

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 endogenous and exogenous variables. What can we say about the causal and probabilistic aspects of variables that appear in these equations without explicitly solving the equations? We make use of Simon's causal ordering algorithm (Simon, 1953) to construct a *causal ordering graph* and prove that it expresses the effects of soft and perfect interventions on the equations under certain unique solvability assumptions. We further construct a *Markov ordering graph* and prove that it encodes conditional independences in the distribution implied by the equations with independent random exogenous variables, under a similar unique solvability assumption. We discuss how this approach reveals and addresses some of the limitations of existing causal modelling frameworks, such as causal Bayesian networks and structural causal models.

Keywords: Causality, Conditional Independence, Structure Learning, Causal Ordering, Graphical Models, Equilibrium Systems, Cycles, Comparative Statics

1. Introduction

The discovery of causal relations is a fundamental objective in many scientific endeavours. The process of the scientific method usually involves a hypothesis, such as a causal graph or a set of equations, that explains observed phenomena. Such a graph structure can be learned automatically from conditional independences in observational data via causal discovery algorithms, e.g., the well-known PC and FCI algorithms (Spirtes et al., 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 mixed graphs can actually simultaneously encode the causal semantics

and the conditional independence constraints of a system.¹ We explicitly define soft and perfect interventions on sets of equations and demonstrate that, for some models, a single graph expressing conditional independences between variables via d-separations does not represent the effects of these interventions in an unambiguous way, while graphs that also have vertices representing equations do encode both the dependence and causal structure implied by these models. 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.

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 hypothesis, such as a causal graph or set of equations, that are then verified or rejected through experimentation. We show how testable predictions can be derived automatically from sets of equations via the *causal ordering algorithm*, introduced by Simon (1953). We adapt and extend the algorithm to construct a *directed cluster graph* that we call the *causal ordering graph*. From this, we can construct a directed graph that we call the *Markov ordering graph*. We prove that, under a certain unique solvability assumption, the latter implies conditional independences between variables which can be tested in observational data and the former represents the effects of soft and certain perfect interventions which can be verified through experimentation. We believe that 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 associated with a Structural Causal Model (SCM) (see Pearl (2000); Bongers et al. (2020)), which are also commonly referred to as Structural Equation Models (SEMs).² 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 observations in Iwasaki and Simon (1994); Dash (2005). Throughout this work, we discuss an example in Iwasaki and Simon (1994) to illustrate our ideas. Here, we use it to highlight the contributions of this paper and to provide 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_{v_I} and it flows out of the tub through a drain with diameter X_{v_K} . An ensemble of such bathtubs that have faucets and drains with different rates and diameters can be modelled by the equations f_K and f_I below:*

$$f_K : \quad X_{v_K} = U_{w_K}, \tag{1}$$

$$f_I : \quad X_{v_I} = U_{w_I}, \tag{2}$$

1. See, for example, (Dawid, 2010) and references therein for a discussion.
 2. The latter term has been used by econometricians since the 1950s. Note that, in the past some econometricians have used (cyclic/non-recursive) “structural models” without requiring that there is a specified one-to-one correspondence between endogenous variables and equations; see e.g., Basmann (1963). Recent usage is consistent with the implication that there is a specified variable on the left-hand side for each equation as is common in the SCM framework.

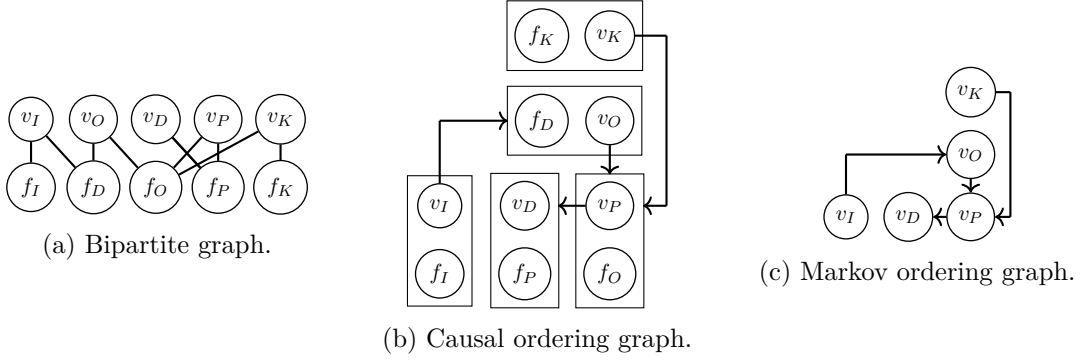


Figure 1: Three graphical representations for the bathtub system in equilibrium. The bipartite graph in Figure 1a is a representation of the structure of equations $F = \{f_K, f_I, f_P, f_O, f_D\}$ where the vertices $V = \{v_K, v_I, v_P, v_O, v_D\}$ correspond to endogenous variables and there is an 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 1b, 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 1c.

where U_{w_K} and U_{w_I} are independent random variables both taking value in $\mathbb{R}_{>0}$. When the faucet is turned on, the water level X_{v_D} in the bathtub increases as long as the inflow X_{v_I} of the water exceeds the outflow X_{v_O} of water. The differential equation $\dot{X}_{v_D}(t) = U_{w_1}(X_{v_I}(t) - X_{v_O}(t))$ defines the mechanism for the rate of change in $X_{v_D}(t)$, where U_{w_1} is a constant or a random variable taking value in $\mathbb{R}_{>0}$. At equilibrium the rate of change is equal to zero, resulting in the equilibrium equation

$$f_D : \quad U_{w_1}(X_{v_I} - X_{v_O}) = 0. \quad (3)$$

As the water level X_{v_D} increases, the pressure X_{v_P} that is exerted by the water increases as well. The mechanism for the change in pressure is defined by the differential equation $\dot{X}_{v_P}(t) = U_{w_2}(gU_{w_3}X_{v_D}(t) - X_{v_P}(t))$, where g is the gravitational acceleration and U_{w_2}, U_{w_3} are constants or random variables both taking value in $\mathbb{R}_{>0}$. After equilibration, we obtain

$$f_P : \quad U_{w_2}(gU_{w_3}X_{v_D} - X_{v_P}) = 0. \quad (4)$$

The higher the pressure X_{v_P} or the bigger the size of the drain X_{v_K} , the faster the water flows through the drain. The differential equation $\dot{X}_{v_O}(t) = U_{w_4}(U_{w_5}X_{v_K}X_{v_P}(t) - X_{v_O}(t))$ models the outflow rate of the water, where U_{w_4}, U_{w_5} are constants or random variables both taking value in $\mathbb{R}_{>0}$. The equilibrium equation f_O is given by

$$f_O : \quad U_{w_4}(U_{w_5}X_{v_K}X_{v_P} - X_{v_O}) = 0. \quad (5)$$

We will study the conditional independences that are implied by equilibrium equations (1) to (5). In Sections 5.1 and 5.2 we will define the notion of soft and perfect interventions on sets of equations as a generalization of soft and perfect interventions on SCMs. The causal properties of sets of equilibrium equations are examined by comparing the equilibrium

distribution before and after an intervention. Our approach is related to the comparative statics analysis that is used in economics to study the change in equilibrium distribution after changing exogenous variables or parameters in the model, see also Simon and Iwasaki (1988). In this work, we will additionally consider the effects on the equilibrium distribution of perfect interventions targeting endogenous variables in the equilibrium equations.

Graphical representations. A set of equations can be represented by a bipartite graph. In the case of the filling bathtub, the structure of equilibrium equations (1) to (5) is represented by the bipartite graph in Figure 1a. 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 labelled v_i appears in the equation with label f_j . A formal definition of a system of constraints and its associated bipartite graph will be provided in Section 1.1. The causal ordering algorithm, introduced by Simon (1953) and 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 1b. In Section 4 we will show how the Markov ordering graph can be constructed from a causal ordering graph. For the equilibrium equations of the filling bathtub, the Markov ordering graph is given in Figure 1c. The causal ordering algorithm of Simon (1953) can only be applied to bipartite graphs that have the property that they are self-contained. In Section 3 we introduce an extended causal ordering algorithm that can also be applied to bipartite graphs that are not self-contained.

Markov property. The Markov ordering graph in Figure 1c encodes conditional independences between the equilibrium solutions X_{v_K} , X_{v_I} , X_{v_P} , X_{v_O} , and X_{v_D} of the equilibrium equations. In particular, d -separations between variable vertices in the Markov ordering graph imply conditional independences between the corresponding variables under certain solvability conditions, as we will prove in Theorem 17 in Section 4. In Figure 1c, the variable vertices v_I and v_D are d -separated by v_P . It follows that at equilibrium the inflow rate X_{v_I} and the water level X_{v_D} are independent given the outflow rate X_{v_P} . In Sections 3 and 4.4 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 σ -separations.³

Soft interventions. The causal ordering graph in Figure 1b encodes the effects of soft interventions targeting (equilibrium) equations. This type of intervention is often also referred to as a mechanism change. We assume that the variables in each cluster can be solved uniquely from the equations in their cluster both before and after the intervention.⁴ A soft intervention has no effect on a variable if there is no directed path from the intervention

3. Forré and Mooij (2017) introduced the notion of σ -separations to replace d -separations in directed graphs that may contain cycles. See Section A.2 for more details.

4. For the underlying dynamical model this assumption means that we assume that the equations of the model define a unique equilibrium to which the system converges and that the system also converges to a unique equilibrium that is defined by the model equations after an intervention on one of the parameters or exogenous variables in the model. For some dynamical systems, extra equations are required that describe the dependence of the equilibrium distribution on initial conditions. Their causal semantics

target to the cluster containing the variable, as we will prove in Theorem 20 in Section 5.1. Consider an experiment where the value of the gravitational acceleration 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 $\{v_K, v_I, v_P, v_O\}$ in the causal ordering graph in Figure 1b. Since the conditions of Theorem 20 are satisfied, the soft intervention on f_P has no effect on $\{X_{v_K}, X_{v_I}, X_{v_P}, X_{v_O}\}$ but it may have an effect on X_{v_D} (depending on the precise functional form of the equations and the values of the parameters).

Perfect interventions. The causal ordering graph in Figure 1b also encodes the effects of perfect interventions on clusters, under the assumption that variables can be solved uniquely from the equations of their clusters in the causal ordering graph before and after intervention. We will formally prove this in Theorem 23 in Section 5.2. Consider a perfect intervention on the cluster $\{f_K, v_K\}$ (i.e., fixing the diameter X_{v_K} of the drain by altering the equation f_K) in Figure 1b. This intervention may change the solution for $\{X_{v_K}, X_{v_P}, X_{v_D}\}$ because v_K is targeted by the intervention and there are directed paths from the cluster of v_K to the clusters of v_P and v_D . It has no effect on $\{X_{v_I}, X_{v_O}\}$ because there are no directed paths from the cluster of v_K to the clusters of v_I and v_O .

1.1 System of constraints

Our formal treatment of sets of equations mirrors the definition of a structural causal model in the sense that we separate the model from the endogenous random variables that solve it. An introduction to cyclic SCMs will be provided in Appendix A.2, while the related graph terminology and background regarding Markov properties can be found in Appendix A.1 and Appendix A.3, respectively. Here, we introduce a mathematical object that we call a *system of constraints* to represent equations together with their structure as a bipartite graph.

Definition 1 A system of constraints is a tuple $\langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} = \langle V, F, E \rangle \rangle$ where

1. $\mathcal{X} = \bigotimes_{v \in V} \mathcal{X}_v$, where each \mathcal{X}_v is a standard measurable space and the domain of a variable X_v ,
2. $\mathbf{X}_W = (X_w)_{w \in W}$ is a family of independent random variables taking value in \mathcal{X}_W with $W \subseteq V$ a set of indices corresponding to exogenous variables,⁵
3. $\Phi = (\Phi_f)_{f \in F}$ 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}_f ,
 - (c) $\phi_f : \mathcal{X}_{V(f)} \rightarrow \mathcal{Y}_f$ a measurable function,
4. $\mathcal{B} = \langle V, F, E \rangle$ is a bipartite graph with:

cannot be modelled in the standard SCM framework (Blom et al., 2019). For these systems, Blom et al. (2019) introduced the more general class of Causal Constraints Models.

5. This means that the nodes $V \setminus W$ correspond to endogenous variables.

- (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. We will often refer to the bipartite graph in a system of constraints as the ‘associated bipartite graph’. 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: $V(f) = \text{adj}_{\mathcal{B}}(f)$. For a set $S_F \subseteq F$, we will let $\text{adj}_{\mathcal{B}}(S_F) = V(S_F) = \cup_{f \in S_F} V(f)$ denote the adjacencies of the vertices $f \in S_F$.

When modelling some system with a system of constraints, we are implicitly assuming that the constraints are *reversible* in the sense that the causal relations between the endogenous variables are flexible and may depend in principle on the entire set of constraints in the system. However, there is an important modelling choice regarding which of the variables to consider as *endogenous* (“internal” to the system) and which variables to consider as *exogenous* (“external” to the system). The implicit assumption here is that *the endogenous variables cannot cause the exogenous variables*. This is the (only) causal “background knowledge” that is expressed formally by a system of constraints. As Simon (1953) showed, and as we will explicate in later sections, the causal relations between the endogenous variables can then be obtained by applying Simon’s causal ordering algorithm.

Example 2 Consider two variables: the temperature in a room (X_1) and the reading of a thermometer in the same room (X_2). One can think of different systems of constraints to model these variables. One possibility is the single constraint ($X_1 - X_2 = 0$) in which both X_1 and X_2 are considered to be endogenous variables. As it turns out, we will then not be able to draw any conclusion regarding the causal relation between X_1 and X_2 . Another possibility would be to use the same constraint, but now considering X_1 to be exogenous and X_2 to be endogenous. Then, one will find that X_1 causes X_2 , but not vice versa, which may appear to be a realistic model. Yet another possibility with the same constraint would be to consider X_2 to be the exogenous variable and X_1 to be endogenous. This model would be considered less realistic in most situations (except perhaps in somewhat unnatural settings where the thermometer would be broken, but its reading would be used by some agent to adjust the heating in order to control the room temperature).

Thus, the constraint $X_1 - X_2 = 0$ on its own does not lead to any conclusions regarding the causal relations between variables X_1 and X_2 ; it is only through the additional background knowledge (represented by the distinction between endogenous and exogenous variables) that the causal directionality is fixed. In cases with more than one endogenous variable (like in Example 1), the causal ordering algorithm can be used to “propagate” the causal directionality from exogenous to endogenous variables, and a causal ordering of the endogenous variables can be obtained.

1.2 Related work and contributions

Graphical models are a popular statistical tool to model probabilistic aspects of complex systems. 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 direct causal relations between corresponding variables (Pearl, 2000). The strong assumptions that are necessary for this viewpoint have been the topic of debate (Dawid, 2010). This work contributes to this discussion by revisiting an example in Iwasaki and Simon (1994), and discussing how it seems that, in this case, the presence of vertices representing equations is required to simultaneously express both conditional independences and the effects of interventions in a single graph.

Throughout this work, we discuss the application of the causal ordering algorithm to the equilibrium equations of the bathtub model that we discussed in Example 1. In the literature, feedback processes that have reached equilibrium have been represented by e.g., chain graphs (Lauritzen and Richardson, 2002) and cyclic directed graphs (Spirtes, 1995; Mooij et al., 2013; Bongers and Mooij, 2018). For the latter it was shown that they imply conditional independences in the equilibrium distribution via the d-separation criterion in the linear or discrete case (Forré and Mooij, 2017) but that the directed global Markov property may fail if the underlying model is neither linear nor discrete (Spirtes, 1995). The alternative criterion that Spirtes (1995) formulated for the “collapsed graph” was recently reformulated in terms of σ -separations and shown to hold in very general settings (Forré and Mooij, 2017). Constraint-based causal discovery algorithms for the cyclic setting under various assumptions are given in Richardson (1996); Forré and Mooij (2018); Strobl (2018); Mooij et al. (2020); Mooij and Claassen (2020). The causal properties of dynamical systems at equilibrium were previously studied by Fisher (1970); Mooij et al. (2013); Hyttinen et al. (2012); Lauritzen and Richardson (2002); Mooij et al. (2011); Bongers and Mooij (2018); Blom et al. (2019), who consider graphical and causal models that arise from studying the stationary behaviour of dynamical models. For the deterministic case, Mooij et al. (2013) propose to map first-order differential equations to labelled equilibrium equations and then to the structural equations of an SCM. This idea was recently generalized to the stochastic case and higher order differential equations (Bongers and Mooij, 2018). For certain systems, such as the bathtub model in Example 1, this construction may lead to a cyclic SCM with self-cycles (Bongers and Mooij, 2018). The causal and conditional independence properties of cyclic SCMs (possibly with self-cycles) have been studied by Bongers et al. (2020). In other work assumptions on the underlying dynamical model have been made to avoid the complexities of SCMs with self-cycles. Here, we will consider potential benefits (e.g., obtaining a stronger Markov property) of applying the technique of causal ordering to the structural equations of the cyclic SCM for the equilibrium equations of dynamical systems such as the bathtub system.

Our work generalizes the causal ordering algorithm that 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. There also exists a different, computationally more efficient, algorithm for causal ordering (Nayak, 1995; Gonçalves and Porto, 2016). We formally prove that this algorithm is equivalent to the one in Simon (1953). This 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. Using methods to determine the upper-triangular form of a matrix in Pothen and Fan (1990), we further extend the causal ordering algorithm so that it can be applied to any bipartite graph.

In Section 6 we will present a detailed discussion of how our work relates to that of Iwasaki and Simon (1994); Bongers and Mooij (2018); Bongers et al. (2020); Dash (2005). We show that what Iwasaki and Simon (1994) call the “causal graph” 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. Because Simon and Iwasaki (1988) assume that a one-to-one correspondence between variables and equations is known in advance, they can use the Markov ordering graph to read off the effects of soft interventions. We argue that the causal ordering graph, and not the Markov ordering graph, should be used to represent causal relations when the matching between variables and equations is not known before-hand. This sheds some new light on the work of Dash (2005) on (causal) structure learning and equilibration in dynamical systems. We further discuss the advantages and disadvantages of our causal ordering approach compared to the SCM framework.

2. Causal ordering

In this section, we adapt the causal ordering algorithm of Simon (1953), rephrase it in terms of *self-contained* bipartite graphs, and define the output of the algorithm as a *directed cluster graph*.⁶ We then prove that Simon’s causal ordering algorithm is well-defined and has a unique output.

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

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 3.

6. The notion of a directed cluster graph corresponds to the box representation of a collapsed graph in Richardson (1996), Chapter 4.

Definition 3 Let $\mathcal{B} = \langle V, F, E \rangle$ be a bipartite graph. A subset $F' \subseteq F$ is said to be self-contained if

1. $|F'| = |\text{adj}_{\mathcal{B}}(F')|$,
2. $|F''| \leq |\text{adj}_{\mathcal{B}}(F'')|$ for all $F'' \subseteq F'$.⁷

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 set⁸ if all its non-empty strict subsets are not self-contained.

Example 3 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.

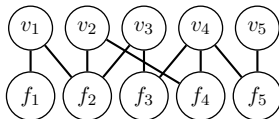


Figure 2: A self-contained bipartite graph $\mathcal{B} = \langle V, F, E \rangle$ with $V = \{v_1, v_2, v_3, v_4, v_5\}$ and $F = \{f_1, f_2, f_3, f_4, f_5\}$. The sets $\{f_1\}$, $\{f_1, f_2, f_3, f_4\}$, and $\{f_1, f_2, f_3, f_4, f_5\}$ are self-contained, and $\{f_1\}$ is the only minimal self-contained 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. An important assumption is that the mechanisms of the system do not cause the exogenous variables. 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 4 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:

$$\begin{aligned} \Phi_{f_1} : \quad & X_{v_1} - X_{w_1} = 0, \\ \Phi_{f_2} : \quad & X_{v_2} - X_{v_1} - X_{w_2} = 0. \end{aligned}$$

The associated bipartite graph $\mathcal{B} = \langle V, F, E \rangle$ is given in Figure 3a. It has vertices V that 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 Φ_{f_1} and Φ_{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 Φ_f). Since $|V| \neq |F|$, the associated bipartite graph is not self-contained.

