Causal calculus in the presence of cycles, latent confounders and selection bias

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Abstract

We prove the main rules of causal calculus (also called do-calculus) for interventional structural causal models (iSCMs), a generalization of a recently proposed general class of non-/linear structural causal models that allow for cycles, latent confounders and arbitrary probability distributions. We also generalize adjustment criteria and formulas from the acyclic setting to the general one (i.e. iSCMs). Such criteria then allow to estimate (conditional) causal effects from observational data that was (partially) gathered under selection bias and cycles. This generalizes the backdoor criterion, the selection-backdoor criterion and extensions of these to arbitrary iSCMs. Together, our results thus enable causal reasoning in the presence of cycles, latent confounders and selection bias.

1 INTRODUCTION

Statistical models are governed by the rules of probability (e.g. sum and product rule), which link joint distributions with the corresponding (conditional) marginal ones. Causal models follow additional rules, which relate the observational distributions with the interventional ones. In contrast to the rules of probability theory, which directly follow from their axioms, the rules of causal calculus need to be proven, when based on the definition of structural causal models (SCMs). As SCMs will among other things depend on the underlying graphical structure (e.g. with or without cycles or bidirected edges, etc.), the used function classes (e.g. linear or non-linear, etc.) and the allowed probability distributions (e.g. discrete, continuous, singular or mixtures, etc.) the respective endeavour is not immediate.

Such a framework of causal calculus contains rules about when one can 1.) insert/delete observations, 2.) exchange action/observation, 3.) insert/delete actions; and about when and how to recover from interventions and/or selection bias (backdoor and selection-backdoor criterion), etc. (see [1,8,5,12,18,21,23,24,28,30]). While these rules have been extensively studied for acyclic causal models, e.g. (semi-)Markovian models, which are attached to directed acyclic graphs (DAGs) or acyclic directed mixed graphs (ADMGs) (see [1,8,5,12,18,21,23,24,28,30]), the case of causal models with cycles stayed in the dark.

To deal with cycles and latent confounders at the same time in this paper we will introduce the class of interventional structural causal models (iSCMs), a “conditional” version of the recently proposed class of modular structural causal models (mSCMs) (see [8,9]) to also include external nodes that can play the role of parameter/action/intervention nodes. They have several desirable properties: iSCMs allow for arbitrary probability distributions, non-/linear functional relations, latent confounders and cycles. They can also model non-/probabilistic external and probabilistic internal nodes in one framework. Furthermore, the class of iSCMs is closed under arbitrary marginalisations and interventions. All causal models that are based on acyclic graphs like DAGs, ADMGs or mDAGs (see [7,25]) can be interpreted as special acyclic iSCMs. Thus iSCMs generalize all these classes of causal models in one framework, but also allow for cycles and external non-/probabilistic nodes. Also the generalized directed global Markov property for mSCMs (see [8,9]) generalizes to iSCMs, i.e. iSCMs entail the conditional independence relations that follow from the σ-separation criterion in the underlying graph, where σ-separation generalizes the usual d-separation (also called m- or m∗-separation, see [7,17,21,25,33]) from acyclic graphs to directed mixed graphs (DMGs) (and even HEDGes and σ-CGs) with or without cycles in a non-naive way.

This paper now aims at proving the mentioned main rules
of causal calculus for iSCMs and derive adjustment criteria with corresponding adjustment formulas like generalized (selection-)backdoor adjustments.

The paper is structured as follows: We will first give the precise definition and main constructions of interventional structural causal models (iSCMs) closely mirroring mSCMs from \[8,9\]. We then will review the definition of $\sigma$-separation and generalize its criterion from mSCMs (see \[8,9\]) to iSCMs. As a preparation for the causal calculus, which relates observational and interventional distributions, we will then show how one can extend a given iSCM to one that also incorporates additional interventional variables indicating the regime of interventions onto the observed nodes. We will then basically show how the rules of causal calculus directly follow from the existence of such an extended iSCM and the $\sigma$-separation criterion applied to it. Finally, we will derive the mentioned general adjustment criteria with corresponding adjustment formulas.

2 INTERVENTIONAL STRUCTURAL CAUSAL MODELS

In this section we will define *interventional structural causal models* (iSCMs), which could be seen as a “conditional” version of modular structural causal models (mSCMs) defined in \[8,9\]. We will then construct marginalized iSCMs and intervened iSCMs. To allow for cycles we first need to introduce the notion of loop of a graph and its strongly connected components.

