induced by  $(V \cup F) \setminus W$  is self-contained. Assume that it is uniquely solvable w.r.t.  $\operatorname{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$  and let  $\mathbf{X}^*$  be a solution of  $\mathcal{M}$ . Let  $S_F \subseteq F$  and  $S_V \subseteq V \setminus W$  be such that  $(S_F \cup S_V) \in \mathcal{V}$ . Assume that the intervened system  $\mathcal{M}_{\operatorname{do}(S_F,S_V,\boldsymbol{\xi}_{S_V})}$  is uniquely solvable w.r.t.  $\operatorname{CO}(\mathcal{B}_{\operatorname{do}(S_F,S_V)})$  and let  $\mathbf{X}'$  be a solution of  $\mathcal{M}_{\operatorname{do}(S_F,S_V,\boldsymbol{\xi}_{S_V})}$ . If there is no directed path from any  $x \in S_V$  to  $v \in V$  in  $\operatorname{CO}(\mathcal{B})$  then  $X_v^* = X_v'$  almost surely. Conversely, if there is  $x \in S_V$  such that there is a directed path x to v in  $\operatorname{CO}(\mathcal{B})$  then  $X_v^*$  may have a different distribution than  $X_v'$ .

Let  $v \in S_V$ . Since the variable vertices  $S_V$  are targeted by the perfect intervention, we have that  $X'_v = \xi_v$ , which is generically different from the solution component  $X_v^*$ . Consider  $v \in V \setminus S_V$  and its cluster cl(v) in  $CO(\mathcal{B})$ . Since the causal ordering graph is acyclic by construction, there exists a topological ordering  $V^{(1)}, \ldots, V^{(i)} =$  $cl(v), \ldots V^{(n)}$  of the clusters in  $CO(\mathcal{B})$  (where *n* is the amount of clusters in  $CO(\mathcal{B})$ ) such that  $V^{(j)} \prec cl(v)$  implies that there is a directed path from some vertex in  $V^{(j)}$  to the cluster cl(v) in  $CO(\mathcal{B})$ . By assumption, the solution component  $X_v^*$ can be solved from the constraints and variables in  $V^{(i)} = cl(v)$  by plugging in the solution for variables in  $V^{(1)}, \ldots, V^{(i-1)}$ . Let  $s_f^1, \ldots, s_f^m$  and  $s_v^1, \ldots, s_v^m$  denote the ordered vertices in  $S_F$  and  $S_V$  respectively and suppose that  $S_V \cup S_F = V^{(k)}$ for some  $k \in \{1, \ldots, n\}$ . By definition of a perfect intervention on a cluster we know that  $V^{(1)}, \ldots, V^{(k-1)}, \{s_f^1, s_v^1\}, \ldots, \{s_f^m, s_v^m\}, V^{(k+1)}, \ldots, V^{(n)}$  is a topological ordering of clusters in  $CO(\mathcal{B})_{do(S_F, S_V)} = CO(\mathcal{B}_{do(S_F, S_V)})$  (by Proposition 3).

Suppose that  $V^{(k)} \succ V^{(i)}$  in the topological ordering for  $\operatorname{CO}(\mathcal{B})$ . By assumption of unique solvability w.r.t.  $\operatorname{CO}(\mathcal{B})_{\operatorname{do}(S_F,S_V)}$ ,  $X'_v$  can be solved from the constraints and variables in  $V^{(i)}$  by plugging in the solution for variables in  $V^{(1)}, \ldots, V^{(i-1)}$ . It follows that  $X^*_v = X'_v$  almost surely and by construction of the topological ordering there is no directed path from any  $x \in S_V$  to v in  $\operatorname{CO}(\mathcal{B})$ . Suppose that  $V^{(k)} \prec \operatorname{cl}(v)$  in the topological ordering for  $\operatorname{CO}(\mathcal{B})$ . By assumption of unique solvability w.r.t.  $\operatorname{CO}(\mathcal{B})_{\operatorname{do}(S_F,S_V)}$ , we know that  $X'_v$  can be solved from the constraints and variables in  $V^{(i)}$  by plugging in the solution for variables in  $V^{(1)}, \ldots, V^{(k-1)}, \{s_f^1, s_v^1\}, \ldots, \{s_f^m, s_v^m\}, V^{(k+1)}, \ldots, V^{(i-1)}$ . It follows that  $X^*_v$  and  $X'_v$  generically have a different distribution, and by construction of the topological ordering there is a directed path from a vertex in  $S_V$  to the cluster  $\operatorname{cl}(v)$  in  $\operatorname{CO}(\mathcal{B})$ .