7. This condition is also called the Hall Property (Hall, 1986).

8. In this case the Strong Hall Property holds, that is $|F''| < |\text{adj}_{\mathcal{B}}(F'')|$ for all $\emptyset \subsetneq F'' \subsetneq F'$ (Hall, 1986).



Figure 3: The bipartite graph in Figure 3a is associated with the constraints in Example 4. Exogenous variables are indicated by dashed circles. The directed cluster graph that is obtained by applying Algorithm 1 is shown in Figure 3b.

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 below has been adapted for systems of constraints with exogenous variables. The input is 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 $\mathcal{B}' = \langle V', F', E' \rangle$ 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 self-contained set $S_F \subseteq F$ in \mathcal{B}' . Together with the set of adjacent variable vertices $S_V = \text{adj}_{\mathcal{B}'}(S_F)$ a cluster $S_F \cup S_V$ is formed and added to \mathcal{V} . For each $v \in V$, an edge $(v \rightarrow (S_F \cup S_V))$ is added to \mathcal{E} if $v \notin S_V$ and $v \in \text{adj}_{\mathcal{B}}(S_F)$. 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 $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$.

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 its subgraph induced by $(V \setminus W) \cup F$ is self-contained

Output: directed cluster graph $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$

$\mathcal{E} \leftarrow \emptyset$ // initialization

$\mathcal{V} \leftarrow \{\{w\} : w \in W\}$ // initialization

$\mathcal{B}' \leftarrow \langle V', F', E' \rangle$ subgraph induced by $(V \setminus W) \cup F$ // initialization

while \mathcal{B}' is not the null graph **do**

$S_F \leftarrow$ a minimal self-contained set of F'

$C \leftarrow S_F \cup \text{adj}_{\mathcal{B}'}(S_F)$ // construct cluster

$\mathcal{V} \leftarrow \mathcal{V} \cup \{C\}$ // add cluster

for $v \in \text{adj}_{\mathcal{B}}(S_F) \setminus \text{adj}_{\mathcal{B}'}(S_F)$ **do**

$\mathcal{E} \leftarrow \mathcal{E} \cup \{(v \rightarrow C)\}$ // add edges to cluster

$\mathcal{B}' \leftarrow$ subgraph of \mathcal{B}' induced by $(V' \cup F') \setminus C$ // remove cluster

Theorem 4 shows that the output of causal ordering via minimal self-contained sets is well-defined and unique.

Theorem 4 *The output of Algorithm 1 is well-defined and unique.*

The following example shows how the causal ordering algorithm works on the bipartite graph in Figure 3a.

Example 5 *Consider the set of equations in Example 4 and its associated bipartite graph in Figure 3a. 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}' 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 $(w_1 \rightarrow \{v_1, f_1\})$ to \mathcal{E} . Finally, we add $\{v_2, f_2\}$ to \mathcal{V} and the edges $(v_1 \rightarrow \{v_2, f_2\})$ and $(w_2 \rightarrow \{v_2, f_2\})$ to \mathcal{E} . The output of the causal ordering algorithm is the directed cluster graph in Figure 3b. This reflects how one would solve the system of equations Φ_{f_1}, Φ_{f_2} with respect to X_{v_1}, X_{v_2} in terms of X_{w_1}, X_{w_2} by hand.*

3. Extending the causal ordering algorithm

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 algorithm suggested by Nayak (1995). Gonçalves and Porto (2016) proved that Simon’s classic algorithm makes use of a subroutine that solves an NP-hard problem, whereas the computational complexity of Nayak’s algorithm is bounded by $\mathcal{O}(|V||E|)$, where $|V|$ is the number of nodes and $|E|$ is the number of edges in the bipartite graph. Here, we provide a proof for the fact that causal ordering via minimal self-contained sets is equivalent to causal ordering via perfect matchings. There are many systems of equations with a unique solution that consist of more equations than there are endogenous variables, most notably in the case of non-linear equations, or in the presence of cycles. In that case the bipartite graph associated with these equations may not be self-contained. In this section, we show how Nayak’s algorithm can be extended using maximum matchings so that it can be applied to any bipartite graph.

3.1 Causal ordering via perfect matchings

Given a bipartite graph \mathcal{B} , the *associated directed graph* can be constructed from a matching M by *orienting edges*. A directed cluster graph can then be constructed via the operations that *construct clusters* and *merge clusters* in Definition 5 below.

Definition 5 *Let $\mathcal{B} = \langle V, F, E \rangle$ be a self-contained bipartite graph and M a perfect matching for \mathcal{B} .*

1. *Orient edges: For each $(v-f) \in E$ the edge set E_{dir} has an edge $(v \leftarrow f)$ if $(v-f) \in M$ and an edge $(v \rightarrow f)$ if $(v-f) \notin M$. E_{dir} has no additional edges. The associated directed graph is $\mathcal{G}(\mathcal{B}, M) = \langle V \cup F, E_{\text{dir}} \rangle$.*

2. Construct clusters: Let \mathcal{V}' be a partition of vertices $V \cup F$ into strongly connected components in $\mathcal{G}(\mathcal{B}, M)$. For each $(x \rightarrow w) \in E_{\text{dir}}$ the edge set \mathcal{E}' has an edge $(x \rightarrow \text{cl}(w))$ if $x \notin \text{cl}(w)$, where $\text{cl}(w) \in \mathcal{V}'$ is the strongly connected component of w in $\mathcal{G}(\mathcal{B}, M)$. The edge set \mathcal{E}' has no additional edges. The associated clustered graph is $\text{clust}(\mathcal{G}(\mathcal{B}, M)) = \langle \mathcal{V}', \mathcal{E}' \rangle$.
3. Merge clusters: Let $\mathcal{V} = \{S \cup M(S) : S \in \mathcal{V}'\}$. For each $(x \rightarrow S) \in \mathcal{E}'$ with $x \notin M(S)$ the edge set \mathcal{E} contains an edge $(x \rightarrow S \cup M(S))$. The edge set \mathcal{E} has no additional edges. The associated clustered and merged graph is $\text{merge}(\text{clust}(\mathcal{G}(\mathcal{B}, M))) = \langle \mathcal{V}, \mathcal{E} \rangle$.⁹

Algorithm 2: Causal ordering via perfect matching.

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  $(V \setminus W) \cup F$  // initialization
 $M \leftarrow$  perfect matching for  $\mathcal{B}'$  // initialization
 $E_{\text{dir}} \leftarrow \emptyset$  // orient edges
for  $(v - f) \in E$  with  $f \in F$  do
    if  $(v - f) \in M$  then
         $\perp$  Add  $(v \leftarrow f)$  to  $E_{\text{dir}}$ 
    else
         $\perp$  Add  $(v \rightarrow f)$  to  $E_{\text{dir}}$ 
 $\mathcal{V}' \leftarrow$  strongly connected components of  $\langle V \cup F, E_{\text{dir}} \rangle$  // clustering
 $\mathcal{E}' \leftarrow \emptyset$ 
for  $(x \rightarrow w) \in E_{\text{dir}}$  do
    for  $S \in \mathcal{V}'$  do
        if  $w \in S$  and  $x \notin S$  then
             $\perp$  Add  $(x \rightarrow S)$  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  $(x \rightarrow S) \in \mathcal{E}'$  do
        if  $x \notin M(S)$  then
             $\perp$  Add  $(x \rightarrow S \cup M(S))$  to  $\mathcal{E}$ 
    
```

For *causal ordering via perfect matching* we require as input 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. 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 matching¹⁰

9. In Theorem 6 we will show that this is the causal ordering graph $\text{CO}(\mathcal{B})$.

10. Note that a bipartite graph has a perfect matching if and only if it is self-contained (Hall, 1986). See also Theorem 38 and Corollary 39 in Appendix B.4.

for \mathcal{B}' ,¹¹ 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.¹² Finally, the merge operation is applied to construct the causal ordering graph. Theorem 6 below shows that causal ordering via perfect matchings is equivalent to causal ordering via minimal self-contained sets.

Theorem 6 *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.

Example 6 *Consider the bipartite graph \mathcal{B} in Figure 4a. The subgraph induced by the vertices $V = \{v_1, \dots, v_5\}$ and $F = \{f_1, \dots, f_5\}$ 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 $V = \{v_1, \dots, v_5\}$ and $F = \{f_1, \dots, f_5\}$ 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 $(w_1 \rightarrow C_1)$ 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 $(v_1 \rightarrow C_2)$, $(w_2 \rightarrow C_2)$, $(w_3 \rightarrow C_2)$, $(w_4 \rightarrow C_2)$, and $(w_5 \rightarrow C_2)$ 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 $(v_4 \rightarrow C_3)$ and $(w_6 \rightarrow C_3)$ to \mathcal{E} . The directed cluster graph $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ is given in Figure 4e.

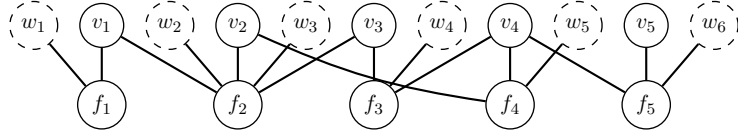
For causal ordering via perfect matchings, we consider the following two perfect matchings of the self-contained bipartite graph in Figure 2:

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

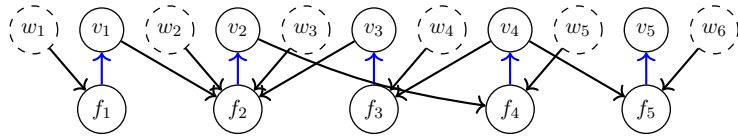
We use these one-to-one correspondences between endogenous variable vertices and constraint vertices in the orientation step in Definition 5 to obtain the associated directed graphs $\mathcal{G}(\mathcal{B}, M_1)$ and $\mathcal{G}(\mathcal{B}, M_2)$ in Figures 4b and 4c respectively. Application of the clustering step in Definition 5 to either $\mathcal{G}(\mathcal{B}, M_1)$ or $\mathcal{G}(\mathcal{B}, M_2)$ results in the clustered graph $\text{clust}(\mathcal{G}(\mathcal{B}, M_2)) = \text{clust}(\mathcal{G}(\mathcal{B}, M_1))$ in Figure 4d. The final step is to merge clusters in this directed cluster graph. We find that the causal ordering graph $\text{merge}(\text{clust}(\mathcal{G}(\mathcal{B}, M_1))) = \text{merge}(\text{clust}(\mathcal{G}(\mathcal{B}, M_2)))$ in Figure 4e does not depend on the choice of perfect matching, as is implied by Theorem 6. Note that the output of causal ordering with minimal self-contained sets coincides with the output of causal ordering via perfect matchings.

11. 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).

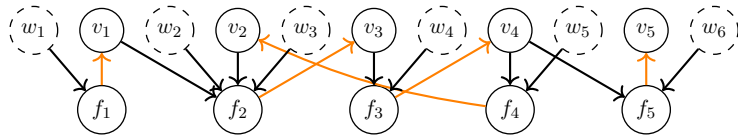
12. Tarjan's algorithm, which runs in $\mathcal{O}(|V| + |E|)$ time, can be used to find the strongly connected components in a directed graph (Tarjan, 1972).



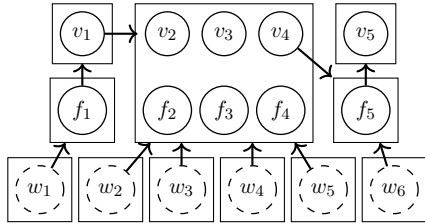
(a) Bipartite graph \mathcal{B} where dashed vertices indicate exogenous variables.



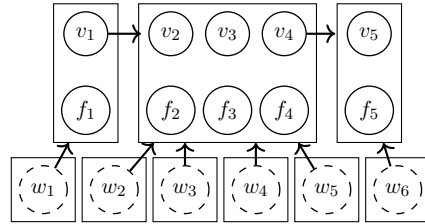
(b) Associated directed graph $\mathcal{G}(\mathcal{B}, M_1)$.



(c) Associated directed graph $\mathcal{G}(\mathcal{B}, M_2)$.



(d) Clustered graph $\text{clust}(\mathcal{G}(\mathcal{B}, M_1))$.



(e) Causal ordering graph $\text{CO}(\mathcal{B})$.

Figure 4: Causal ordering with two different perfect matchings M_1 and M_2 applied to the bipartite graph in Figure 4a. The results of subsequently orienting edges, constructing clusters, and merging clusters as in Definition 5 are given in Figures 4b to 4e. The edges in M_1 that are oriented from variables to equations in Figure 4b are indicated with blue edges. Likewise, edges in M_2 are indicated with orange edges in Figure 4c. The clustered graph in Figure 4d coincides with $\text{clust}(\mathcal{G}(\mathcal{B}, M_2))$ and for the causal ordering graph in Figure 4e we have that $\text{CO}(\mathcal{B}) = \text{merge}(\text{clust}(\mathcal{G}(\mathcal{B}, M_1))) = \text{merge}(\text{clust}(\mathcal{G}(\mathcal{B}, M_2)))$.

3.2 Coarse decomposition via maximum matchings

The extension that we propose relies on the *coarse decomposition* of bipartite graphs in Pothen and Fan (1990), which was originally proposed by Dulmage and Mendelsohn (1958). The main idea is that a set of equations (i.e., a system of constraints) can be divided into an *incomplete* part that has fewer equations than variables, an *over-complete* part that has more equations than variables, and a part that is self-contained. The *coarse decomposition* in Definition 7 below uses the notions of a *maximum matching* and an *alternating path* for a maximum matching. The former is a matching so that there are no matchings with a greater cardinality, while the latter is a sequence of distinct vertices and edges $(v_1, e_1, v_2, e_2, \dots, e_{n-1}, v_n)$ so that edges e_i are alternatingly in and out a maximum matching M . Proposition 8 by Pothen (1985) shows that the coarse decomposition is unique.¹³ In this section we loosely follow the exposition of the coarse decomposition in Van Diepen (2019) and Pothen and Fan (1990).

Definition 7 *Let M be a maximum matching for a bipartite graph $\mathcal{B} = \langle V, F, E \rangle$ and let V_{un} and F_{un} denote the unmatched vertices in V and F respectively. The incomplete set $T_I \subseteq V \cup F$ and overcomplete set $T_O \subseteq V \cup F$ are given by:*

$$\begin{aligned} T_I &:= \{x \in V \cup F : \text{there is an alternating path between } x \text{ and some } y \in V_{\text{un}}\}, \\ T_O &:= \{x \in V \cup F : \text{there is an alternating path between } x \text{ and some } y \in F_{\text{un}}\}. \end{aligned}$$

The complete set is given by $T_C = V \cup F \setminus (T_I \cup T_O)$. The coarse decomposition $\text{CD}(\mathcal{B}, M)$ is given by $\langle T_I, T_C, T_O \rangle$. The incomplete graph \mathcal{B}_I is the subgraph of \mathcal{B} induced by vertices T_I , the complete graph \mathcal{B}_C is the subgraph of \mathcal{B} induced by vertices T_C , and the overcomplete graph \mathcal{B}_O is the subgraph of \mathcal{B} induced by vertices T_O .

Note that T_I and T_O are necessarily disjoint, for more details see Lemma 36 in Appendix B.2.

Proposition 8 *[Pothen (1985)] The coarse decomposition of a bipartite graph \mathcal{B} is independent of the choice of the maximum matching.*

There exist fast algorithms that are able to find a maximum matching in a bipartite graph $\mathcal{B} = \langle V, F, E \rangle$, such as the Hopcraft-Karp-Karzanov algorithm, which runs in $\mathcal{O}(|E|\sqrt{|V \cup F|})$ time (Hopcraft and Karp, 1973; Karzanov, 1973). In the following example we manually searched for maximum matchings to illustrate the result in Proposition 8 that the coarse decomposition is unique.

Example 7 *Consider the bipartite graph \mathcal{B}' in Figure 5b, which has the following four maximum matchings.*

$$M_1 = \{(v_1 - f_2), (v_2 - f_3), (v_3 - f_4), (v_4 - f_5)\}, \tag{6}$$

$$M_2 = \{(v_1 - f_1), (v_2 - f_3), (v_3 - f_4), (v_5 - f_5)\}, \tag{7}$$

$$M_3 = \{(v_1 - f_2), (v_2 - f_3), (v_3 - f_4), (v_5 - f_5)\}, \tag{8}$$

$$M_4 = \{(v_1 - f_1), (v_2 - f_3), (v_3 - f_4), (v_4 - f_5)\}. \tag{9}$$

¹³. For completeness, we have included a proof of this theorem in Appendix B.2.

By Proposition 8 we know that the coarse decomposition $\text{CD}(\mathcal{B}', M)$, with $M \in \{M_1, M_2, M_3, M_4\}$, does not depend on the choice of maximum matching. The coarse decomposition is displayed in Figure 5c. It is a straightforward exercise to verify that applying Definition 7 to each of the maximum matchings results in the same coarse decomposition. Note that if the vertices $\{f_1, \dots, f_5\}$ are associated with equations, and the vertices $\{v_1, \dots, v_5\}$ are associated with variables, then the incomplete graph \mathcal{B}_I has fewer equations than variables, whereas the over-complete graph \mathcal{B}_O has more equations than variables. The complete graph \mathcal{B}_C is self-contained.

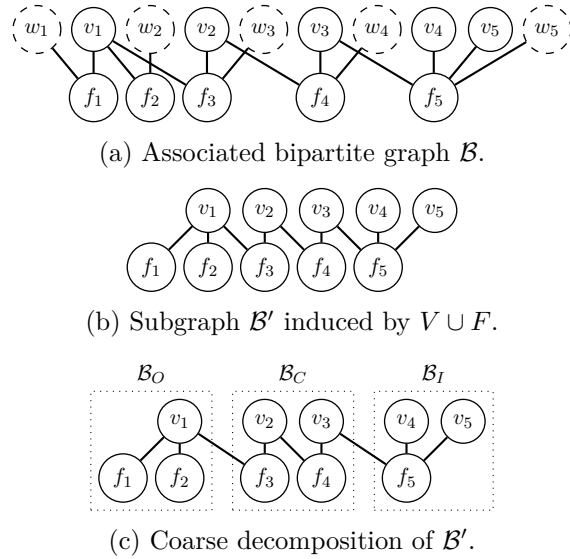


Figure 5: The bipartite graph \mathcal{B} associated with the system of equations in Example 8 is given in Figure 5a. Its subgraph \mathcal{B}' induced by $V = \{v_1, \dots, v_5\}$ and $F = \{f_1, \dots, f_5\}$ in Figure 5b is not self-contained. The coarse decomposition of \mathcal{B}' is given in Figure 5c.

3.3 Causal ordering via coarse decomposition

Here we present the extended causal ordering algorithm. It relies on the unique coarse decomposition of a bipartite graph into its incomplete, complete, and over-complete parts. Lemma 9, due to Pothén (1985), shows that the complete graph has a perfect matching. Together, Lemma 9 and Lemma 10 justify the steps in Algorithm 3 to construct a causal ordering graph. The proofs are provided in Appendix B.2.

Lemma 9 [Pothén (1985)] *Let \mathcal{B} be a bipartite graph with coarse decomposition $\langle T_I, T_C, T_O \rangle$. The subgraph \mathcal{B}_C of \mathcal{B} induced by vertices in T_C has a perfect matching and is self-contained.*

Lemma 10 [Pothén (1985)] *Let $\mathcal{B} = \langle V, F, E \rangle$ be a bipartite graph with a maximum matching M . Let $\text{CD}(\mathcal{B}, M) = \langle T_I, T_C, T_O \rangle$ be the associated coarse decomposition. No edge joins a vertex in $T_I \cap V$ with a vertex in $(T_C \cup T_O) \cap F$ and no edge joins a vertex in $T_C \cap V$ with a vertex in $T_O \cap F$.*

Algorithm 3 takes a set of exogenous vertices $W \subseteq V$ and a bipartite graph $\mathcal{B} = \langle V, F, E \rangle$ as input. In contrast with Algorithms 1 and 2, the subgraph of \mathcal{B} induced by $(V \cup F) \setminus W$ need not be self-contained. The output is a causal ordering graph $\langle \mathcal{V}, \mathcal{E} \rangle$. The algorithm first uses a maximum matching M for the subgraph \mathcal{B}' of \mathcal{B} induced by $(V \setminus W) \cup F$ to construct the coarse decomposition $\langle T_I, T_C, T_O \rangle$ of \mathcal{B}' . Since the complete graph \mathcal{B}_C is self-contained (by Lemma 9) the causal ordering algorithm for self-contained bipartite graphs can be applied to obtain the directed cluster graph $\text{CO}(\mathcal{B}_C) = \langle \mathcal{V}_C, \mathcal{E}_C \rangle$. The cluster set \mathcal{V} consists of the clusters in \mathcal{V}_C and the connected components in \mathcal{B}_I and \mathcal{B}_O . The edge set \mathcal{E} contains all edges in \mathcal{E}_C . For edges between vertices $v \in T_O \cap V$ and $f \in T_C \cap F$ in \mathcal{B} an edge $(v \rightarrow \text{cl}_{\mathcal{V}}(f))$ is added to \mathcal{E} .¹⁴ Similarly, for edges between vertices $v \in (T_O \cup T_C) \cap V$ and $f \in T_I \cap F$ an edge $(v \rightarrow \text{cl}_{\mathcal{V}}(f))$ is also added to \mathcal{E} . By Lemma 10 there are no other edges between the incomplete, complete, and over-complete graphs. Finally, edges from exogenous vertices W are added to the causal ordering graph. The details can be found in Algorithm 3.

Algorithm 3: Causal ordering via coarse decomposition.