**Definition 2.1 (Loops).** Let $G = (V,E)$ be a directed graph (with or without cycles).

1. A set of nodes $S \subseteq V$ is called a loop of $G$ if for every two nodes $v_1, v_2 \in S$ there are two directed paths $v_1 \rightarrow \cdots \rightarrow v_2$ and $v_2 \rightarrow \cdots \rightarrow v_1$ in $G$ such that all the intermediate nodes are also in $S$ (if any). The sets $S = \{v\}$ are also considered as loops.

2. The set of loops of $G$ is written as $L(G)$.

3. The strongly connected component of $v$ in $G$ is defined to be: $\operatorname{Sc}^G(v) := \operatorname{Anc}^G(v) \cap \operatorname{Desc}^G(v)$.

**Remark 2.2.** Let $G = (V,E)$ be a directed graph.

1. We always have $v \in \operatorname{Sc}^G(v)$ and $\operatorname{Sc}^G(v) \subseteq \{v\}$.

2. If $G$ is acyclic then: $\operatorname{L}(G) = \{\{v\} \mid v \in V\}$.

In the following, all spaces are meant to be equipped with $\sigma$-algebras, forming standard measurable spaces, and all maps to be measurable.

**Definition 2.3 (Interventional Structural Causal Model).** An interventional structural causal model (iSCM) by definition consists of:

1. A set of nodes $V^+ = V \cup U \cup J$, where elements of $V$ correspond to observed variables, elements of $U$ to latent variables and elements of $J$ to intervention variables.

2. An observation/latent/action space $X_v$ for every $v \in V^+$, $X := \prod_{v \in V^+} X_v$.

3. A product probability measure $\mathbb{P} = \otimes_{u \in U} \mathbb{P}_u$ on the latent space $X_U := \prod_{u \in U} X_u$.

4. A directed graph structure $G^+ = (V^+, E^+)$ with the properties:
   
   (a) $V = \text{Ch}^G(U)$,
   (b) $\text{Pa}^G(U \cup J) = \emptyset$,
   
   where $\text{Ch}^G$ and $\text{Pa}^G$ stand for children and parents in $G$, resp.

5. A system of structural equations $g = (g_S)_{S \subseteq L(G^+)}$:

   $$g_S : \prod_{v \in \text{Pa}^G(S) \setminus S} X_v \rightarrow \prod_{v \in S} X_v$$

   that satisfy the following global compatibility conditions: For every nested pair of loops $S' \subseteq S \subseteq V$ of $G^+$ and every element $x_{\text{Pa}^G(S) \setminus S} \in \prod_{v \in \text{Pa}^G(S) \setminus S} X_v$ we have the implication:

   $$g_S(x_{\text{Pa}^G(S) \setminus S}) = x_S \implies g_{S'}(x_{\text{Pa}^G(S') \setminus S'}) = x_{S'},$$

   where $x_{\text{Pa}^G(S') \setminus S'}$ and $x_S$ denote the corresponding components of $x_{\text{Pa}^G(S) \setminus S}$.

The iSCM will be denoted by $M = (G^+, X, \mathbb{P}_U, g)$.

**Definition 2.4 (Modular structural causal model, see \[8,9\]).** A modular structural causal model (mSCM) is an iSCM without intervention nodes, i.e. $J = \emptyset$.

**Remark 2.5 (Relation between iSCMs and mSCMs).** Given an iSCM $M = (G^+, X, \mathbb{P}_U, g)$ with graph $G^+ = (V \cup U \cup J, E^+)$ we can construct a well-defined mSCM by specifying a product distribution $\mathbb{P}_J := \otimes_{j \in J} \mathbb{P}_j$ on $X_J := \prod_{j \in J} X_j$. For every node $j \in J$ we can decide to change $j$ either to a latent node (U) or to an observed node (V). In the latter case we then formally need to add a latent node $u_j$ to $U$ and an edge $u_j \rightarrow j$ to $G^+$, put $X_{u_j} := X_j$ and $g(j) := \text{id}_{X_j}$ and consider $\mathbb{P}_J$ to live on the latent space $X_{u_j}$ (corresponding to $u_j$ rather then to $j$ directly).

The actual joint distributions on the observed space $X_V$ and thus the random variables attached to any iSCM will be defined in the following.

**Definition 2.6.** Let $M = (G^+, X, \mathbb{P}_U, g)$ be an iSCM with $G^+ = (V \cup U \cup J, E^+)$. We fix a value $x_j \in X_j$. The following constructions will depend on the choice of $x_j$.