# 8.7 Proof of Proposition 3

**Proposition 3.** Let  $\mathcal{B} = \langle V, F, E \rangle$  be a bipartite graph and W a set of exogenous variables such that the subgraph of  $\mathcal{B}$  induced by  $(V \cup F) \setminus W$  is self contained. Let  $CO(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$  be the corresponding causal ordering graph. Let  $S_F \subseteq F$  and  $S_V \subseteq V \setminus W$  be such that  $(S_F \cup S_V) \in \mathcal{V}$ . Then:

$$\mathrm{CO}(\mathcal{B}_{\mathrm{do}(S_F,S_V)}) = \mathrm{CO}(\mathcal{B})_{\mathrm{do}(S_F,S_V)}.$$

Let  $S_V = \langle s_v^1, \ldots, s_v^m \rangle$  and  $S_F = \langle s_f^1, \ldots, s_f^m \rangle$  denote the targeted variables and constraints. We consider the output  $\operatorname{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$  of the causal ordering algorithm. Suppose that the order in which clusters  $V^{(i)}$  are added to  $\mathcal{V}_1$  is given by

$$V^{(1)}, \dots, V^{(k)} = (S_F \cup S_V), \dots, V^{(n)}.$$

Consider  $\operatorname{CO}(\mathcal{B}_{\operatorname{do}(S_F,S_V)}) = \langle \mathcal{V}', \mathcal{E}' \rangle$ . It follows from Definition 11, Lemma 2, Lemma 3, and the definition of Algorithm 1 that

$$V^{(1)}, \ldots, V^{(k-1)}, \{s_f^1, s_v^1\}, \ldots, \{s_f^m, s_v^m\}, V^{(k+1)}, \ldots, V^{(n)}$$

is an order in which clusters could be added to  $\mathcal{V}'$ . This shows that there are two differences between  $\operatorname{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$  and  $\operatorname{CO}(\mathcal{B}_{\operatorname{do}(S_F,S_V)}) = \langle \mathcal{V}', \mathcal{E}' \rangle$ : first  $(S_F \cup S_V) \in \mathcal{V}$  whereas  $\{\{s_f^i, s_v^i\} : i = 1, \ldots, m\} \subseteq \mathcal{V}'$  and second the clusters  $(S_F \cup S_V)$ may have parents in  $\operatorname{CO}(\mathcal{B})$  but the clusters  $\{s_f^i, s_v^i\}$  (with  $i \in \{1, \ldots, m\}$ ) have no parents in  $\operatorname{CO}(\mathcal{B}_{\operatorname{do}(S_F,S_V)})$ . The result follows directly from Definition 12.  $\Box$ 