```

Input: a set of exogenous vertices  $W$ , a bipartite graph  $\mathcal{B} = \langle V \cup W, F, E \rangle$ .
Output: directed cluster graph  $\langle \mathcal{V}, \mathcal{E} \rangle$ 
 $\mathcal{B}' \leftarrow$  subgraph of  $\mathcal{B}$  induced by  $(V \setminus W) \cup F$ 
 $M \leftarrow$  maximum matching for  $\mathcal{B}'$ 
 $\langle T_I, T_C, T_O \rangle \leftarrow \text{CD}(\mathcal{B}', M)$  // coarse decomposition
 $\mathcal{B}_C \leftarrow$  subgraph of  $\mathcal{B}'$  induced by  $T_C$ 
 $\mathcal{B}_I \leftarrow$  subgraph of  $\mathcal{B}'$  induced by  $T_I$ 
 $\mathcal{B}_O \leftarrow$  subgraph of  $\mathcal{B}'$  induced by  $T_O$ 
 $\langle \mathcal{V}_C, \mathcal{E}_C \rangle \leftarrow$  causal ordering graph for  $\mathcal{B}_C$  // construct clusters
 $\mathcal{V}_I \leftarrow$  partition of  $T_I$  into connected components in  $\mathcal{B}_I$ 
 $\mathcal{V}_O \leftarrow$  partition of  $T_O$  into connected components in  $\mathcal{B}_O$ 
 $\mathcal{V} \leftarrow \mathcal{V}_I \cup \mathcal{V}_C \cup \mathcal{V}_O \cup \{\{w\} : w \in W\}$ 
 $\mathcal{E} \leftarrow \mathcal{E}_C$  // find edges
for  $(v - f) \in E$  do
    if  $v \in (T_O \cup T_C) \cap V$  and  $f \in T_I \cap F$  then
         $\perp$  Add  $(v \rightarrow \text{cl}_{\mathcal{V}}(f))$  to  $\mathcal{E}$ 
    else if  $v \in T_O \cap V$  and  $f \in T_C \cap F$  then
         $\perp$  Add  $(v \rightarrow \text{cl}_{\mathcal{V}}(f))$  to  $\mathcal{E}$ 
for  $w \in W$  do
     $\perp$  add  $(w \rightarrow \text{cl}_{\mathcal{V}}(f))$  to  $\mathcal{E}$  for all  $f \in \text{adj}_{\mathcal{B}}(w)$  // exogenous vertices
    