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1To have a “reduced” form of the latent space one can in addition impose the condition: $\text{Ch}^G(u_1) \cap \text{Ch}^G(u_2) = \emptyset$ for every two distinct $u_1, u_2 \in U$. This can always be achieved by gathering latent nodes together if $\text{Ch}^G(u_1) \subseteq \text{Ch}^G(u_2)$.

2Note that the index set runs over all “observable loops” $S \subseteq V$, $S \in L(G^+)$, not just the sets $\{v\}$ for $v \in V$. 

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1. The latent variables are given by \((X_u)_{u \in U} \sim \mathbb{P}_U\), i.e. by the canonical projections \(X_u : X_U \to X_u\), which are jointly \(P_1\)-independent. These are still independent of \(x_j\), but we put \(X_u^{\text{do}(x_j)} := X_u\).

2. For \(j \in J\) we put \(X_j^{\text{do}(x_j)} := x_j\), the constant variable given by the \(j\)-component of \(x_j\).

3. The observed variables \((X_v^{\text{do}(x_j)})_{v \in V}\) are inductively defined by:

\[
X_v^{\text{do}(x_j)} := g_S(v(X_v^{\text{do}(x_j)})_{w \in \text{Pa}^+(S) \setminus S}),
\]

where \(S := \text{Se}^+(v) := \text{Anc}^+(v) \cap \text{Desc}^+(v)\) and the second index \(v\) refers to the \(v\)-component of \(g_S\). The induction is taken over any topological order of the strongly connected components of \(G^+\), which always exists (see [14]).

4. By the compatibility condition for \(g\) we then have that for every \(S \in \mathcal{L}(G^+)\) with \(S \subseteq V\) the following equality holds:

\[
X_S^{\text{do}(x_j)} = g_S(X_S^{\text{do}(x_j)})_{w \in \text{Pa}^+(S) \setminus S},
\]

where we put \(X_A := \prod_{v \in A} X_v\) and \(X_A := (X_v)_{v \in A}\) for subsets \(A\).

5. We define the family of conditional distributions:

\[
\mathbb{P}_U(X_A | X_B, X_J = x_j) := \mathbb{P}_U(X_A | X_B, \text{do}(X_J = x_j)) := \mathbb{P}_U(X_A^{\text{do}(x_j)} | X_B^{\text{do}(x_j)}),
\]

for \(A, B \subseteq V\) and \(x_j \in X_J\). Note that in the following we will use the \(\text{do}\) and the \(\text{do-free notation}\) (only) for the \(J\)-variables interchangeably.

6. If we, furthermore, specify a product distribution \(\mathbb{P}_J = \bigotimes_{j \in J} \mathbb{P}_J\) on \(X_J\), then we get a joint distribution \(\mathbb{P}\) on \(X_{V \cup J}\) by setting:

\[
\mathbb{P}(X_V, X_J) := \mathbb{P}_U(X_V | \text{do}(X_J)) \mathbb{P}_J(X_J).
\]

**Remark 2.7.** Let \(M = (G^+, \mathcal{X}, \mathbb{P}_U, g)\) be an iSCM with \(G^+ = (V \cup U \cup J, \mathcal{E}^+)\). For every subset \(A \subseteq V\) we get a well defined map \(g_A : X_{\text{Pa}^+(A)\setminus A} \to X_A\), by recursively plugging in the \(g_S\) into each other for the biggest occurring loops \(S \subseteq A\) by the same arguments as before. These then are all globally compatible by construction and satisfy:

\[
X_A^{\text{do}(x_j)} = g_A(X_A^{\text{do}(x_j)}).\]

Similar to mSCMs (see [8, 9]) we can define the marginalisation of an iSCM.

**Definition 2.8 (Marginalisation of iSCMs).** Let \(M = (G^+, \mathcal{X}, \mathbb{P}, g)\) be an iSCM with \(G^+ = (V \cup U \cup J, \mathcal{E}^+)\) and \(W \subseteq V\) a subset. The marginalised iSCM \(M^W\) w.r.t. \(W\) can be defined by plugging the functions \(g_S\) related to \(W\) into each other. For example, when marginalizing out \(W = \{w\}\) we can define (for the non-trivial case \(w \in \text{Pa}^+(S) \setminus S\)):

\[
g_{S', v}(x_{\text{Pa}^+(S) \setminus S'} | x_S) := g_{S, v}(x_{\text{Pa}^+(S) \setminus (S \cup \{w\})}, g(w(x_{\text{Pa}^+(w) \setminus \{w\}})),
\]

where \((G^+)^W\) is the marginalised graph of \(G^+, S' \subseteq V^W := V \setminus W\) is any loop of \((G^+)^W\) and \(S\) the corresponding induced loop in \(G^+\).