# 8.8 Directed edges in the graph of the SCM

The SCM for the bathtub system that we discussed in Section 3.3 does not have a unique solution under every possible intervention on the SCM. Therefore, according to Bongers, Forré, et al. (2020), the graph of this SCM does not have a straightforward causal interpretation. Instead, we may apply Proposition 7.1.1 in Bongers, Forré, et al. (2020), which gives a sufficient condition for detecting an edge  $(v_i \rightarrow v_j)$  in the graph of an SCM. For an edge  $(v_i \rightarrow v_j)$  in the bathtub system, it says to consider  $\boldsymbol{\xi}_I \in \mathbb{R}^3_{>0}$  (with  $I = \{K, I, P, O, D\} \setminus \{i, j\}$ ) such that the SCM has a unique solution under the intervention do $(I, \boldsymbol{\xi}_I)$ . The edge  $(v_i \to v_j)$  is present if there exist distinct values  $\xi_i, \tilde{\xi}_i \in \mathbb{R}_{>0}$  such that the SCM has a unique solution after subsequently applying the interventions  $do(I, \boldsymbol{\xi}_I)$  and  $do(i, \boldsymbol{\xi}_i)$  that does not coincide with the unique solution after subsequently applying the interventions  $do(I, \xi_I)$  and  $do(i, \xi_i)$ . From the second column in Table 5 we can read off that the directed edges  $(v_K \to v_O)$ ,  $(v_P \to v_O)$ , and  $(v_D \to v_O)$  are implied by the proposition. Proposition 7.1.1 in Bongers, Forré, et al. (2020) also provides a sufficient condition for the presence of edges  $(v_i \rightarrow v_j)$  in the latent projection onto  $\{i, j\}$ . If there exists distinct  $\xi_i, \xi_i \in \mathbb{R}_{>0}$  such that the SCM has a unique solution under the intervention  $do(i, \xi_i)$  that does not coincide with the unique solution after the intervention  $do(i, \tilde{\xi}_i)$ . From the third column in Table 5 we can read off that the edges  $(v_K \to v_P), (v_K \to v_D), (v_I \to v_P), (v_I \to v_O), (v_I \to v_D),$  $(v_D \rightarrow v_P)$ , and  $(v_D \rightarrow v_O)$  are present in the corresponding latent projections onto two variables.

Note that the effects of interventions on  $\{f_K, v_K\}$  and  $\{f_I, v_I\}$  implied by Table 5 agree with those presented in Table 3. Interestingly, the proposition implies that the edge  $(v_K \to v_O)$  is present in the graph of the SCM, while it does not imply the presence of this edge in the latent projection onto  $\{v_K, v_O\}$ .

Table 5: The presence of directed edges in the graph of the SCM for the bathtub system that is implied by Proposition 7.1.1 in Bongers, Forré, et al. (2020). We also consider the implied presence of directed edges in the graph of an SCM in which only two out of five variables are observed. Under interventions targeting  $\{v_K, v_I, v_P, v_O\}$  or there is no unique solution for  $X_D$ . Under interventions targeting  $\{v_K, v_I, v_P, v_O\}$  the intervention values there is no solution if the values  $\xi_I$  or  $\xi_O$  are varied individually. Similarly, for interventions targeting either  $v_O$  or  $v_P$  there are no two distinct interventions values under which the intervened system is solvable.

Edge $(x \to y)$	Graph of the SCM	Latent projection onto $\boldsymbol{x},\boldsymbol{y}$
$v_K \rightarrow v_I$	not implied	not implied
$v_K \rightarrow v_P$	not implied	present
$v_K \rightarrow v_O$	present	not implied
$v_K \to v_D$	solution $X_D$ not unique	present
$v_I \rightarrow v_K$	not implied	not implied
$v_I \rightarrow v_P$	not implied	present
$v_I \rightarrow v_O$	not implied	present
$v_I \rightarrow v_D$	cannot vary $X_I$	present
$v_P \rightarrow v_K$	not implied	cannot vary $X_P$
$v_P \rightarrow v_I$	not implied	cannot vary $X_P$
$v_P \rightarrow v_O$	present	cannot vary $X_P$
$v_P \rightarrow v_D$	solution $X_D$ not unique	cannot vary $X_P$
$v_O \rightarrow v_K$	not implied	cannot vary $X_O$
$v_O \rightarrow v_I$	not implied	cannot vary $X_O$
$v_O \rightarrow v_P$	not implied	cannot vary $X_O$
$v_O \rightarrow v_D$	cannot vary $X_O$	cannot vary $X_O$
$v_D \rightarrow v_K$	not implied	not implied
$v_D \rightarrow v_I$	not implied	not implied
$v_D \rightarrow v_P$	present	present
$v_D \rightarrow v_O$	not implied	present