```

Corollary 11 *The output of Algorithm 3 is well-defined and unique.*

Proof This follows directly from Theorem 4 and Proposition 8. ■

Corollary 11 shows that the output of causal ordering via coarse decomposition does not depend on the choice of the maximum matching (i.e., the output is unique). The following

14. Note that $\text{cl}_{\mathcal{V}}(x)$ denotes the cluster in the partition \mathcal{V} that contains the vertex x .

example provides a manual demonstration of the causal ordering algorithm via the coarse decomposition.

Example 8 We apply the causal ordering algorithm via coarse decomposition (i.e., Algorithm 3) to the bipartite graph in Figure 5a. Its subgraph induced by endogenous variables and equations is the bipartite graph in Figure 5b and its coarse decomposition is given in Figure 5c. Since, by Lemma 9, \mathcal{B}_C is self-contained we can apply the causal ordering algorithm (Algorithm 1) to the complete subgraph resulting in the directed cluster graph $\text{CO}(\mathcal{B}_C) = \langle \mathcal{V}_C, \mathcal{E}_C \rangle$ where $\mathcal{V}_C = \{\{v_2, f_3\}, \{v_3, f_4\}\}$ and $\mathcal{E}_C = \{(v_2 \rightarrow \{v_3, f_4\})\}$. The cluster set is then given by $\mathcal{V} = \mathcal{V}_C \cup \{\{v_4, v_5, f_5\}\} \cup \{\{v_1, f_1, f_2\}\}$. We then add singleton clusters $\{w_1\}, \{w_2\}, \{w_3\}, \{w_4\}, \{w_5\}$ for each exogenous vertex. Next we add the edges \mathcal{E}_C , $(v_1 \rightarrow \{v_2, f_3\})$ and $(v_3 \rightarrow \{v_4, v_5, f_5\})$ to the edge set \mathcal{E} . Finally, we add edges $(w_1 \rightarrow \{v_1, f_1, f_2\})$, $(w_2 \rightarrow \{v_1, f_1, f_2\})$, $(w_3 \rightarrow \{v_2, f_3\})$, $(w_4 \rightarrow \{v_3, f_4\})$ and $(w_5 \rightarrow \{v_4, v_5, f_5\})$ to the edge set \mathcal{E} . The resulting causal ordering graph $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ is given in Figure 6.

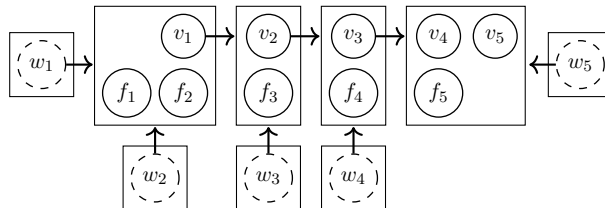


Figure 6: Causal ordering graph for the bipartite graph in Figure 5a.

4. Markov ordering graph

First we consider (unique) solvability assumptions for systems of constraints. We will then construct the *Markov ordering graph* and prove that it implies conditional independences between variables that appear in constraints. We also apply our method to the model for the filling bathtub in Example 1. Finally, we present a novel result regarding the generalized directed global Markov property for solutions of systems of constraints and an *associated directed graph*.

4.1 Solvability for systems of constraints

In this section, 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 12 We say that a measurable mapping $g : \mathcal{X}_W \mapsto \mathcal{X}_{V \setminus W}$ that maps values of the exogenous variables to values of the endogenous variables is a solution to a system of constraints $\langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$ if

$$\phi_f(g_{V(f) \setminus W}(\mathbf{X}_W), \mathbf{X}_{V(f) \cap W}) = c_f, \quad \forall f \in F, \quad \mathbb{P}_{\mathbf{X}_W}\text{-a.s.}$$

We say that the system of constraints is uniquely solvable (or “has a unique solution”) if all its solutions are $\mathbb{P}_{\mathbf{X}_W}$ -a.s. equal.

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

Example 9 Consider a system of constraints $\langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$ with $\mathcal{X} = \mathbb{R}^4$ and independent exogenous random variables $\mathbf{X}_W = (X_w)_{w \in \{w_1, w_2\}}$ taking value in \mathbb{R}^2 . Suppose that Φ consists of the constraints

$$\Phi_{f_1} = \langle X_{V(f_1)} \mapsto X_{v_1} - X_{w_1}, 0, \{v_1, w_1\} \rangle, \quad (10)$$

$$\Phi_{f_2} = \langle X_{V(f_2)} \mapsto X_{v_2}^2 - |X_{w_2}|, 0, \{v_2, w_2\} \rangle. \quad (11)$$

This system of constraints has solutions with different distributions. One solution is given by $(X_{v_1}^*, X_{v_2}^*) = (X_{w_1}, \sqrt{|X_{w_2}|})$ and another solution is $(X'_{v_1}, X'_{v_2}) = (X_{w_1}, \text{sgn}(X_{w_1})\sqrt{|X_{w_2}|})$. 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.

Underspecified (and overspecified) systems of constraints can be avoided by the requirement that it is *uniquely solvable*. In Definition 13 below we give a sufficient condition under which a unique solution can be obtained by solving variables in clusters from equations in these clusters.

Definition 13 A system of constraints $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$ is solvable w.r.t. constraints $S_F \subseteq F$ and endogenous variables $S_V \subseteq V(S_F) \setminus W$ if there exists a measurable function $\mathbf{g}_{S_V} : \mathcal{X}_{V(S_F) \setminus S_V} \rightarrow \mathcal{X}_{S_V}$ s.t. $\mathbb{P}_{\mathbf{X}_W}$ -a.s., for all $\mathbf{x}_{V(S_F) \setminus W} \in \mathcal{X}_{V(S_F) \setminus W}$:

$$\phi_f(\mathbf{x}_{V(f) \setminus W}, \mathbf{X}_{V(f) \cap W}) = c_f, \quad \forall f \in S_F \iff \mathbf{x}_{S_V} = \mathbf{g}_{S_V}(\mathbf{x}_{V(S_F) \setminus (S_V \cup W)}, \mathbf{X}_{V(S_F) \cap W}).$$

\mathcal{M} is uniquely solvable w.r.t. constraints S_F and endogenous variables S_V if the converse implication also holds.

The following condition suffices for the existence of a unique solution that can be obtained by solving for variables from equations in their cluster along a topological ordering of the clusters in the causal ordering graph. This weakens the assumptions made in Simon (1953) who requires both unique solvability w.r.t. every subset of equations (and the endogenous variables that appear in them) and self-containedness of the bipartite graph.

Definition 14 We say that \mathcal{M} is uniquely solvable w.r.t. the causal ordering graph $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ if it is uniquely solvable w.r.t. $S \cap F$ and $S \cap V$ for all $S \in \mathcal{V}$ with $S \cap W = \emptyset$.

For systems of constraints for cyclic models or with non-linear equations, for which the incomplete subgraph is not the empty graph, the condition of unique solvability with respect to the causal ordering graph is not always satisfied. This is illustrated by Example 10 below.

Example 10 Let $V = \{v_1, \dots, v_5\}$ be an index set for endogenous variables X_{v_1}, \dots, X_{v_5} taking value in \mathbb{R} , $W = \{w_1, \dots, w_5\}$ an index set for independent exogenous random variables U_{w_1}, \dots, U_{w_5} taking value in \mathbb{R} , and p_1, p_2 parameters with values in \mathbb{R} . Consider the following non-linear system of constraints:

$$\Phi_{f_1} : \quad X_{v_1}^2 - U_{w_1} = 0, \quad (12)$$

$$\Phi_{f_2} : \quad \text{sgn}(X_{v_1}) - \text{sgn}(U_{w_2}) = 0, \quad (13)$$

$$\Phi_{f_3} : \quad X_{v_2} - p_1 X_{v_1} - U_{w_3} = 0, \quad (14)$$

$$\Phi_{f_4} : \quad X_{v_3} - p_2 X_{v_2} - U_{w_4} = 0, \quad (15)$$

$$\Phi_{f_5} : \quad X_{v_3} + X_{v_4} + X_{v_5} - U_{w_5} = 0. \quad (16)$$

The associated bipartite graph \mathcal{B} is given in Figure 5a and the corresponding causal ordering graph is given in Figure 6. It is easy to check that the system of constraints is uniquely solvable with respect to the clusters $\{v_1, f_1, f_2\}$, $\{v_2, f_3\}$, and $\{v_3, f_4\}$ in the causal ordering graph. Equation f_5 does not provide a unique solution for the variables v_4 and v_5 and hence the system is not uniquely solvable with respect to the cluster $\{v_4, v_5, f_5\}$.

Generally speaking, systems of constraints are not uniquely solvable with respect to the clusters in the incomplete set of vertices in the associated bipartite graph. In order to derive a Markov property for the complete and overcomplete sets of vertices in the associated bipartite graph, we use the condition in Definition 15 below, which is slightly weaker than the one in Definition 13. Since self-contained bipartite graphs do not have an incomplete part there is no difference between the two conditions in that case.

Definition 15 Let $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$ be a system of constraints. Denote its coarse decomposition by $\text{CD}(\mathcal{B}) = \langle T_I, T_C, T_O \rangle$ and its causal ordering graph by $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$. We say that \mathcal{M} is maximally uniquely solvable if it is

1. uniquely solvable w.r.t. $S \cap F$ and $S \cap V$ for all $S \in \mathcal{V}$ with $S \cap W = \emptyset$ and $S \cap T_I = \emptyset$, and
2. solvable with respect to $T_I \cap F$ and $(T_I \cap V) \setminus W$.

This condition suffices to guarantee the existence of a solution, and that it is unique on the (over)complete part $(T_O \cup T_C) \cap V \setminus W$.

4.2 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 16 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 $V = \cup_{S \in \mathcal{V}} S$ and $(v \rightarrow w) \in E$ if and only if $(v \rightarrow \text{cl}(w)) \in \mathcal{E}$. For a system of constraints $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$ with $\mathcal{B} = \langle V, F, E \rangle$, we say that $\text{MO}(\mathcal{B}) = D(\text{CO}(\mathcal{B}))_{\text{mar}(F)}$ is the Markov ordering graph.

Under the assumption that systems of constraints are uniquely solvable with respect to the (over)complete part of their causal ordering graph, Theorem 17 relates d-separations between vertices in the Markov ordering graph to conditional independences between the corresponding components of a solution of the system of constraints.

Theorem 17 *Let $\mathbf{X}^* = \mathbf{h}(\mathbf{X}_W)$ with $\mathbf{h} : \mathcal{X}_W \rightarrow \mathcal{X}_{V \setminus W}$ be a solution of a system of constraints $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$ with coarse decomposition $\text{CD}(\mathcal{B}) = \langle T_I, T_C, T_O \rangle$. Let $\text{MO}_{\text{CO}}(\mathcal{B})$ denote the subgraph of the Markov ordering graph induced by $T_C \cup T_O$ and let \mathbf{X}_{CO}^* denote the corresponding solution components. If \mathcal{M} is maximally uniquely solvable then the pair $(\text{MO}_{\text{CO}}(\mathcal{B}), \mathbb{P}_{\mathbf{X}_{\text{CO}}^*})$ satisfies the directed global Markov property (see Definition 31).*

In particular, when the incomplete and overcomplete sets are empty (i.e., when $T_I = \emptyset$ and $T_O = \emptyset$) and the system is uniquely solvable with respect to the causal ordering graph, Theorem 17 tells us that the pair $(\text{MO}(\mathcal{B}), \mathbb{P}_{\mathbf{X}^*})$ satisfies the directed global Markov property.

Example 11 *Consider the system of constraints in Example 10. The Markov ordering graph for the associated bipartite graph in Figure 5a can be constructed from the causal ordering graph in Figure 6 and is given in Figure 7. One can check that the system of constraints is uniquely solvable with respect to the clusters in the complete and overcomplete sets. The Markov ordering graph can be used to read off conditional independences from d-separations between vertices that are not in the incomplete part. For example, since v_1 is d-separated from v_3 given v_2 , we deduce that $X_{v_1} \perp\!\!\!\perp X_{v_3} \mid X_{v_2}$, for any solution of the constraints.*

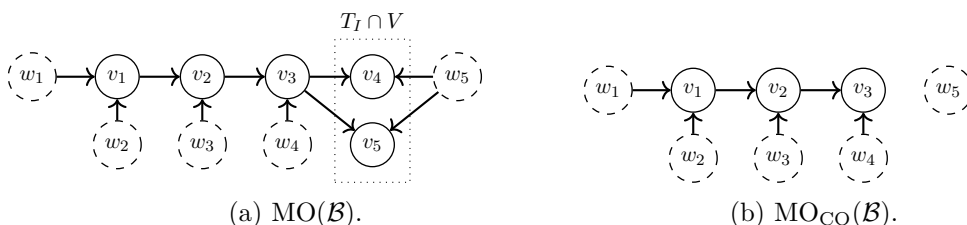


Figure 7: (a) The Markov ordering graph associated with the system of constraints in Example 10. It can be constructed from the causal ordering graph in Figure 6. The vertices in the incomplete graph are indicated by the dashed rectangle. (b) Its subgraph induced by $T_C \cap T_O$. Theorem 17 shows that d-separations in $\text{MO}_{\text{CO}}(\mathcal{B})$ imply conditional independences.

4.3 Application to the filling bathtub

In Example 1 we informally described an equilibrium model for a filling bathtub. The endogenous variables of the system are the diameter X_{v_K} of the drain, the rate X_{v_I} at which water flows from the faucet, the water pressure X_{v_P} , the rate X_{v_O} at which the water goes through the drain and the water level X_{v_D} . The model is formally represented by a system of constraints $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$ where:

1. $\mathcal{X} = \mathbb{R}_{>0}^{12}$ is a product of standard measurable spaces corresponding to the domain of variables that are indexed by $\{v_K, v_I, v_P, v_O, v_D, w_K, w_I, w_1, \dots, w_5\}$,
2. $\mathbf{X}_W = \{U_{w_I}, U_{w_K}, U_{w_1}, \dots, U_{w_5}\}$ is a family of independent exogenous random variables,
3. Φ is a family of constraints:

$$\begin{aligned}
 \Phi_{f_K} &= \langle X_{V(f_K)} \mapsto X_{v_K} - U_{w_K}, & 0, & \quad V(f_K) = \{v_K, w_K\}, \\
 \Phi_{f_I} &= \langle X_{V(f_I)} \mapsto X_{v_I} - U_{w_I}, & 0, & \quad V(f_I) = \{v_I, w_I\}, \\
 \Phi_{f_P} &= \langle X_{V(f_P)} \mapsto U_{w_1}(gU_{w_2}X_{v_D} - X_{v_P}), & 0, & \quad V(f_P) = \{v_D, v_P, w_1, w_2\}, \\
 \Phi_{f_O} &= \langle X_{V(f_O)} \mapsto U_{w_3}(U_{w_4}X_{v_K}X_{v_P} - X_{v_O}), & 0, & \quad V(f_O) = \{v_K, v_P, v_O, w_3, w_4\}, \\
 \Phi_{f_D} &= \langle X_{V(f_D)} \mapsto U_{w_5}(X_{v_I} - X_{v_O}), & 0, & \quad V(f_D) = \{v_I, v_O, w_5\},
 \end{aligned}$$

4. The associated bipartite graph $\mathcal{B} = \langle V, F, E \rangle$ is as in Figure 8. The vertices $F = \{f_K, f_I, f_P, f_O, f_D\}$ correspond to constraints and the vertices $V \setminus W = \{v_K, v_I, v_P, v_O, v_D\}$ and $W = \{w_I, w_K, w_1, \dots, w_5\}$ correspond to endogenous and exogenous variables respectively. Note that the subgraph induced by the endogenous vertices $V \setminus W$ is the self-contained bipartite graph presented in Figure 1a.

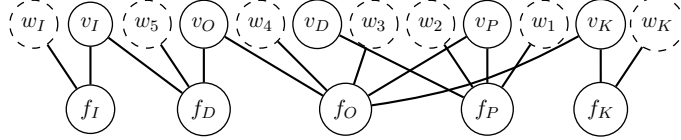


Figure 8: The bipartite graph associated with the equilibrium equations of the bathtub system.

Solvability with respect to the causal ordering graph: Applying Algorithm 1 to the bipartite graph results in the causal ordering graph $\text{CO}(\mathcal{B})$ in Figure 9. Since the bipartite graph induced by the endogenous variables and equations is self-contained, there is no incomplete or overcomplete subgraph. The assumption of maximal unique solvability in Theorem 17 then reduces to the assumption of unique solvability with respect to the causal ordering graph. Through explicit calculations, it is easy to verify that \mathcal{M} is (maximally) uniquely solvable with respect to $\text{CO}(\mathcal{B})$, whenever $g \neq 0$:

1. For the cluster $\{f_K, v_K\}$ we have that $X_{v_K} - U_{w_K} = 0 \iff X_{v_K} = U_{w_K}$.
2. For the cluster $\{f_I, v_I\}$ we have that $X_{v_I} - U_{w_I} = 0 \iff X_{v_I} = U_{w_I}$.
3. For $\{f_O, v_P\}$ we have that $U_{w_3}(U_{w_4}X_{v_K}X_{v_P} - X_{v_O}) = 0 \iff X_{v_P} = \frac{X_{v_O}}{U_{w_3}X_{v_K}}$.
4. For $\{f_D, v_O\}$ we have that $U_{w_5}(X_{v_I} - X_{v_O}) \iff X_{v_O} = X_{v_I}$.
5. For $\{f_P, v_D\}$ we have that $U_{w_1}(gU_{w_2}X_{v_D} - X_{v_P}) \iff X_{v_D} = \frac{X_{v_P}}{gU_{w_2}}$.

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 $\mathbf{A}\mathbf{X} = \mathbf{Y}$, we may use the fact that this assumption is satisfied when the matrix of coefficients \mathbf{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).¹⁵ We consider detailed analysis of conditions under which (maximal) unique solvability is guaranteed to be outside the scope of this paper. Note that, under the assumption of (maximal) unique solvability, the conditional independences can be read off from the Markov ordering graph without the requirement of calculating explicit solutions.

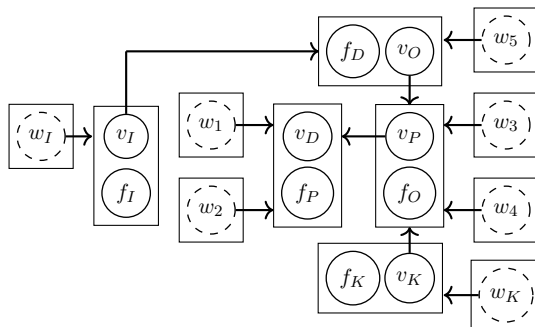


Figure 9: The causal ordering graph for the equilibrium equations of the bathtub system.

Markov ordering graph: Application of declustering and marginalization of vertices in F , as in Definition 16, to the causal ordering graph in Figure 9 results in the Markov ordering graph in Figure 10a. Since \mathcal{M} is uniquely solvable with respect to $\text{CO}(\mathcal{B})$, Theorem 17 tells us that the pair $(\text{MO}(\mathcal{B}), \mathbb{P}_{\mathbf{X}^*})$ satisfies the directed global Markov property, where \mathbf{X}^* is a solution of \mathcal{M} .¹⁶

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

15. In particular, Hadamard’s global implicit function theorem in Krantz and Parks (2013) states the following (Hadamard, 1906). Let $\mathbf{f} : \mathbb{R}^n \mapsto \mathbb{R}^n$ be a C^2 mapping. Suppose that $\mathbf{f}(\mathbf{0}) = \mathbf{0}$ and that the Jacobian determinant is non-zero at each point. Further suppose that whenever $K \subseteq \mathbb{R}^n$ is compact then $\mathbf{f}^{-1}(K)$ is compact (i.e., \mathbf{f} is proper). Then \mathbf{f} is one-to-one and onto. In the literature, several conditions have been formulated yielding global inverse theorems in different or more general settings, see for example Idczak (2016); Gutú (2017).

16. Recall that there is no incomplete and overcomplete part of the bipartite graph. Therefore we have that $\text{MO}_{\text{CO}}(\mathcal{B}) = \text{MO}(\mathcal{B})$.

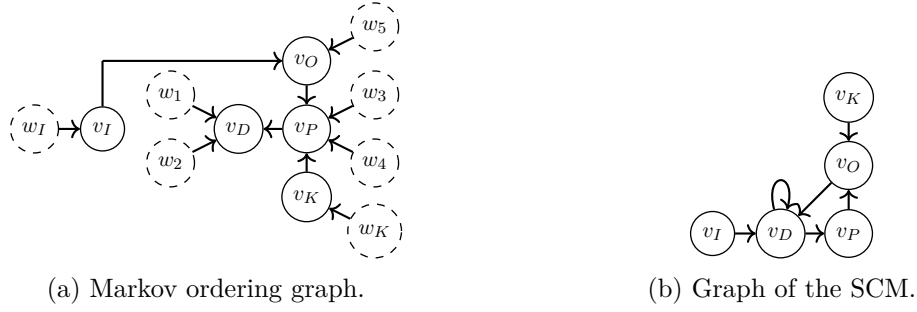


Figure 10: The Markov ordering graph for the equilibrium equations of the filling bathtub system, obtained by applying Definition 16 to the causal ordering graph in Figure 9 is given in Figure 10a. The d-separations in the Markov ordering graph imply conditional independences between corresponding endogenous variables. Most of these conditional independences cannot be read off from the graph for the SCM of the bathtub system in Figure 10b, except for $X_{v_I} \perp\!\!\!\perp X_{v_K}$.

independences between the corresponding endogenous variables. For example:

$$\begin{aligned}
 v_K \stackrel{d}{\perp}_{\text{MO}(\mathcal{B})} v_O &\implies X_{v_K} \perp\!\!\!\perp X_{v_O}, \\
 v_K \stackrel{d}{\perp}_{\text{MO}(\mathcal{B})} v_D \mid v_P &\implies X_{v_K} \perp\!\!\!\perp X_{v_D} \mid X_{v_P}, \\
 v_I \stackrel{d}{\perp}_{\text{MO}(\mathcal{B})} v_P \mid v_O &\implies X_{v_I} \perp\!\!\!\perp X_{v_P} \mid X_{v_O}, \\
 v_O \stackrel{d}{\perp}_{\text{MO}(\mathcal{B})} v_D \mid v_P &\implies X_{v_O} \perp\!\!\!\perp X_{v_D} \mid X_{v_P}.
 \end{aligned}$$

For $g > 0$, every solution to the system of constraints has the same distribution, and this distribution is d-faithful to the Markov ordering graph. When $g = 0$, the system of constraints only has a solution if $U_{w_I} = 0$ almost surely; in that case the corresponding distribution is not d-faithful w.r.t. the Markov ordering graph in Figure 10a.

Comparison to SCM representation: The (random) differential equations that describe the system of a bathtub can be *equilibrated to an SCM* that has a self-cycle. Bongers et al. (2020) show that the equilibrated model has the following structural equations:

$$\begin{aligned}
 X_{v_K} &= U_{w_K}, \\
 X_{v_I} &= U_{w_I}, \\
 X_{v_P} &= gU_{w_3}X_{v_D}, \\
 X_{v_O} &= U_{w_5}X_{v_K}X_{v_P}, \\
 X_{v_D} &= X_{v_D} + U_{w_1}(X_{v_I} - X_{v_O}).
 \end{aligned}$$

The graph of this SCM is depicted in Figure 10b. Because the SCM is uniquely solvable w.r.t. the strongly connected components $\{v_I\}$, $\{v_D, v_P, v_O\}$ and $\{v_K\}$, the σ -separations in this graph imply conditional independences (Theorem 6.3 in Bongers et al., 2020). Most

of the conditional independences implied by the Markov ordering graph cannot be read off from the graph of this SCM in Figure 10b via the σ -separation criterion, except for $X_{v_I} \perp\!\!\!\perp X_{v_K}$. Clearly the distribution of a solution to the system of constraints is not faithful to the graph of the SCM and causal ordering on the equilibrium equations provides a stronger Markov property than equilibration to an SCM.

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, in the case of the bathtub model, a one-to-one correspondence between variables and constraints is obtained automatically by the causal ordering algorithm. In general, the bipartite graph of a set of structural equations is self-contained and perfect matchings connect each variable to an equation. If the SCM is acyclic then the associated bipartite graph has a unique perfect matching that retrieves the correspondence between variables and equations in the SCM. We further discuss applications of the technique of causal ordering to structural equations in Section 6.2.

4.4 Generalized directed global Markov property

For systems of constraints with no over- or incomplete parts, the associated directed graph that is constructed in the causal ordering algorithm via perfect matchings also yields a Markov property. Theorem 18 below shows that for systems that are uniquely solvable with respect to the causal ordering graph, the σ -separations between variable vertices in the directed graph $\mathcal{G}(\mathcal{B}, M)_{\text{mar}(F)}$ imply conditional independences between the corresponding solution components.

Theorem 18 *Let $\mathbf{X}^* = \mathbf{g}(\mathbf{X}_W)$ be a solution of a system of constraints $\langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$, 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 $S_F = (S \cup M(S)) \cap F$ then the pair $(\mathcal{G}(\mathcal{B}, M)_{\text{mar}(F)}, \mathbb{P}_{\mathbf{X}^*})$ satisfies the generalized directed global Markov property (Definition 31).*

Example 12 *Consider a system of constraints $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$ with $W = \{w_1, \dots, w_6\}$, $V \setminus W = \{v_1, \dots, v_5\}$, $F = \{f_1, \dots, f_5\}$, and $\mathcal{B} = \langle V, F, E \rangle$ as in Figure 4a. Suppose that $\mathcal{X} = \mathbb{R}^{11}$ and Φ consists of constraints:*

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

It is easy to check that this linear system of equations can be uniquely solved in the order prescribed by the causal ordering graph $\text{CO}(\mathcal{B})$ in Figure 4e. Therefore, according to Theorem 17 the d -separations among endogenous variables in the corresponding Markov

ordering graph $\text{MO}(\mathcal{B})$ imply conditional independences between the corresponding endogenous variables. It follows that d -separations in the Markov ordering graph $\text{MO}(\mathcal{B})_{\text{mar}(W)}$ for the endogenous variables in Figure 11b 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 $X_{v_1}^* \perp\!\!\!\perp X_{v_5}^* \mid X_{v_4}^*$. One may note that d -separations in $\text{MO}(\mathcal{B})_{\text{mar}(W)}$ coincide with σ -separations in both associated directed graphs $\mathcal{G}(\mathcal{B}, M_1)_{\text{mar}(F \cup W)}$ and $\mathcal{G}(\mathcal{B}, M_2)_{\text{mar}(F \cup W)}$, which are depicted in Figures 11c and 11d respectively. It can be seen from the proof of Theorem 18 in Appendix B.5 that this result holds in general. It follows from Theorem 18 that the σ -separations in $\mathcal{G}(\mathcal{B}, M_1)_{\text{mar}(F \cup W)}$ and $\mathcal{G}(\mathcal{B}, M_2)_{\text{mar}(F \cup W)}$ imply conditional independences between the corresponding variables. For example, we see that v_1 and v_5 are σ -separated by v_4 in both graphs, and hence $X_{v_1}^* \perp\!\!\!\perp X_{v_5}^* \mid X_{v_4}^*$ for a solution \mathbf{X}^* .

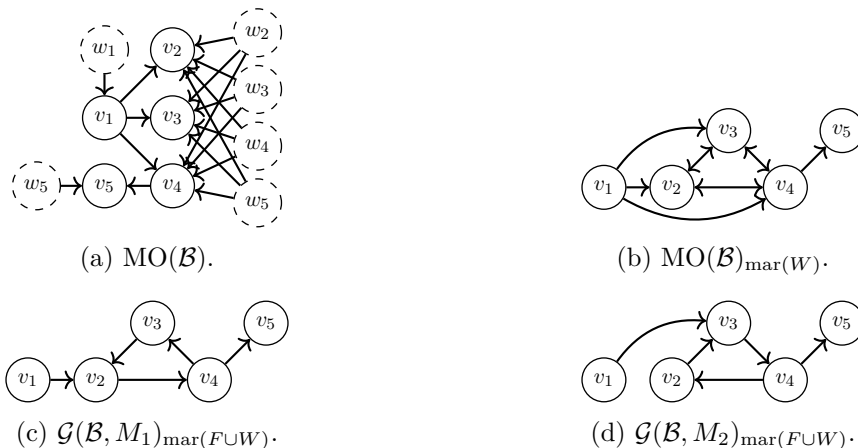


Figure 11: The Markov ordering graph of the causal ordering graph in Figure 4e is given in Figure 11a. Marginalization of the exogenous vertices W results in the directed mixed graph in Figure 11b. The directed graphs in Figures 11c and 11d are obtained by marginalizing out the constraint vertices F and exogenous vertices W from the directed graphs $\mathcal{G}(\mathcal{B}, M_1)$ and $\mathcal{G}(\mathcal{B}, M_2)$ in Figures 4b and 4c respectively.

5. Causal implications of sets of equations

Nowadays, it is common to relate causation directly to the effects of manipulation (Woodward, 2003; Pearl, 2000). In the context of sets of equations there are many ways to model manipulations on these equations. Assuming that the manipulations correspond to feasible actions in the real world that is modelled by the equations, the effects of manipulations correspond to causal relations. 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 on sets of equations.¹⁷ We prove that the causal ordering graph represents the effects of both *soft interventions on equations* and *perfect interventions on*

17. Our definitions in the context of systems of constraints may deviate from conventional definitions of interventions on SCMs. In an SCM, each variable is associated with a single structural equation. The

clusters in the causal ordering graph. We also show that these interventions 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 19 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'_f a constant taking value in a measurable space \mathcal{Y} , and $\phi'_f : \mathcal{X}_{V(f)} \rightarrow \mathcal{Y}$ a measurable function. A soft intervention $\text{si}(f, \phi'_f, c'_f)$ targeting Φ_f results in the intervened system $\mathcal{M}_{\text{si}(f, \phi'_f, c'_f)} = \langle \mathcal{X}, \mathbf{X}_W, \Phi_{\text{si}(f, \phi'_f, c'_f)}, \mathcal{B} \rangle$ where $\Phi_{\text{si}(f, \phi'_f, c'_f)} = (\Phi \setminus \{\Phi_f\}) \cup \{\Phi'_f\}$ with $\Phi'_f = \langle \phi'_f, c'_f, V(f) \rangle$.

For systems of constraints that are maximally uniquely solvable w.r.t. the causal ordering graph, both before and after a soft intervention, Theorem 20 shows that such a soft intervention does not have an effect on variables that cannot be reached by a directed path from that constraint in the causal ordering graph, while it may have an effect on other variables.¹⁸

Theorem 20 Let $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$ be a system of constraints with coarse decomposition $\text{CD}(\mathcal{B}) = \langle T_I, T_C, T_O \rangle$. Suppose that \mathcal{M} is maximally uniquely solvable w.r.t. the causal ordering graph $\text{CO}(\mathcal{B})$ and let $\mathbf{X}^* = \mathbf{g}(\mathbf{X}_W)$ be a solution of \mathcal{M} . Let $f \in (T_C \cup T_O) \cap F$ and assume that the intervened system $\mathcal{M}_{\text{si}(f, \phi'_f, c'_f)}$ is also maximally uniquely solvable w.r.t. $\text{CO}(\mathcal{B})$. Let $\mathbf{X}' = \mathbf{h}(\mathbf{X}_W)$ be a solution of $\mathcal{M}_{\text{si}(f, \phi'_f, c'_f)}$. If there is no directed path from f to $v \in (T_C \cup T_O) \cap V$ in $\text{CO}(\mathcal{B})$ then $X_v^* = X'_v$ almost surely. On the other hand, if there is a directed path from f to v in $\text{CO}(\mathcal{B})$ then X_v^* may have a different distribution than X'_v , depending on the details of the model \mathcal{M} .

Example 13 shows that the presence of a directed path in the causal ordering graph for the equilibrium equations of the bathtub system implies a causal effect for almost all parameter values. This illustrates that non-effects and *generic* effects can be read off from the causal ordering graph.¹⁹

notion of a perfect intervention on an SCM does not carry over to systems of constraints because there is no imposed one-to-one correspondence between equations and variables.

18. Our result generalizes Theorem 6.1 in Simon (1953) for linear self-contained systems of equations. The proof of our theorem is similar.

19. If a model contains finitely many parameters, and if a directed path from an equation vertex f to a variable vertex v implies that for almost all values (w.r.t. Lebesgue measure on the parameter space) of the parameters there exists an intervention on f that changes the distribution of the solution component X_v , then we say that there is a *generic* causal effect of f on v . We will make no attempts to define this notion of genericity more generally in this work, because (i) it is not directly obvious how this should be done in non-parametric settings, and (ii) the unique solvability conditions may impose additional constraints on the parameters in case of cycles, complicating matters further. We thank an anonymous referee for pointing out the latter complication.

Table 1: The effects of soft interventions on constraints in the causal ordering graph for the bathtub system in Figure 9.

target	generic effect	non-effect
f_K	$X_{v_K}, X_{v_P}, X_{v_D}$	X_{v_I}, X_{v_O}
f_I	$X_{v_I}, X_{v_P}, X_{v_O}, X_{v_D}$	X_{v_K}
f_P	X_{v_D}	$X_{v_K}, X_{v_I}, X_{v_P}, X_{v_O}$
f_O	X_{v_P}, X_{v_D}	$X_{v_K}, X_{v_I}, X_{v_O}$
f_D	$X_{v_P}, X_{v_O}, X_{v_D}$	X_{v_K}, X_{v_I}

Example 13 Recall the system of constraints for the filling bathtub in Section 4.3. Think of an experiment where the gravitational acceleration 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 accelerating the bathtub system or by moving the bathtub system to another planet. We can model the effect on the equilibrium distribution in such an experiment by a soft intervention targeting f_P that replaces the constraint Φ_{f_P} by

$$\langle X_{V(f_P)} \mapsto U_{w_1}(g'U_{w_2}X_{v_D} - X_{v_P}), 0, V(f_P) = \{v_D, v_P, w_1, w_2\} \rangle. \quad (17)$$

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 9. There is no directed path from f_P to v_K, v_I, v_P or v_O . Therefore, perhaps surprisingly, Theorem 20 tells us that the soft intervention targeting f_P neither has an effect on the pressure X_{v_P} at equilibrium nor on the outflow rate X_{v_O} at equilibrium. Since there is a directed path from f_P to v_D , the water level X_{v_D} at equilibrium may be different after a soft intervention on f_P . If the gravitational acceleration g is equal to zero, then the system of constraints for the bathtub is not maximally uniquely solvable w.r.t. the causal ordering graph (except if $U_{w_1} = 0$ almost surely). For all other values of the parameter g the generic effects and non-effects of soft interventions on other constraints of the bathtub system can be read off from the causal ordering graph and are presented in Table 1.

5.2 The effects of perfect interventions

A *perfect intervention* acts on a variable and a constraint. Definition 21 shows that it replaces the targeted constraint by a constraint that sets the targeted variable equal to a constant. Note that this definition of perfect interventions is very general and allows interventions for which the intervened system of constraints is not maximally uniquely solvable w.r.t. the causal ordering graph. In this work, we will only consider the subset of perfect interventions that target clusters in the causal ordering graph, for which the intervened system is also maximally uniquely solvable w.r.t. the causal ordering graph. We consider an analysis of necessary conditions on interventions for the intervened system to be maximally uniquely solvable beyond the scope of this work.

Definition 21 Let $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} = \langle V, F, E \rangle \rangle$ be a system of constraints and let $\xi_v \in \mathcal{X}_v$. A perfect intervention $\text{do}(f, v, \xi_v)$ targeting the variable $v \in V \setminus W$ and the constraint $f \in F$ results in the intervened system $\mathcal{M}_{\text{do}(f, v, \xi_v)} = \langle \mathcal{X}, \mathbf{X}_W, \Phi_{\text{do}(f, v, \xi_v)}, \mathcal{B}_{\text{do}(f, v)} \rangle$ where

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

Perfect interventions on a set of variable-constraint pairs $\{(f_1, v_1), \dots, (f_n, v_n)\}$ in a system of constraints are denoted by $\text{do}(S_F, S_V, \xi_{S_V})$ where $S_F = \langle f_1, \dots, f_n \rangle$ and $S_V = \langle v_1, \dots, v_n \rangle$ are tuples. For a bipartite graph \mathcal{B} so that its subgraph induced by $(V \cup F) \setminus W$ is self-contained, Lemma 22 shows that the subgraph of the intervened bipartite graph $\mathcal{B}_{\text{do}(S_F, S_V)}$ induced by $(V \cup F) \setminus W$ is also self-contained when $S = (S_F \cup S_V)$ is a cluster in $\text{CO}(\mathcal{B})$ with $S \cap W = \emptyset$.

Lemma 22 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 $(V \cup F) \setminus W$ is self-contained. Consider an intervention $\text{do}(S_V, S_F)$ on a cluster $S = S_F \cup S_V$ with $S \cap W = \emptyset$ in the causal ordering graph $\text{CO}(\mathcal{B})$. The subgraph of $\mathcal{B}_{\text{do}(S_F, S_V)}$ induced by $(V \cup F) \setminus W$ is self-contained.

Theorem 23 shows how the causal ordering graph can be used to read off the (generic) effects and non-effects of *perfect interventions on clusters* in the complete and overcomplete sets of the associated bipartite graph under the assumption of unique solvability with respect to the complete and overcomplete sets in the causal ordering graph.

Theorem 23 Let $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} = \langle V, F, E \rangle \rangle$ be a system of constraints with coarse decomposition $\text{CD}(\mathcal{B}) = \langle T_I, T_C, T_O \rangle$. Assume that \mathcal{M} is maximally uniquely solvable w.r.t. $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ and let \mathbf{X}^* be a solution of \mathcal{M} . Let $S_F \subseteq (T_C \cup T_O) \cap F$ and $S_V \subseteq (T_C \cup T_O) \cap (V \setminus W)$ be such that $(S_F \cup S_V) \in \mathcal{V}$. Consider the intervened system $\mathcal{M}_{\text{do}(S_F, S_V, \xi_{S_V})}$ with coarse decomposition $\text{CD}(\mathcal{B}_{\text{do}(S_F, S_V)}) = \langle T'_I, T'_C, T'_O \rangle$. Let \mathbf{X}' be a solution of $\mathcal{M}_{\text{do}(S_F, S_V, \xi_{S_V})}$. If there is no directed path from any $x \in S_V$ to $v \in (T_C \cup T_O) \cap V$ in $\text{CO}(\mathcal{B})$ then $X_v^* = X'_v$ almost surely. On the other hand, if there is $x \in S_V$ such that there is a directed path from x to $v \in (T_C \cup T_O) \cap V$ in $\text{CO}(\mathcal{B})$ 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. In particular, when the distribution of a solution component is different for almost all parameter values, then we say that there is a generic effect.¹⁹ In this way, we can establish the generic effects of a perfect intervention without solving the equations by relying on a solvability assumption. Example 14 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 generic effects and non-effects of perfect interventions on clusters can be read off from the causal ordering graph.

Table 2: Solutions for system of constraints describing the bathtub system in Section 4.3 without interventions (i.e., the observed system) and after perfect interventions $\text{do}(f_P, v_D, \xi_D)$, $\text{do}(f_D, v_O, \xi_O)$, and $\text{do}(f_D, v_D, \xi_D)$.

	observed	$\text{do}(f_P, v_D, \xi_D)$	$\text{do}(f_D, v_O, \xi_O)$	$\text{do}(f_D, v_D, \xi_D)$
$X_{v_K}^*$	U_{w_K}	U_{w_K}	U_{w_K}	U_{w_K}
$X_{v_I}^*$	U_{w_I}	U_{w_I}	U_{w_I}	U_{w_I}
$X_{v_P}^*$	$\frac{U_{w_I}}{(U_{w_4}U_{w_K})}$	$\frac{U_{w_I}}{(U_{w_4}U_{w_K})}$	$\frac{\xi_O}{(U_{w_4}U_{w_K})}$	$gU_{w_2}\xi_D$
$X_{v_O}^*$	U_{w_I}	U_{w_I}	ξ_O	$U_{w_4}U_{w_K}gU_{w_2}\xi_D$
$X_{v_D}^*$	$\frac{U_{w_I}}{(U_{w_4}U_{w_K}gU_{w_2})}$	ξ_D	$\frac{\xi_O}{(U_{w_4}U_{w_K}gU_{w_2})}$	ξ_D

Table 3: The effects of perfect interventions on clusters of variables and constraints in the causal ordering graph for the bathtub system in Figure 9 obtained by Theorem 23. Since $\{f_D, v_D\}$ is not a cluster in the causal ordering graph, the effects of this intervention cannot be read off from the causal ordering graph.

target	generic effect	non-effect
f_K, v_K	$X_{v_K}, X_{v_P}, X_{v_D}$	X_{v_I}, X_{v_O}
f_I, v_I	$X_{v_I}, X_{v_P}, X_{v_O}, X_{v_D}$	X_{v_K}
f_P, v_D	X_{v_D}	$X_{v_K}, X_{v_I}, X_{v_P}, X_{v_O}$
f_O, v_P	X_{v_P}, X_{v_D}	$X_{v_K}, X_{v_I}, X_{v_O}$
f_D, v_O	$X_{v_P}, X_{v_O}, X_{v_D}$	X_{v_K}, X_{v_I}
$f_P, f_D, f_O, v_P, v_D, v_O$	$X_{v_P}, X_{v_O}, X_{v_D}$	X_{v_K}, X_{v_I}

Example 14 Recall the system of constraints \mathcal{M} for the filling bathtub at equilibrium in Section 4.3 and consider the perfect interventions $\text{do}(f_P, v_D, \xi_D)$, $\text{do}(f_D, v_O, \xi_O)$, and $\text{do}(f_D, v_D, \xi_D)$. These interventions model experiments that can, at least in principle, be conducted in practice:

1. The intervention $\text{do}(f_P, v_D, \xi_D)$ replaces the constraint f_P by a constraint that sets the water level X_{v_D} equal to a constant and leaves all other constraints unaffected. This could correspond to an experimental set-up where the constant g in the constraint Φ_{f_P} is controlled by accelerating and decelerating the bathtub system precisely in such a way that the water level X_{v_D} is forced to take on a constant value ξ_D both in time and across the ensemble of bathtubs. We observe the system once it has reached equilibrium.
2. The interventions $\text{do}(f_D, v_O, \xi_O)$ and $\text{do}(f_D, v_D, \xi_D)$ 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_{v_O} or the water level X_{v_D} is kept at a constant level both in time and across the ensemble of bathtubs. The system is observed when it has reached equilibrium.

Note that the cluster $\{f_D, v_D\}$ is not a cluster in the causal ordering graph in Figure 9. However, the system of constraints $\mathcal{M}_{\text{do}(f_D, v_D, \xi_D)}$ is maximally uniquely solvable with respect to the causal ordering graph $\text{CO}(\mathcal{B}_{\text{do}(f_D, v_D)})$, and therefore the effects of the intervention are well-defined.²⁰ 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 $\text{do}(f_P, v_D, \xi_D)$ does not change the solution for the variables $X_{v_K}, X_{v_I}, X_{v_P}, X_{v_O}$, but it generically does change the solution for X_{v_D} . We further find that $\text{do}(f_D, v_D, \xi_D)$ and $\text{do}(f_D, v_O, \xi_D)$ affect the solution for the variables $X_{v_P}, X_{v_O}, X_{v_D}$ but not of X_{v_K} and X_{v_I} .

The causal ordering graph $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ for the bathtub system is given in Figure 9. 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 maximally uniquely solvable w.r.t. its causal ordering graph, we can apply Theorem 23 and read off the generic effects and non-effects 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 $\text{do}(f_P, v_D, \xi_D)$ and $\text{do}(f_D, v_O, \xi_O)$, 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 10b in Section 6.

5.3 Interventions commute with causal ordering

Given a system of constraints we can obtain the causal ordering graph after a perfect intervention on one of its clusters in the original causal ordering graph by running the causal ordering algorithm on the bipartite graph in the intervened system of constraints. In this section we will define an operation of “perfect intervention” directly on the clusters in a causal ordering graph and show that the causal ordering graph that is obtained after a perfect intervention coincides with the causal ordering graph of the intervened system (i.e., perfect interventions on clusters in the causal ordering graph commute with the causal ordering algorithm). 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 24 Let $\mathcal{B} = \langle V, F, E \rangle$ be a bipartite graph and W a set of exogenous variables. Let $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ be the corresponding causal ordering graph and consider $S \in \mathcal{V}$ with $S \cap W = \emptyset$. Let $S_F = \langle f_i : i = 1, \dots, n \rangle$ and $S_V = \langle v_i : i = 1, \dots, n \rangle$ 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 $\text{do}(S_F, S_V)$ on a cluster $\{S_F, S_V\}$ results in the directed cluster graph $\text{CO}(\mathcal{B})_{\text{do}(S_F, S_V)} = \langle \mathcal{V}', \mathcal{E}' \rangle$ where²¹

1. $\mathcal{V}' = (\mathcal{V} \setminus \{S\}) \cup \{\{v_i, f_i\} : i = 1, \dots, n\}$,

20. The intervention on $\{f_D, v_D\}$ is interesting because it removes the constraint that the water flowing through the faucet X_{v_I} must be equal to the water flowing through the drain X_{v_O} . This can be accomplished by adding a hose to the system through which additional water can flow in and out of the bathtub to ensure that X_{v_D} remains at a constant level. Notice that, in this example, the *total* inflow and *total* outflow of water remain equal, while the inflow *through the faucet* and the outflow *through the drain* may differ.

21. A perfect intervention $\text{do}(S_F, S_V, \xi_V)$ replaces constraints Φ_{f_i} with causal constraints $\Phi'_{f_i} = \langle X_{v_i} \mapsto X_{v_i}, \xi_{v_i}, \{v_i\} \rangle$. Notice that the labels f_i of the constraints are unaltered, and therefore only

$$2. \mathcal{E}' = \{(x \rightarrow T) \in \mathcal{E} : T \neq S\}.$$

A soft intervention on a system of constraints has no effect on the bipartite graphical structure of the constraints and the variables that appear in them. Since the bipartite graph of the system is 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 25 *Let $\mathcal{B} = \langle V, F, E \rangle$ be a bipartite graph and W a set of exogenous variables. Let $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ 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:*

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

The bipartite graph in Figure 12a has the causal ordering graph depicted in Figure 12b. The perfect intervention $\text{do}(S_F, S_V)$ 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 12d. Since perfect interventions on clusters commute with causal ordering, this graph can also be obtained by applying the causal ordering algorithm to the intervened bipartite graph in Figure 12c. Proposition 25 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. We will use this result in Section 6.3 to elucidate the commutation properties of equilibration and interventions in dynamical models as defined in Dash (2005) and Bongers and Mooij (2018).

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. 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 observe here that the Markov ordering graph in Figure 10a does not have an unambiguous causal interpretation, 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 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 from a contemporary perspective on interventions and causality.

the edges in the bipartite graph and causal ordering graph change after an intervention, as well as the clusters in the causal ordering graph, while the labels of vertices are preserved.

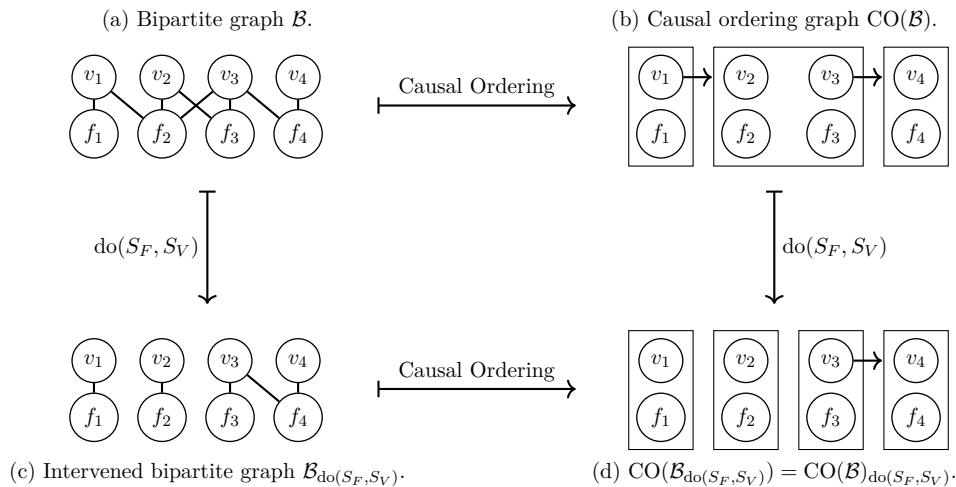


Figure 12: The intervention $\text{do}(S_F, S_V)$ with ordered sets $S_F = \langle f_2, f_3 \rangle$ and $S_V = \langle v_2, v_3 \rangle$ commutes with causal ordering. Application of causal ordering and the intervention to the bipartite graph in 12a results in the causal ordering graph in 12b and the intervened bipartite graph in 12c respectively. The directed cluster graph in 12d can be obtained either by applying causal ordering to the intervened bipartite graph or by intervening on the causal ordering graph.

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 13a. The corresponding Markov ordering graph in Figure 13c 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 implies certain conditional independences between components of solutions of equations.²²

Soft interventions. We first consider the representation of 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 13c because there is no vertex f_D . 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 Markov ordering graph in Figure 13c 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 . In earlier work, Simon and Iwasaki (1988) assumed that a matching between variable and equation vertices is known in advance, allowing them to read off effects of soft interventions. We

22. Iwasaki and Simon (1994) consider deterministic systems of equations and therefore it would not have made sense to consider Markov properties. In earlier work, the vanishing partial correlations implied by linear systems with three variables and normal errors were studied by Simon (1954).

conclude that the Markov ordering graph, by itself, does not represent the effects of soft interventions on equations in general.

Perfect interventions. In Example 14, the perfect intervention $\text{do}(f_D, v_D, \xi_D)$ has 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 13c 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 intervention $\text{do}(f_P, v_D, \xi_D)$ or $\text{do}(f_D, v_O, \xi_O)$. 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 $\text{do}(f_P, v_D, \xi_D)$ which targets the cluster containing v_D corresponds to a perfect intervention on D in the Markov ordering graph in Figure 13c. Since it is not clear from the Markov ordering 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 either.

Causal ordering graph. The causal ordering graph for the bathtub system is given in Figure 1b. 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 Theorems 17 and 23). 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 equation 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 are easily applicable to other modelling frameworks, such as the popular SCM framework (Pearl, 2000; Bongers et al., 2020). Application of causal ordering to the structural equations of an SCM with self-cycles may result in a different ordering than the one implied by the SCM. In particular, causal ordering may lead to a stronger Markov property and 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 non-effects of arbitrary perfect interventions, one can still obtain those by first intervening on the bipartite graph, then applying the causal ordering algorithm, and finally reading off the descendants of the intervention targets (under appropriate maximal unique solvability conditions).

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 endogenous variables are derived automatically by the causal ordering algorithm. Consider, for example, the following

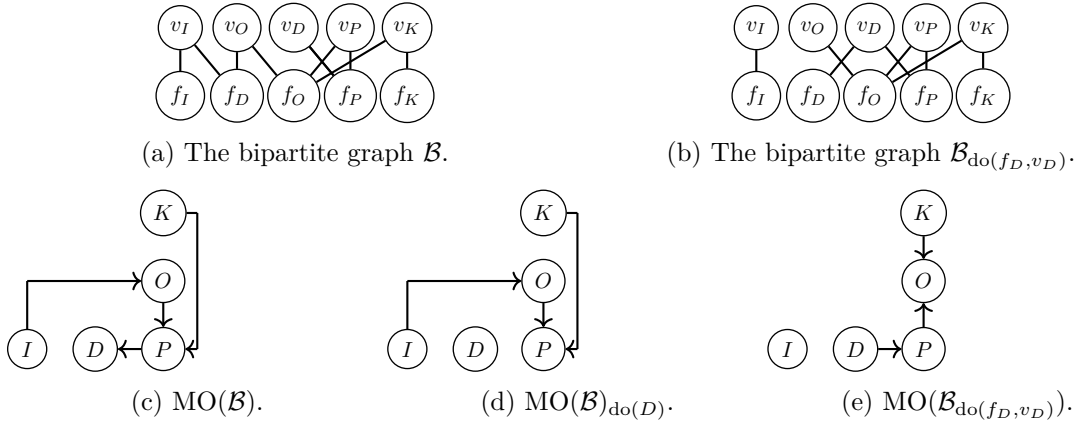


Figure 13: The bipartite graph for the bathtub system without exogenous variables is given in Figure 13a. The intervened bipartite graph is given in Figure 13b. The Markov ordering graphs for the observed and intervened bathtub system are given in Figures 13c and 13e respectively. Figure 13d shows the 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 in Figure 13e.

structural equations:

$$X_1 = U_1 \quad (18)$$

$$X_2 = aX_1 + U_2, \quad (19)$$

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

$$X_1 - U_1 = 0, \quad (20)$$

$$X_2 - aX_1 - U_2 = 0. \quad (21)$$

Note that any set of structural equations implies a self-contained set of equations.²³ 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 4), the structure that is provided by the structural equations is actually redundant if the structural equations contain no cycles.

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

$$\begin{aligned} f_K : \quad X_{v_K} &= U_{w_K}, & f_O : \quad X_{v_O} &= U_{w_5} X_{v_K} X_{v_P}, \\ f_I : \quad X_{v_I} &= U_{w_I}, & f_D : \quad X_{v_D} &= X_{v_D} + U_{w_1} (X_{v_I} - X_{v_O}), \\ f_P : \quad X_{v_P} &= g U_{w_3} X_{v_D}. \end{aligned}$$

23. 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 38 in Appendix B.4).

The graph of this SCM is depicted in Figure 10b, and the descendants and non-descendants of vertices are given in Table 4. Can we use this table to read off generic causal effects of perfect interventions targeting $\{f_K, v_K\}$, $\{f_I, v_I\}$, $\{f_P, v_P\}$, $\{f_O, v_O\}$, and $\{f_D, v_D\}$? The graph of the SCM contains (self-)cycles and the SCM does not have a (unique) solution under each of these perfect interventions.²⁴ Therefore, the graph of this SCM may not have a straightforward causal interpretation. Indeed, Bongers et al. (2020) pointed out that for SCMs with cycles or self-cycles, the absence (presence) of directed edges and directed paths between vertices may not correspond one-to-one to the absence (generic presence) of direct and indirect causal effects, as it does in DAGs. (Self-)cycles may even lead to (in)direct causal effects without a corresponding directed edge or path being present in the graph of the SCM. For the bathtub example, that unusual behaviour does not occur, but instead it illustrates another behaviour: certain causal effects are absent, even though one would naïvely expect these to be generically present based on the graph of the SCM.²⁵ For example, 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_{v_O} does *not* change after the perfect intervention $\text{do}(f_K, v_K)$. That this causal relation is absent can actually be read off from the causal ordering graph in Figure 1b.

For the bathtub system, the causal ordering algorithm can exploit the fact that equation f_D can be replaced by $f'_D : 0 = U_{w_1}(X_{v_I} - X_{v_O})$, which does not involve v_D , whereas for the SCM this self-cycle cannot be removed. This causes the following differences in the results of the two approaches:

1. The d-separations in the Markov ordering graph in Figure 10a imply more conditional independences than those implied by the σ -separations in the graph of the SCM in Figure 10b (as was discussed in detail in Section 4.3).
2. The graph of the SCM and the causal ordering graph represent different perfect intervention targets. In the graph of the SCM, we have minimal perfect intervention targets of the form $\{f_i, v_i\}$ with $i \in \{K, I, P, O, D\}$, while the causal ordering graph represents minimal perfect interventions on clusters $\{f_K, v_K\}$, $\{f_I, v_I\}$, $\{f_P, v_P\}$, $\{f_O, v_O\}$, and $\{f_D, v_D\}$. In both cases, the set of all perfect intervention targets that are represented by the graph are obtained by taking unions of minimal perfect intervention targets.
3. The causal ordering graph of the bathtub has a straightforward causal interpretation because the bathtub system still has a unique solution under interventions on clusters in the causal ordering graph. 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.

We conclude that the causal ordering approach yields a more “faithful” representation of the bathtub than the SCM framework.

24. There is no (unique) solution if one fixes the outflow rate of the system X_{v_O} to a value that is not equal to X_{v_I} for the perfect interventions targeting $\{f_O, v_O\}$ and $\{f_P, v_P\}$. In the dynamical model for the bathtub, these perfect interventions would correspond with the water level becoming (plus or minus) infinity.

25. Such behaviour is a characteristic of perfectly adaptive dynamical systems (Blom and Mooij, 2021).

Other frameworks. Since the causal ordering algorithm can be applied to any 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 et al., 2019). The causal ordering algorithm can be directly applied to a 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 10b.

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

In this subsection we will discuss in more detail the relation between our work and other closely related work, in particular that of Dash (2005).

Dynamical models in terms of first order differential equations can be *equilibrated to a set of equations* by equating each time-derivative to zero (Mooij et al., 2013; Bongers and Mooij, 2018). They can be *equilibrated and mapped to a causal ordering graph* by applying the causal ordering algorithm to the resulting set of equilibrium equations. They can also be *equilibrated and mapped to a Markov ordering graph* by subsequently applying Definition 16 to this causal ordering graph. The bathtub system provides an example of what Dash (2005) calls a “violation of the Equilibration Manipulation Commutability property”.²⁶

Consider the dynamical system version of the filling bathtub, with dynamical equations

$$\begin{aligned}
 f_K : \quad & X_{v_K} = U_{w_K}, \\
 f_I : \quad & X_{v_I} = U_{w_I}, \\
 f_D : \quad & \dot{X}_{v_D}(t) = U_{w_1}(X_{v_I}(t) - X_{v_O}(t)), \\
 f_P : \quad & \dot{X}_{v_P}(t) = U_{w_2}(gU_{w_3}X_{v_D}(t) - X_{v_P}(t)), \\
 f_O : \quad & \dot{X}_{v_O}(t) = U_{w_4}(U_{w_5}X_{v_K}X_{v_P}(t) - X_{v_O}(t)).
 \end{aligned}$$

26. We argue that this is confusing terminology in two ways. First, what Dash calls “equilibration” is what we would call equilibration to a set of equations, composed with the mapping to the Markov ordering graph. Second, Dash follows Iwasaki and Simon (1994) in referring to the Markov ordering graph as the “causal graph”. 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. This terminological confusion explains the apparent contradiction with the result of Bongers and Mooij (2018), who prove that equilibration to an SCM commutes with manipulation (for perfect interventions).

Equilibration yields the equilibrium equations f_K , f_I , f_D , f_P , and f_O in equations (1) to (5). It is clear in this particular case that any perfect intervention $\text{do}(S_F, S_V, \xi_V)$ (where we extended Definition 21 to dynamical equations) commutes with equilibration (substituting zeroes for all first-order derivatives).²⁷ This type of commutation relation actually holds also in more general settings (see Mooij et al. (2013) and Bongers and Mooij (2018)).

On the other hand, mapping a set of equations to the corresponding Markov ordering graph does not necessarily commute with perfect interventions. For example, for the perfect intervention $\text{do}(f_D, v_D)$, the Markov ordering graphs $\text{MO}(\mathcal{B})_{\text{do}(v_D)}$ and $\text{MO}(\mathcal{B}_{\text{do}(f_D, v_D)})$ are wildly different, as can be seen by comparing Figures 13d and 13e respectively. Since perfect interventions do commute with equilibration, one can conclude that also the composition of equilibration followed by mapping to the Markov ordering graph fails to commute with this perfect intervention. This is the phenomenon that Dash (2005) pointed out.

This lack of commutability does not hold for *all* perfect interventions. For example, one can easily check that the perfect intervention $\text{do}(f_K, v_K)$ commutes with the composition of equilibration followed by mapping to the Markov ordering graph. More generally, Proposition 25 tells us that for the bathtub, the clusters in the causal ordering graph ($\{f_K, v_K\}$, $\{f_I, v_I\}$, $\{f_P, v_D\}$, $\{f_O, v_P\}$, and $\{f_D, v_O\}$) represent the minimal perfect interventions targets for which both operations do commute. This means that of the perfect interventions that Dash (2005) considers ($\text{do}(\{v_K, f_K\})$, $\text{do}(\{v_I, f_I\})$, $\text{do}(\{v_D, f_D\})$, $\text{do}(\{v_O, f_O\})$, $\text{do}(\{v_P, f_P\})$, and combinations thereof), exactly three commute with the mapping to the Markov ordering graph (namely $\text{do}(\{f_K, v_K\})$, $\text{do}(\{f_I, v_I\})$, $\text{do}(\{f_P, v_P, f_O, v_O, f_D, v_D\})$, and combinations thereof). Hence, these are also the three minimal perfect interventions in that set that commute with equilibration followed by mapping to the Markov ordering graph.

As pointed out by Dash (2005), this lack of commutability has important implications when one tries to discover causal relations through structure learning, which we will briefly discuss in the next subsection.

6.4 Structure learning

We have shown that, under a solvability assumption, d-separations in the Markov ordering graph (or σ -separations in the directed graph associated with a particular perfect matching) imply conditional independences between variables in a system of constraints (see Theorem 17 and Theorem 18). Constraint-based causal discovery algorithms relate conditional independences in data to graphs under the Markov condition and the corresponding d- or σ -faithfulness assumption. 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 13c. The usual assumption is then that the Markov ordering graph equals the causal graph, where directed edges express direct causal relations

27. Note that it is crucially important here to ensure that the *labelling* of the equations is not changed by the equilibration operation.

between variables. In this work we have shown that this learned Markov ordering graph does *not* have such a straightforward causal interpretation.

7. Conclusion and future work

In this work, we 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 a *causal ordering graph* and a *Markov ordering graph* from a set of equations, without calculating explicit global solutions to the system of equations. The novelties of this paper include an extension of the causal ordering algorithm for general bipartite graphs, and proving that the corresponding Markov ordering graph implies conditional independences between variables, whereas the corresponding 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 on SCMs. 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 any obvious causal interpretation in terms of soft or perfect interventions. We showed that the causal ordering graph, on the other hand, does encode the effects of soft and certain perfect interventions. The main take-away is that we need to make a distinction between variables and equations in graphical representations of the probabilistic and causal aspects of models with feedback. By making this distinction, we clarified the correct interpretation of some existing observations in the literature. Additionally, we shed new light on discussions in causal discovery about the justification of using a single directed graph with endogenous variables as vertices to simultaneously represent causal relations and conditional independences. In recent work, we show that the phenomenon where the Markov ordering graph does not encode causal semantics in the usual way manifests itself in certain biological or econometric models with feedback at equilibrium (Blom and Mooij, 2020, 2021).

We have introduced two different graphical objects that represent causal relations and conditional independences respectively. A more parsimonious solution would be to use a bipartite graph together with a perfect matching to construct a single *partially oriented bipartite graph*. In that case, edges of the bipartite graph are oriented using the perfect matching (see Definition 5) if they do not lie on an alternating path that starts and ends with the same vertex. By construction, this ensures that edges are not oriented if their orientation varies across perfect matchings. To read off conditional independences from this graph, a Markov property would need to be defined for this graphical object, which would then be applicable to a set of equations and a set of declared exogenous variables. We believe that this would be an interesting direction for future work.

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Appendix A. Preliminaries

A.1 Graph terminology

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 $\text{adj}_{\mathcal{B}}(x) = \{y \in V \cup F : (x - y) \in E\}$ for its *adjacencies*, and for $X \subseteq V \cup F$ we write $\text{adj}_{\mathcal{B}}(X) = \bigcup_{x \in X} \text{adj}_{\mathcal{B}}(x)$ 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 x and 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.

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 $(v \rightarrow w)$ between vertices $v, w \in V$. A *directed 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 . If a directed mixed graph $\langle V, E, B \rangle$ has an edge $(v \rightarrow v) \in E$ then we say that it has a *self-cycle*. We say that a vertex v is a *parent* of w if $(v \rightarrow w) \in E$ and write $v \in \text{pa}_{\mathcal{G}}(w)$. Similarly we say that w is a *child* of v if $(v \rightarrow w) \in E$ and write $w \in \text{ch}_{\mathcal{G}}(v)$. A *path* is a sequence of distinct vertices and edges $(v_1, e_1, v_2, e_2, \dots, e_{n-1}, v_n)$ where for $i = 1, \dots, n - 1$ we have that $e_i = (v_i \rightarrow v_{i+1})$, $e_i = (v_i \leftarrow v_{i+1})$, or $e_i = (v_i \leftrightarrow v_{i+1})$. The path is called *open* if there is no $v_i \in \{v_2, \dots, v_{n-1}\}$ such that there are two arrowheads at v_i on the path (i.e., there is no collider on the path). A *directed path* $(v \rightarrow \dots \rightarrow w)$ 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 $v \in \text{an}_{\mathcal{G}}(w)$. We say that w is a *descendant* of v if there is a directed path from v to w and write $w \in \text{de}_{\mathcal{G}}(v)$.

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

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

Since the relation is reflexive, symmetric, and transitive this is an equivalence relation. The equivalence classes $\text{sc}_{\mathcal{G}}(v)$ are called the *strongly connected components* of \mathcal{G} . A directed graph without self-cycles is *acyclic* if and only if all of its strongly connected components are singletons. A directed graph with no directed cycles is called a Directed Acyclic Graph (DAG).

A *perfect intervention* $\text{do}(I)$ on a directed mixed graph $\mathcal{G} = \langle V, E, B \rangle$ removes all edges with an arrowhead at any of the nodes $i \in I \subseteq V$. That is, $\mathcal{G}_{\text{do}(I)} = \langle V, E', B' \rangle$ where $E' = \{(x \rightarrow y) \in E : y \notin I\}$ and $B' = \{(x \leftrightarrow y) \in B : x \notin I, y \notin I\}$. *Marginalizing* out a set of nodes $W \subseteq V$ from a directed mixed graph $\mathcal{G} = \langle V, E, B \rangle$ results in a directed mixed graph $\mathcal{G}_{\text{mar}(W)} = \langle V \setminus W, E_{\text{mar}(W)}, B_{\text{mar}(W)} \rangle$ (also known as the *latent projection*) where:

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

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

A.2 Cyclic SCMs

Structural causal models are a popular causal modelling framework that form the basis of many statistical methods for causal inference (Pearl, 2000). Their origins can be traced back to early work in genetics (Wright, 1921), econometrics (Wright, 1928; Haavelmo, 1943), and the social sciences (Goldberger and Duncan, 1973). The properties of acyclic SCMs (i.e., recursive SEMs) have been widely studied and are well-understood, see for example Lauritzen et al. (1990); Spirtes et al. (2000); Pearl (2000). For systems that have causal cycles the class of cyclic SCMs has been proposed as an appropriate modelling class (Spirtes, 1995; Mooij et al., 2013). Recently, Forré and Mooij (2017); Bongers et al. (2020) showed that *modular* and *simple* SCMs retain many of the attractive properties of acyclic SCMs. Notably, they induce a unique distribution over variables, they obey a Markov property, and their graphs have an intuitive causal interpretation. Here, we will closely follow Bongers et al. (2020) for a succinct introduction to cyclic SCMs and their properties. We also discuss literature on how they may arise from equilibrating dynamical models.

The definition of an SCM in Bongers et al. (2020) slightly deviates from previous notions of (acyclic) SCMs because it separates the model from the (endogenous) random variables that solve it. Due to this change, interventions on SCMs are always well-defined, even if the resulting *intervened* SCM does not have a (unique) solution. In Definition 26 below, we explicitly include exogenous random variables, which may be observed or unobserved, and the graph of the SCM. The endogenous random variables that solve an SCM are defined in Definition 27.

Definition 26 *A structural causal model (SCM) is a tuple $\langle \mathcal{X}, \mathbb{P}_W, \mathbf{f}, \mathcal{G} \rangle$ where*

1. $\mathcal{X} = \bigotimes_{v \in V} \mathcal{X}_v$, where each \mathcal{X}_v is a standard measurable space and the domain of a variable X_v ,
2. $\mathbb{P}_W = \prod_{w \in W} \mathbb{P}_w$ specifies the exogenous distribution, a product probability measure on $\bigotimes_{w \in W} \mathcal{X}_w$, where each \mathbb{P}_w is a probability measure on \mathcal{X}_w , with $W \subseteq V$ a set of indices corresponding to exogenous variables,²⁸
3. $\mathbf{f} : \mathcal{X}_V \rightarrow \mathcal{X}_{V \setminus W}$ is a measurable function that specifies causal mechanisms.²⁹
4. $\mathcal{G} = \langle V, E \rangle$ is a directed graph with:
 - (a) a set of nodes V corresponding to variables,
 - (b) a set of edges $E = \{(v_i \rightarrow v_j) : v_i \text{ is a parent of } v_j\}$.³⁰

28. This means that the nodes $V \setminus W$ correspond to endogenous variables.

29. The structural equations of the model are given by $x_v = f_v(\mathbf{x})$, $\mathbf{x} \in \mathcal{X}$ for $v \in V \setminus W$.

30. We say that v_i is a parent of v_j if and only if $v_j \in V \setminus W$ and there does not exist a measurable function $\tilde{f}_j : \mathcal{X}_{V \setminus \{v_i\}} \rightarrow \mathcal{X}_j$ such that for \mathbb{P}_W -almost every $\mathbf{x}_W \in \mathcal{X}_W$ and for all $\mathbf{x}_{V \setminus W} \in \mathcal{X}_{V \setminus W}$ we have $x_j = f_j(\mathbf{x}) \iff x_j = \tilde{f}_j(\mathbf{x}_{V \setminus \{v_i\}})$, see Definition 2.7 in Bongers et al. (2020).

Definition 27 We say that a random variable \mathbf{X} taking value in \mathcal{X} is a solution to an SCM $\langle \mathcal{X}, \mathbb{P}_W, \mathbf{f}, \mathcal{G} \rangle$ if $\mathbb{P}^{\mathbf{X}_W} = \mathbb{P}_W$ (i.e., if the marginal distribution of \mathbf{X} on \mathcal{X}_W equals the exogenous distribution specified by the SCM), and

$$\mathbf{X}_{V \setminus W} = \mathbf{f}(\mathbf{X}) \quad a.s. \quad (22)$$

The notion of *unique solvability w.r.t. a subset* is given in Definition 28 below.

Definition 28 An SCM $\langle \mathcal{X}, \mathbb{P}_W, \mathbf{f}, \mathcal{G} \rangle$ is *uniquely solvable w.r.t. $S \subseteq V \setminus W$* if there exists a measurable function $\mathbf{g}_S : \mathcal{X}_{\text{pa}_{\mathcal{G}}(S) \setminus S} \rightarrow \mathcal{X}_S$ such that for \mathbb{P}_W -almost every $\mathbf{x}_W \in \mathcal{X}_W$ and for all $\mathbf{x}_{V \setminus W} \in \mathcal{X}_{V \setminus W}$

$$\mathbf{x}_S = \mathbf{g}_S(\mathbf{x}_{\text{pa}_{\mathcal{G}}(S) \setminus S}) \iff \mathbf{x}_S = \mathbf{f}_S(\mathbf{x}). \quad (23)$$

SCMs that are uniquely solvable w.r.t. every subset of variables are called *simple SCMs* (Bongers et al., 2020). It can be shown that SCMs with acyclic graphs are simple SCMs (Proposition 3.6 in Bongers et al. (2020)). Furthermore, SCMs are uniquely solvable w.r.t. a single variable if and only if there is no self-cycle at that variable (Proposition 3.9 in Bongers et al. (2020)). The notion of (perfect) interventions on an SCM is given in Definition 29.

Definition 29 Let $\mathcal{M} = \langle \mathcal{X}, \mathbb{P}_W, \mathbf{f}, \mathcal{G} \rangle$ be an SCM, $I \subseteq V \setminus W$ an intervention target and $\xi_I \in \mathcal{X}_I$ the intervention value. A *perfect intervention* $\text{do}(I, \xi_I)$ on the SCM maps it to an *intervened SCM* $\mathcal{M}_{\text{do}(I, \xi_I)} = \langle \mathcal{X}, \mathbb{P}_W, \tilde{\mathbf{f}}, \mathcal{G}_{\text{do}(I)} \rangle$ with

$$\tilde{f}_v(\mathbf{x}) := \begin{cases} \xi_v & v \in I \\ f_v(\mathbf{x}) & v \in V \setminus (W \cup I). \end{cases} \quad (24)$$

Cyclic SCMs may have no solution, multiple solutions with different distributions, or all solutions may have the same distribution. This may even change as a result of a perfect intervention. Because changes in the solution after an intervention may not be compatible with the structure of the functional relations between variables, the causal interpretation of the graph of a cyclic SCM may not be intuitive (Bongers et al., 2020). It can be shown that the graph of a simple SCM, whose unique solvability is preserved under intervention (Proposition 8.2 in Bongers et al. (2020)), has an intuitive causal interpretation; direct and indirect causal effects can be read off from the graph of the SCM by checking for the presence of directed edges and directed paths between variables (Bongers et al., 2020). For general cyclic models, Bongers et al. (2020) give a sufficient condition for detecting direct and indirect causes in an SCM with cycles. Roughly speaking, an indirect cause v_i of v_j can be detected if by controlling v_i we can bring about a change in the distribution of v_j and a direct cause v_d of v_j can be detected if by controlling v_d and keeping all other variables constant we can bring about a change in the distribution of v_j . For the exact formulation we refer to Proposition 7.1 in Bongers et al. (2020).

Cyclic SCMs have been used to represent the equilibrium distribution of dynamical models (Fisher, 1970; Spirtes, 1995; Richardson, 1996; Lauritzen and Richardson, 2002; Mooij et al., 2013; Bongers and Mooij, 2018). Under certain stability assumptions, an SCM can be obtained by *equilibrating* a dynamical model (Mooij et al., 2013; Bongers and

Mooij, 2018). In the deterministic setting, Mooij et al. (2013) showed that a set of first-order differential equations in a globally asymptotically stable system can be mapped to a set of *labelled equilibrium equations* by setting the time derivatives of variables equal to zero and labelling them as belonging to the time derivative of particular variables. If each labelled equilibrium equation can be solved for the corresponding variable then the labelled equilibrium equations can be mapped to a cyclic SCM without self-cycles. The idea that a dynamical model can be *equilibrated to an SCM* was formalized in a general stochastic setting with zeroth and higher order differential equations by Bongers and Mooij (2018), who also show how to equilibrate the *causal dynamics model* of the bathtub system that we discussed in Example 1 to an SCM with self-cycles.

A.3 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., Lauritzen et al. (1990); Pearl (2000); Spirtes et al. (2000); Forré and Mooij (2017). For 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 the ‘collapsed graph’ representation of Spirtes (1995) inspired Forré and Mooij (2017) to introduce the σ -separation criterion.

Definition 30 *For a directed mixed graph $\mathcal{G} = \langle V, E, B \rangle$ we say that a path (v_1, \dots, v_n) is σ -blocked by $Z \subseteq V$ if*

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

The path is d-blocked by Z if it is σ -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 σ -separated by $Z \subseteq V$ if every path in \mathcal{G} with one end-vertex in X and one end-vertex in Y is σ -blocked by Z , and write

$$X \perp_{\mathcal{G}}^{\sigma} Y \mid Z.$$

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

$$X \perp_{\mathcal{G}}^d Y \mid Z.$$

It can be shown that σ -separation implies d-separation and that the two are equivalent for acyclic graphs (Forré and Mooij, 2017). In general, d-separation does not imply σ -separation. The d-separations or σ -separations in a probabilistic graphical model may imply conditional independences via the Markov properties in Definition 31 below.

Definition 31 For a directed mixed graph $\mathcal{G} = \langle V, E, B \rangle$ and a probability distribution $\mathbb{P}_{\mathbf{X}}$ on a product $\mathcal{X} = \otimes_{v \in V} \mathcal{X}_v$ 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 $W, Y, Z \subseteq V$:

$$W \perp_{\mathcal{G}}^d Y \mid Z \implies \mathbf{X}_W \perp_{\mathbb{P}_{\mathbf{X}}} \mathbf{X}_Y \mid \mathbf{X}_Z.$$

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

$$W \perp_{\mathcal{G}}^{\sigma} Y \mid Z \implies \mathbf{X}_W \perp_{\mathbb{P}_{\mathbf{X}}} \mathbf{X}_Y \mid \mathbf{X}_Z.$$

Since σ -separations imply d-separations but not the other way around, the generalized directed global Markov property is strictly weaker than the directed global Markov property (Bongers et al., 2020). For acyclic SCMs the induced probability distribution on endogenous variables and the corresponding DAG satisfy the directed global Markov property (Lauritzen et al., 1990). The variables that solve a simple SCM obey the generalized directed global Markov property relative to the graph of the SCM (Bongers et al., 2020), while d-separation is limited to more specific settings such as acyclic models, discrete variables, or continuous variables with linear relations (Forré and Mooij, 2017). A comprehensive account of different Markov properties for graphical models is provided by Forré and Mooij (2017).

Constraint-based causal discovery algorithms require an additional faithfulness assumption. A probability distribution is *d-faithful* to a directed mixed graph when each conditional independence implies a d-separation in that graph. Similarly, a probability distribution is *σ -faithful* to a directed mixed graph when each conditional independence implies a σ -separation in that graph. In non-linear, non-discrete, cyclic settings the σ -faithfulness assumption is a natural extension of the common d-faithfulness assumption with σ -separation replacing d-separation. In the acyclic setting, d-separation has been shown to be strongly complete in the discrete and linear-Gaussian cases without latent confounders (Meek, 1995), which means that d-faithfulness holds for almost all values of the parameters (with respect to Lebesgue measure in the natural parametrization). This is often used to motivate the assumption of d-faithfulness for constraint-based causal discovery. No analogous results are known regarding the completeness of σ -separation in the general non-linear, non-discrete cyclic setting (although Spirtes (1995) conjectures its completeness in the setting where latent confounders are absent).

Various constraint-based causal discovery algorithms have been proposed for the cyclic case. Under the additional assumption of causal sufficiency (i.e., no latent confounding variables), the NL-CCD algorithm was shown to be sound under the generalized directed Markov property and the weaker d-faithfulness assumption (Chapter 4 in Richardson (1996)). Recently, Forré and Mooij (2018); Mooij et al. (2020); Mooij and Claassen (2020) proved soundness for a variety of causal discovery algorithms under the generalized directed Markov property and the σ -faithfulness assumption. Strobl (2018) proved soundness of a causal discovery algorithm under the directed Markov property and the d-faithfulness assumption, allowing for latent confounding and selection bias.

Appendix B. Proofs

In this section of the appendix, all proofs are provided.

B.1 Causal ordering via minimal self-contained sets

In this section we prove Theorem 4 below.

Theorem 4 *The output of Algorithm 1 is well-defined and unique.*

Lemma 32 below shows that the minimal self-contained sets in a self-contained bipartite graph are disjoint. Lemma 33 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 32 and 33 to prove Lemma 34 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 32 *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*

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

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 3, we have that

$$|S_1 \cap S_2| < |\text{adj}_{\mathcal{B}}(S_1 \cap S_2)|. \quad (25)$$

Consider the following equations:

$$|\text{adj}_{\mathcal{B}}(S_1)| + |\text{adj}_{\mathcal{B}}(S_2)| - |S_1 \cap S_2| \quad (26)$$

$$= |S_1| + |S_2| - |S_1 \cap S_2| \quad (27)$$

$$= |S_1 \cup S_2| \leq |\text{adj}_{\mathcal{B}}(S_1 \cup S_2)| \quad (28)$$

$$\begin{aligned} &= |\text{adj}_{\mathcal{B}}(S_1) \cup \text{adj}_{\mathcal{B}}(S_2)| \\ &= |\text{adj}_{\mathcal{B}}(S_1)| + |\text{adj}_{\mathcal{B}}(S_2)| - |\text{adj}_{\mathcal{B}}(S_1) \cap \text{adj}_{\mathcal{B}}(S_2)| \\ &\leq |\text{adj}_{\mathcal{B}}(S_1)| + |\text{adj}_{\mathcal{B}}(S_2)| - |\text{adj}_{\mathcal{B}}(S_1 \cap S_2)|, \end{aligned} \quad (29)$$

where equality (27) holds by condition 1 of Definition 3, since \mathcal{B} is self-contained inequality (28) holds by condition 2 of Definition 3, and inequality (29) holds because $\text{adj}_{\mathcal{B}}(S_1 \cap S_2) \subseteq \text{adj}_{\mathcal{B}}(S_1) \cap \text{adj}_{\mathcal{B}}(S_2)$. It follows that

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

This is in contradiction with equation (25), and hence $S_1 \cap S_2 = \emptyset$. This implies that $|\mathcal{S}_1 \cap \mathcal{S}_2| = 0$ and therefore by the inequalities above we have that $|\text{adj}_{\mathcal{B}}(S_1) \cap \text{adj}_{\mathcal{B}}(S_2)| = 0$. Thus $\text{adj}_{\mathcal{B}}(S_1) \cap \text{adj}_{\mathcal{B}}(S_2) = \emptyset$. \blacksquare

Lemma 33 *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*

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

with $S \in \mathcal{S}_F$. Then the following two properties hold:

1. \mathcal{B}' is self-contained, and
2. the sets in $\mathcal{S}_F \setminus \{S\}$ are minimal self-contained in \mathcal{B}' .

Proof

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

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

This shows that condition 1 of Definition 3 is satisfied for \mathcal{B}' . Assume, for the sake of contradiction, that F' does not satisfy condition 2 of Definition 3 in the induced subgraph \mathcal{B}' . Then there exists $S' \subseteq F'$ such that $|S'| > |\text{adj}_{\mathcal{B}'}(S')|$. Consider the following equations:

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

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 3 are satisfied for \mathcal{B}' . This shows that \mathcal{B}' is self-contained.

Let $S_1 \in \mathcal{S}_F$ and $S_2 \in \mathcal{S}_F$ be two distinct minimal self-contained sets in \mathcal{B} . Suppose that \mathcal{B}_1 is a subgraph of \mathcal{B} induced by $V \setminus \text{adj}_{\mathcal{B}}(S_1)$ and $F \setminus S_1$. By Lemma 32 we know that $S_1 \cap S_2 = \emptyset$ and $\text{adj}_{\mathcal{B}}(S_1) \cap \text{adj}_{\mathcal{B}}(S_2) = \emptyset$. It follows that for all $S' \subseteq S_2$ we have that $\text{adj}_{\mathcal{B}}(S') = \text{adj}_{\mathcal{B}_1}(S')$. We find that

$$\begin{aligned} |S_2| &= |\text{adj}_{\mathcal{B}}(S_2)| = |\text{adj}_{\mathcal{B}_1}(S_2)|, \\ |S'| &\leq |\text{adj}_{\mathcal{B}}(S')| = |\text{adj}_{\mathcal{B}_1}(S')|, \end{aligned}$$

for all $S' \subseteq S_2$. This shows that S_2 satisfies the conditions of Definition 3 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 34 *Let $\mathcal{B} = \langle V, F, E \rangle$ be a self-contained bipartite graph. The output $\text{CO}(\mathcal{B})$ 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 $A = (1, 2, \dots, |\mathcal{V}_1|)$ 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, $B = (1, 2, \dots, |\mathcal{V}_2|)$ 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 $i \in (1, 2, \dots, |\mathcal{V}_1|)$ 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 33 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 $B' = B \setminus (b_1, \dots, b_i) = (b'_1, \dots, b'_{|\mathcal{V}_2| - i})$ be an ordered set such that $b'_j \prec b'_{j+1}$ for all $j = 1, \dots, |\mathcal{V}_2| - (i + 1)$.

1. 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 bipartite 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 $S^{(1)} = T^{(b_1)}, \dots, S^{(i)} = T^{(b_i)}$ are subsequently added to \mathcal{V}_1 and removed from the bipartite graph. Therefore, by Lemma 32 and Lemma 33, 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 32 and Lemma 33, either $T^{(b'_1)} = S^{(i+1)}$ (in which case we are done) or $F \cap S^{(i+1)}$ is minimal self-contained in $\mathcal{B}' \setminus T^{(b'_1)}$.
2. 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 bipartite graph is finite, there exists $m \in 1, \dots, |\mathcal{V}_2| - i$ such that $T^{(b'_m)} = S^{(i+1)}$. By definition of \mathcal{B}' there exists $b_{i+1} \in \mathcal{B}$ 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 $\mathcal{G}_1 = \mathcal{G}_2$. ■

B.2 Coarse decomposition

For completeness, we include the proofs of the results in Pothen and Fan (1990) that are necessary to show that the output of the extended causal ordering algorithm (Algorithm 3) is unique. The presentation in this section is based on the exposition of Van Diepen (2019). In order to prove the statements in Lemma 10 and Proposition 8, we require additional results. Lemma 35 and 36 show that the incomplete, complete, and over-complete set are disjoint. The former uses the notion of an *augmented path* for a bipartite graph \mathcal{B} and a matching M , which is an alternating path for M that starts and ends with an unmatched vertex.

Lemma 35 [Berge (1957)] *M is a maximum matching for a bipartite graph \mathcal{B} if and only if \mathcal{B} does not contain any augmenting paths for M .*

Proof The proof can be found in Berge (1957). ■

Lemma 36 [Pothen (1985)] *Let $\mathcal{B} = \langle V, F, E \rangle$ be a bipartite graph with a maximum matching M . The incomplete set T_I and the overcomplete set T_O in Definition 7 are disjoint.*

Proof For the sake of contradiction, assume that there is a vertex $v \in T_I \cap T_O$. Then there is an alternating path from an unmatched vertex in V to v and there is also an alternating path from an unmatched vertex in F to v . By sticking these two paths together we obtain an augmented path. It follows from Lemma 35 that M is not maximum. This is a contradiction and therefore T_I and T_O must be disjoint. ■

Lemma 37 and Lemma 9 show that for a bipartite graph and a maximum matching with coarse decomposition $\text{CD}(\mathcal{B}, M)$, the vertices in T_I, T_C, T_O are matched to vertices in T_I, T_C, T_O respectively. Furthermore the subgraph of \mathcal{B} induced by T_C is self-contained, so that Algorithm 1 can be applied.

Lemma 37 [Pothen (1985)] *Let $\mathcal{B} = \langle V, F, E \rangle$ be a bipartite graph with a maximum matching M . Let $\text{CD}(\mathcal{B}, M) = \langle T_I, T_C, T_O \rangle$ be the associated coarse decomposition. A matched vertex in T_I is matched to a vertex in T_I and a matched vertex in T_O is matched to a vertex in T_O .*

Proof For a matched vertex $x \in T_I$ there is an alternating path starting from an unmatched vertex $u_v \in V$ to x . When $x \in V$, this alternating path ends with a matched edge and hence x is matched to a vertex in T_I . When $x \in F$ the alternating path ends with an unmatched edge. We may extend the alternating path with the edge adjacent to x that is in M , and hence is matched to a vertex in T_I . For a matched vertex $x \in T_O$ there is an alternating path starting from an unmatched vertex $u_f \in F$ to x . When $x \in F$, this alternating path ends with a matched edge and hence x is matched to a vertex in T_O . When $x \in V$, the alternating path ends with an unmatched edge. The alternating path may be extended with the edge adjacent to x that is in M , and hence x is matched to a vertex in T_O . ■

Lemma 9 [Pothen (1985)] *Let \mathcal{B} be a bipartite graph with coarse decomposition $\langle T_I, T_C, T_O \rangle$. The subgraph \mathcal{B}_C of \mathcal{B} induced by vertices in T_C has a perfect matching and is self-contained.*

Proof By Lemma 37 we know that vertices in T_I and T_O can only be matched to a vertex in T_I and T_O , respectively. There are no unmatched vertices in T_C , so vertices in $T_C \cap V$ are perfectly matched to vertices in $T_C \cap F$. It follows from Hall's marriage theorem that \mathcal{B}_C is self-contained (Hall, 1986). ■

The following lemma restricts edges that can be present between the incomplete, complete and overcomplete sets. This shows that clusters of the causal ordering graph that are in the overcomplete set are never descendants of clusters in the incomplete or complete set. Similarly, it also shows that clusters in the incomplete set are never ancestors of the complete or overcomplete sets. Lemma 10 is then used to prove Proposition 8.

Lemma 10 [Pothen (1985)] *Let $\mathcal{B} = \langle V, F, E \rangle$ be a bipartite graph with a maximum matching M . Let $\text{CD}(\mathcal{B}, M) = \langle T_I, T_C, T_O \rangle$ be the associated coarse decomposition. No edge joins a vertex in $T_I \cap V$ with a vertex in $(T_C \cup T_O) \cap F$ and no edge joins a vertex in $T_C \cap V$ with a vertex in $T_O \cap F$.*

Proof Suppose that there is an edge $e = (v - f)$ between a vertex $v \in T_I \cap V$ to a vertex $f \in (T_C \cup T_O) \cap F$. By Lemma 37 the edge is not in the maximum matching. Note that there is an alternating path from an unmatched vertex in $T_I \cap V$ to v that starts with an unmatched edge and ends with a matched edge. By adding the edge $(v - f)$, we obtain again an alternating path so that $f \in T_I$. This is a contradiction, and hence there is no edge between $(v - f)$. The second part of the lemma follows by symmetry. ■

Proposition 8 [Pothen (1985)] *The coarse decomposition of a bipartite graph \mathcal{B} is independent of the choice of the maximum matching.*

Proof Let M be an arbitrary matching and let $\text{CD}(\mathcal{B}, M) = \langle T_I, T_C, T_O \rangle$. Note that all vertices in $(T_I \cap V) \setminus U_V$ are M -matched to vertices in $T_I \cap F$ (by construction and Lemma 37). Also, all vertices in $(T_O \cap F) \setminus U_F$ are M -matched with vertices in $T_O \cap V$. Finally, all vertices in $T_C \cap V$ are M -matched with vertices in $T_C \cap F$ and vice versa by

Lemma 9. By Lemma 10 we have $\text{adj}_{\mathcal{B}}(T_I \cap V) = T_I \cap F$ and $\text{adj}_{\mathcal{B}}(T_O \cap F) = T_O \cap V$, so any matching for \mathcal{B} can only match vertices in $T_I \cap V$ with vertices in $T_I \cap F$ and vertices in $T_O \cap F$ with vertices in $T_O \cap V$.

For the sake of contradiction, assume that there exists a maximum matching M' that matches a vertex in $T_I \cap F$ with a vertex in $(T_C \cup T_O) \cap V$. Write:

$$\begin{aligned} M_V &= \{v \in V : \exists f \in F : v - f \in M\}, & M'_V &= \{v \in V : \exists f \in F : v - f \in M'\}, \\ M_F &= \{f \in F : \exists v \in V : v - f \in M\}, & M'_F &= \{f \in F : \exists v \in V : v - f \in M'\}. \end{aligned}$$

Note that the number of edges in matching M' is bounded by

$$\begin{aligned} |M'| &= |M'_V| \\ &= |M'_V \cap T_I| + |M'_V \cap T_C| + |M'_V \cap T_O| \\ &\leq (|F \cap T_I| - 1) + |V \cap T_C| + |V \cap T_O| \\ &= (|M_V \cap T_I| - 1) + |M_V \cap T_C| + |M_V \cap T_O| \\ &= |M_V| - 1 = |M| - 1, \end{aligned}$$

where we used that (i) vertices in $T_I \cap V$ can only be matched with vertices in $T_I \cap F$, (ii) all nodes in $T_I \cap F$ are M -matched with vertices in $M_V \cap T_I$, (iii) all variable vertices in T_C are M -matched, and (iv) all vertices in $T_O \cap V$ are M -matched. This contradicts the assumption that M' is a maximum matching.

In a similar way, one obtains a contradiction when assuming the existence of a maximum matching M'' that matches a vertex in $T_O \cap V$ with a vertex in $(T_I \cup T_C) \cap F$. Hence any maximum matching of \mathcal{B} must match all vertices in $T_I \cap F$ with vertices in $T_I \cap V$, and all vertices in $T_O \cap V$ with vertices in $T_O \cap F$. We conclude that T_O and T_I do not depend on the choice of maximum matching. By definition T_C is uniquely determined by T_O and T_I . Therefore the coarse decomposition is independent of the choice of maximum matching. \blacksquare

B.3 Markov property via d-separation

In this section we prove Theorem 17 below.

Theorem 17 *Let $\mathbf{X}^* = \mathbf{h}(\mathbf{X}_W)$ with $\mathbf{h} : \mathcal{X}_W \rightarrow \mathcal{X}_{V \setminus W}$ be a solution of a system of constraints $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$ with coarse decomposition $\text{CD}(\mathcal{B}) = \langle T_I, T_C, T_O \rangle$. Let $\text{MO}_{\text{CO}}(\mathcal{B})$ denote the subgraph of the Markov ordering graph induced by $T_C \cup T_O$ and let \mathbf{X}_{CO}^* denote the corresponding solution components. If \mathcal{M} is maximally uniquely solvable then the pair $(\text{MO}_{\text{CO}}(\mathcal{B}), \mathbb{P}_{\mathbf{X}_{\text{CO}}^*})$ satisfies the directed global Markov property (see Definition 31).*

Proof Let $v \in (T_C \cup T_O) \cap (V \setminus W)$ be arbitrary and define $S_V = \text{cl}(v) \cap V$ and $S_F = \text{cl}(v) \cap F$. First, we will show that $V(S_F) \setminus S_V = \text{pa}_{\text{MO}(\mathcal{B})}(v)$. The following equivalences hold for

$x \in V$:

$$\begin{aligned}
 x \in V(S_F) \setminus S_V &\iff x \in \text{adj}_{\mathcal{B}}(S_F) \setminus S_V && \text{(by Definition 1)} \\
 &\iff (x \rightarrow \text{cl}(v)) \text{ in } \text{CO}(\mathcal{B}) && \text{(by definition of Algorithm 3)} \\
 &\iff (x \rightarrow v) \text{ in } D(\text{CO}(\mathcal{B})) && \text{(by Definition 16)} \\
 &\iff (x \rightarrow v) \text{ in } D(\text{CO}(\mathcal{B}))_{\text{mar}(F)} \\
 &\iff (x \rightarrow v) \text{ in } \text{MO}(\mathcal{B}) && \text{(by Definition 16)} \\
 &\iff x \in \text{pa}_{\text{MO}(\mathcal{B})}(v).
 \end{aligned}$$

By assumption, the system of constraints is maximally uniquely solvable w.r.t. $\text{CO}(\mathcal{B})$. Note that $S_V \subseteq V(S_F)$. Hence, there exist measurable functions $g_i : \mathcal{X}_{\text{pa}_{\text{MO}(\mathcal{B})}(v)} \rightarrow \mathcal{X}_i$ for all $i \in S_V$ such that $\mathbb{P}_{\mathbf{X}_W}$ -a.s., for all $\mathbf{x}_{V(S_F) \setminus W} \in \mathcal{X}_{V(S_F) \setminus W}$:

$$\begin{aligned}
 \forall f \in S_F : \phi_f(\mathbf{x}_{V(f) \setminus W}, \mathbf{X}_{V(f) \cap W}) = c_f &\iff \\
 \forall i \in S_V : x_i = g_i(\mathbf{x}_{\text{pa}_{\text{MO}(\mathcal{B})}(v) \setminus W}, \mathbf{X}_{\text{pa}_{\text{MO}(\mathcal{B})}(v) \cap W}).
 \end{aligned}$$

Since $v \in (T_C \cup T_O) \cap (V \setminus W)$ was chosen arbitrarily and $\mathbf{X}^* = \mathbf{h}(\mathbf{X}_W)$ with \mathbf{h} a solution of \mathcal{M} , it follows that

$$\mathbf{X}_v^* = g_v(\mathbf{X}_{\text{pa}_{\text{MO}(\mathcal{B})}(v)}^*) \quad \mathbb{P}_{\mathbf{X}_W}\text{-a.s.},$$

for all $v \in (T_C \cup T_O) \cap (V \setminus W)$. 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 (Pearl, 2000; Lauritzen, 1996). Because the Markov ordering graphs $\text{MO}(\mathcal{B})$ and $\text{MO}_{\text{CO}}(\mathcal{B})$ are acyclic by construction, and $\text{MO}_{\text{CO}}(\mathcal{B})$ is the graph corresponding to this set of structural equations, this completes the proof. \blacksquare

B.4 Causal ordering via perfect matchings

In this section we prove Theorem 6 below.

Theorem 6 *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 38 (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 $|F'| \leq |\text{adj}_{\mathcal{B}}(F')|$ 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 39 *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 3 we know that if \mathcal{B} is self-contained then $|V| = |F|$. Hence, the statement follows from Definition 3 and Theorem 38. \blacksquare

The following technical lemma is used to prove Lemma 41, 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 40 *Let M be a perfect matching for a self-contained bipartite graph $\mathcal{B} = \langle V, F, E \rangle$. Let $S_V^{(1)}, \dots, S_V^{(n)}$ be a topological ordering of the strongly connected components in the graph $\mathcal{G}(\mathcal{B}, M)_{\text{mar}(F)}$. 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:

$$|S_V^{(1)}| = |S_F^{(1)}| \leq |\text{adj}_{\mathcal{B}^{(1)}}(S_F^{(1)})|. \quad (30)$$

By definition of topological ordering and the orientation step in Definition 5 we know that:

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

Together, these two inequalities show that $|S_F^{(1)}| = |\text{adj}_{\mathcal{B}^{(1)}}(S_F^{(1)})|$. Because $\mathcal{B}^{(1)}$ is self-contained, the set $S_F^{(1)}$ satisfies both conditions of Definition 3. 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 3, we have that $|F'| = |\text{adj}_{\mathcal{B}^{(1)}}(F')|$ and $|S_V^{(1)}| = |S_F^{(1)}|$ so that $S_V^{(1)} \setminus \text{adj}_{\mathcal{B}^{(1)}}(F') \neq \emptyset$ and $\text{adj}_{\mathcal{B}^{(1)}}(F') \neq \emptyset$. Furthermore, by Definition 5 (orientation step), we must have that:

$$\text{pa}_{\mathcal{G}^{(1)}}(\text{adj}_{\mathcal{B}^{(1)}}(F')) = M^{(1)}(\text{adj}_{\mathcal{B}^{(1)}}(F')) = F'. \quad (31)$$

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

$$\text{pa}_{\mathcal{G}^{(1)}}(S_V^{(1)} \setminus \text{adj}_{\mathcal{B}^{(1)}}(F')) = M^{(1)}(S_V^{(1)} \setminus \text{adj}_{\mathcal{B}^{(1)}}(F')) = F \setminus F'. \quad (32)$$

Therefore, there can be no directed path from any $v \in S_V^{(1)} \setminus \text{adj}_{\mathcal{B}^{(1)}}(F')$ to any $f \in F'$ in $\mathcal{G}^{(1)}$. This contradicts the assumption that $S_V^{(1)}$ is a strongly connected component in $\mathcal{G}_{\text{mar}(F)}^{(1)}$. 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 39 we therefore know that $\mathcal{B}^{(2)}$ is self-contained. Since $S_V^{(2)}, \dots, S_V^{(n)}$ is a topological ordering for the strongly connected components in $\mathcal{G}_{\text{mar}(F)}^{(2)}$ the above argument can be repeated to show that $S_F^{(2)}$ is minimal self-contained in $\mathcal{B}^{(2)}$. For arbitrary $i \in \{1, \dots, n\}$ this entire argument can be iterated to show that $S_F^{(i)}$ is minimal self-contained in the self-contained bipartite graph $\mathcal{B}^{(i)}$. \blacksquare

Lemma 41 *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 5 coincides with the output $\mathcal{G}_2 = \langle \mathcal{V}_2, \mathcal{E}_2 \rangle$ of Algorithm 1.*

Proof Let $S^{(1)}, \dots, S^{(n)}$ be a topological ordering of the strongly connected components in $\mathcal{G}(M, \mathcal{B})_{\text{mar}(F)}$. By Definition 5 the cluster set \mathcal{V}_1 consists of clusters $S^{(i)} \cup M(S^{(i)})$ with $i \in \{1, \dots, n\}$. By Lemma 40, 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 4 the output of Algorithm 1 is unique and therefore $\mathcal{V}_1 = \mathcal{V}_2$. By Definition 5 the following equivalences hold for $C \in \mathcal{V}_1 = \mathcal{V}_2$ and $v \in V \setminus C$:

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

Let $C \in \mathcal{V}_1 = \mathcal{V}_2$ and $f \in F \cap (\text{adj}_{\mathcal{B}}(C) \setminus C)$. By definition of Algorithm 1 we know that $(f \rightarrow C) \notin \mathcal{E}_2$. Note that $M(C \cap F) = C \cap V$. By Definition 5 there is no edge $(f \rightarrow v)$ with $v \in C \cap V$ in $\mathcal{G}(\mathcal{B}, M)$ and hence by Definition we know that $(f \rightarrow C) \notin \mathcal{E}_2$. By construction, edges $(x \rightarrow C)$ 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 . \blacksquare

Lemma 41 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.

B.5 Markov property via σ -separation

Here, we prove the following theorem.

Theorem 18 *Let $\mathbf{X}^* = \mathbf{g}(\mathbf{X}_W)$ be a solution of a system of constraints $\langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$, 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 $S_F = (S \cup M(S)) \cap F$ then the pair $(\mathcal{G}(\mathcal{B}, M)_{\text{mar}(F)}, \mathbb{P}_{\mathbf{X}^*})$ satisfies the generalized directed global Markov property (Definition 31).*

The proof of this theorem 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 its augmentation (Forré and Mooij, 2017). The acyclification of a directed graph is given in Definition 42.

Definition 42 *Let $\mathcal{G} = \langle V, E \rangle$ be a directed graph. The acyclification of E , denoted by E^{acy} , has edges $(i \rightarrow j) \in E^{\text{acy}}$ if and only if $i \notin \text{sc}_{\mathcal{G}}(j)$ and there exists $k \in \text{sc}_{\mathcal{G}}(j)$ such that $(i \rightarrow k) \in E$.*

Lemma 43 shows that the clustering operation in Definition 5 on directed graphs, followed by the declustering operation in Definition 16, results in the same directed graph as the one that is obtained by applying the acyclification operation to its edge set.

Lemma 43 *Consider a directed graph $\mathcal{G} = \langle V, E \rangle$ be a directed graph. It holds that $\mathcal{G}^{\text{acy}} = \langle V, E^{\text{acy}} \rangle = D(\text{clust}(\mathcal{G}))$.*

Proof This follows from Definitions 16, 5, and 42. ■

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

Proposition 44 *Let $\mathcal{G} = \langle V, E \rangle$ be a directed graph with nodes V and $\mathcal{G}^{\text{acy}} = \langle V, E^{\text{acy}} \rangle$. Then for all subsets $A, B, C \subseteq V$:*

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

Proof The first equivalence is Proposition A.19 in Bongers et al. (2020). The second equivalence follows directly from Lemma 43. ■

We now have all ingredients to finish the proof of Theorem 18. 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, $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ is well-defined by Corollary 39. Let $S_V^{(1)}, \dots, S_V^{(n)}$ be the strongly connected components in \mathcal{G}_{dir} , where $\mathcal{G}_{\text{dir}} := \mathcal{G}(\mathcal{B}, M)_{\text{mar}(F)}$. By Lemma 40 and the definition of Algorithm 1 we know

that \mathcal{V} consists of the clusters $S_V^{(i)} \cup M(S_V^{(i)})$ with $i = 1, \dots, n$. Therefore, \mathcal{M} is uniquely solvable with respect to $\text{CO}(\mathcal{B})$. By Theorem 17 we have that for subsets $A, B, C \subseteq V \setminus W$:

$$A \underset{\text{MO}(\mathcal{B})}{\perp^d} B | C \implies \mathbf{X}_A \underset{\mathbb{P}_{\mathbf{X}}}{\perp\!\!\!\perp} \mathbf{X}_B | \mathbf{X}_C. \quad (33)$$

By Proposition 44 we have that:

$$A \underset{\mathcal{G}_{\text{dir}}}{\perp^\sigma} B | C \iff A \underset{\mathcal{G}_{\text{dir}}^{\text{acy}}}{\perp^d} B | C \iff A \underset{D(\text{clust}(\mathcal{G}_{\text{dir}}))}{\perp^d} B | C. \quad (34)$$

The desired result follows from implications (33) and (34) 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 16 and 5 we have that:

$$D(\langle \mathcal{V}_{\text{mar}(F)}, \mathcal{E} \rangle) = D(\langle \mathcal{V}, \mathcal{E} \rangle)_{\text{mar}(F)} \quad \text{and} \quad \text{clust}(\mathcal{G}_{\text{dir}}) = \langle \mathcal{V}_{\text{mar}(F)}, \mathcal{E} \rangle, \quad (35)$$

respectively. It follows that

$$D(\text{clust}(\mathcal{G}_{\text{dir}})) = D(\text{CO}(\mathcal{B}))_{\text{mar}(F)} = \text{MO}(\mathcal{B}). \quad (36)$$

Note that both d-separations and σ -separations are preserved under marginalization of exogenous vertices W (Forré and Mooij, 2017; Bongers et al., 2020). This finishes the proof.

B.6 Effects of interventions

This section is devoted to the proofs of the results that were presented in Section 5.

Theorem 20 *Let $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} \rangle$ be a system of constraints with coarse decomposition $\text{CD}(\mathcal{B}) = \langle T_I, T_C, T_O \rangle$. Suppose that \mathcal{M} is maximally uniquely solvable w.r.t. the causal ordering graph $\text{CO}(\mathcal{B})$ and let $\mathbf{X}^* = \mathbf{g}(\mathbf{X}_W)$ be a solution of \mathcal{M} . Let $f \in (T_C \cup T_O) \cap F$ and assume that the intervened system $\mathcal{M}_{\text{si}(f, \phi_f', c_f')}$ is also maximally uniquely solvable w.r.t. $\text{CO}(\mathcal{B})$. Let $\mathbf{X}' = \mathbf{h}(\mathbf{X}_W)$ be a solution of $\mathcal{M}_{\text{si}(f, \phi_f', c_f')}$. If there is no directed path from f to $v \in (T_C \cup T_O) \cap V$ in $\text{CO}(\mathcal{B})$ then $X_v^* = X_v'$ almost surely. On the other hand, if there is a directed path from f to v in $\text{CO}(\mathcal{B})$ then X_v^* may have a different distribution than X_v' , depending on the details of the model \mathcal{M} .*

Proof The directed cluster graph $\text{CO}(\mathcal{B})$ 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 $\text{CO}(\mathcal{B})$ then there exists a topological ordering $V^{(1)}, \dots, V^{(n)}$ of the clusters such that $\text{cl}(v)$ comes before $\text{cl}(f)$. Note that clusters of vertices in the incomplete set T_I are never ancestors of clusters in $T_C \cup T_O$ by Lemma 10 (the proof of this lemma will be given in Appendix B.2). Therefore there exists a topological ordering of clusters so that no cluster in T_I precedes a cluster in $T_C \cup T_O$. By the assumption of unique solvability w.r.t. the clusters $T_C \cup T_O$ in $\text{CO}(\mathcal{B})$ we know that the solution component for any variable $v \in V^{(i)} \subseteq T_C \cup T_O$ can be solved from the constraints in $V^{(i)}$ after plugging in the relevant solution components

$\bigcup_{j=1}^{i-1} V^{(j)}$. By the solvability assumption, the solution components X_v^* and X_v' are equal almost surely.

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

Lemma 22 *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 $(V \cup F) \setminus W$ is self-contained. Consider an intervention $\text{do}(S_V, S_F)$ on a cluster $S = S_F \cup S_V$ with $S \cap W = \emptyset$ in the causal ordering graph $\text{CO}(\mathcal{B})$. The subgraph of $\mathcal{B}_{\text{do}(S_F, S_V)}$ 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 $\mathcal{B}_{\text{do}(S_F, S_V)}$ induced by $(V \cup F) \setminus W$. The result follows from Corollary 39. \blacksquare

Proposition 25 *Let $\mathcal{B} = \langle V, F, E \rangle$ be a bipartite graph and W a set of exogenous variables. Let $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ 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:*

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

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

$$V^{(1)}, \dots, V^{(k)} = (S_F \cup S_V), \dots, V^{(n)}. \quad (37)$$

Consider $\text{CO}(\mathcal{B}_{\text{do}(S_F, S_V)}) = \langle \mathcal{V}', \mathcal{E}' \rangle$. It follows from Definition 21, Lemma 32, Lemma 33, and the definition of Algorithm 3 (i.e., the extended causal ordering algorithm) that

$$V^{(1)}, \dots, V^{(k-1)}, \{s_f^1, s_v^1\}, \dots, \{s_f^m, s_v^m\}, V^{(k+1)}, \dots, V^{(n)} \quad (38)$$

is an order in which clusters could be added to \mathcal{V}' . This shows that there are two differences between $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ and $\text{CO}(\mathcal{B}_{\text{do}(S_F, S_V)}) = \langle \mathcal{V}', \mathcal{E}' \rangle$: first $(S_F \cup S_V) \in \mathcal{V}$ whereas $\{\{s_f^i, s_v^i\} : i = 1, \dots, m\} \subseteq \mathcal{V}'$ and second the clusters $(S_F \cup S_V)$ may have parents in $\text{CO}(\mathcal{B})$ but the clusters $\{s_f^i, s_v^i\}$ (with $i \in \{1, \dots, m\}$) have no parents in $\text{CO}(\mathcal{B}_{\text{do}(S_F, S_V)})$. The result follows directly from Definition 24. \blacksquare

Theorem 23 *Let $\mathcal{M} = \langle \mathcal{X}, \mathbf{X}_W, \Phi, \mathcal{B} = \langle V, F, E \rangle \rangle$ be a system of constraints with coarse decomposition $\text{CD}(\mathcal{B}) = \langle T_I, T_C, T_O \rangle$. Assume that \mathcal{M} is maximally uniquely solvable w.r.t. $\text{CO}(\mathcal{B}) = \langle \mathcal{V}, \mathcal{E} \rangle$ and let \mathbf{X}^* be a solution of \mathcal{M} . Let $S_F \subseteq (T_C \cup T_O) \cap F$ and $S_V \subseteq (T_C \cup T_O) \cap (V \setminus W)$ be such that $(S_F \cup S_V) \in \mathcal{V}$. Consider the intervened system $\mathcal{M}_{\text{do}(S_F, S_V, \xi_{S_V})}$ with coarse decomposition $\text{CD}(\mathcal{B}_{\text{do}(S_F, S_V)}) = \langle T'_I, T'_C, T'_O \rangle$. Let \mathbf{X}' be a solution of $\mathcal{M}_{\text{do}(S_F, S_V, \xi_{S_V})}$. If there is no directed path from any $x \in S_V$ to $v \in (T_C \cup T_O) \cap V$ in $\text{CO}(\mathcal{B})$ then $X_v^* = X'_v$ almost surely. On the other hand, if there is $x \in S_V$ such that there is a directed path from x to $v \in (T_C \cup T_O) \cap V$ in $\text{CO}(\mathcal{B})$ then X_v^* may have a different distribution than X'_v .*

Proof First note that $T_C \cup T_O = T'_C \cup T'_O$ by Definition 21. 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 may be different from the solution component X_v^* . Consider $v \in V \setminus S_V$ and its cluster $\text{cl}(v)$ in $\text{CO}(\mathcal{B})$. Since the causal ordering graph is acyclic by construction, there exists a topological ordering $V^{(1)}, \dots, V^{(i)} = \text{cl}(v), \dots, V^{(n)}$ of the clusters in $\text{CO}(\mathcal{B})$ (where n is the amount of clusters in $\text{CO}(\mathcal{B})$) such that $V^{(j)} \prec \text{cl}(v)$ implies that there is a directed path from some vertex in $V^{(j)}$ to the cluster $\text{cl}(v)$ in $\text{CO}(\mathcal{B})$. Note that clusters in T_I are never ancestors of clusters in $T_C \cup T_O$ and that the ordering $V^{(1)}, \dots, V^{(n)}$ is such that no cluster in T_I precedes a cluster in $T_C \cup T_O$. By assumption, the solution component X_v^* can be solved from the constraints and variables in $V^{(i)} = \text{cl}(v)$ by plugging in the solution for variables in $V^{(1)}, \dots, V^{(i-1)}$. Let s_f^1, \dots, s_f^m and s_v^1, \dots, 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 $k \in \{1, \dots, n\}$. By definition of a perfect intervention on a cluster we know that $V^{(1)}, \dots, V^{(k-1)}, \{s_f^1, s_v^1\}, \dots, \{s_f^m, s_v^m\}, V^{(k+1)}, \dots, V^{(n)}$ is a topological ordering of clusters in $\text{CO}(\mathcal{B})_{\text{do}(S_F, S_V)} = \text{CO}(\mathcal{B}_{\text{do}(S_F, S_V)})$ (by Proposition 25). Furthermore, maximal unique solvability w.r.t. $\text{CO}(\mathcal{B})$ implies maximal unique solvability w.r.t. $\text{CO}(\mathcal{B}_{\text{do}(S_F, S_V)})$.

Suppose that $V^{(k)} \succ \text{cl}(v)$ in the topological ordering for $\text{CO}(\mathcal{B})$. By maximal unique solvability w.r.t. $\text{CO}(\mathcal{B})_{\text{do}(S_F, S_V)}$, X'_v can be solved from the constraints and variables in $\text{cl}(v)$ by plugging in the solution for variables in $V^{(1)}, \dots, V^{(i-1)}$. 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 $\text{CO}(\mathcal{B})$. Suppose that $V^{(k)} \prec \text{cl}(v)$ in the topological ordering for $\text{CO}(\mathcal{B})$. By maximal unique solvability w.r.t. $\text{CO}(\mathcal{B})_{\text{do}(S_F, S_V)}$, we know that X'_v can be solved from the constraints and variables in $V^{(i)}$ by plugging in the solution for variables in $V^{(1)}, \dots, V^{(k-1)}, \{s_f^1, s_v^1\}, \dots, \{s_f^m, s_v^m\}, V^{(k+1)}, \dots, V^{(i-1)}$. It follows that X_v^* and X'_v may 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 $\text{cl}(v)$ in $\text{CO}(\mathcal{B})$. \blacksquare

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