Similar to mSCMs (see [8, 9]) we now define what it means to intervene on observed nodes in an iSCM.

**Definition 2.9 (Perfect interventions on iSCMs).** Let \(M = (G^+, \mathcal{X}, \mathbb{P}, g)\) be an iSCM with \(G^+ = (V \cup U \cup J, \mathcal{E}^+)\). Let \(W \subseteq V \cup J\) be a subset. We then define the post-interventional iSCM \(M_{\text{do}(W)}\) w.r.t. \(W\):

1. Define the graph \(G^+_{\text{do}(W)}\) by removing all the edges \(v \rightarrow w\) for all nodes \(w \in W\) and \(v \in \text{Pa}^+(w)\).
2. Put \(V_{\text{do}(W)} := V \setminus W\) and \(J_{\text{do}(W)} := J \cup W\).
3. Remove the functions \(g_S\) for loops \(S\) with \(S \cap W \neq \emptyset\).

The remaining functions then are clearly globally compatible and we get a well-defined iSCM \(M_{\text{do}(W)}\).

### 3 CONDITIONAL INDEPENDENCE

Here we shortly generalize conditional independence for structured families of distributions. The main application will be the distributions \((\mathbb{P}_U(X_V | \text{do}(X_J = x_j)))_{x_j \in X_J}\) coming from iSCMs, but the following definition might be of more general importance.

**Definition 3.1 (Conditional independence).** Let \(X_V := \prod_{v \in V} X_v\) and \(X_J := \prod_{j \in J} X_j\) be product spaces and

\[
\mathbb{P} := (\mathbb{P}_U(X_V | X_J))_{x_j \in X_J}
\]

a family of distributions on \(X_V\) (measurable\(^4\)) parametrized by \(X_J\). For subsets \(A, B, C \subseteq V \cup J\) we write:

\[
X_A \perp X_B | X_C
\]

if and only if for every product distribution \(\mathbb{P}_J = \bigotimes_{j \in J} \mathbb{P}_J\) on \(X_J\) we have:

\[
X_A \perp \mathbb{P}_{V \cup J} X_B | X_C, \quad \text{i.e.:}
\]

\[
\mathbb{P}_{V \cup J}(X_A | X_B, X_C) = \mathbb{P}_{V \cup J}(X_A | X_C) \mathbb{P}_{V \cup J}-a.s.,
\]

where \(\mathbb{P}_{V \cup J}(X_A | X_B, X_C) := \mathbb{P}_U(X_V | X_J) \mathbb{P}_J(X_J)\), the distribution given by \(X_J \sim \mathbb{P}_J\) and then \(X_V \sim \mathbb{P}_U\).

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\(^4\)We require that for every measurable \(F \subseteq X_V\) the map \(x_J \mapsto [0, 1]\) given by \(x_J \mapsto \mathbb{P}_V(X_V \in F | x_J)\) is measurable. Such families of distributions are also called channels or (stochastic) Markov (transition) kernels (see [14]).
Lemma 3.2. Let the situation be like in [3.7]. If $A, B, C$ are pairwise disjoint, $A \cap J = \emptyset$ and $J \subseteq B \cup C$ then we have the equivalence:

1. $X_A \perp \quad P X_B \mid X_C$, if and only if
2. $\Pr\{X_A \mid X_B = x_B, X_C = x_C\}$ is only a function of $x_C$ (for every setting of $X_A$).

Proof. Since the latter does not depend on the choice of $\Pr_J$ it clearly implies the former. Now assume the former. For every two values $x_B \neq x'_B \in X_B$ and every $x_{V \cup J \backslash B} \in X_{V \cup J \backslash B}$ put $\Pr_J := \bigotimes_{j \in B \cup J} \left( \frac{1}{2} \delta_{x_j} + \frac{1}{2} \delta_{x'_j} \right) \otimes \bigotimes_{j \in J \backslash B} \delta_{x_j}$. Since the former holds for every $\Pr_J$ of product form we get:

$$\Pr\{X_A \mid X_B, X_C\} = \Pr\{\bigcup_{J \subseteq X_B \cup X_C} \Pr\{X_A \mid X_B, X_C, \Pr_J\} \bigcup J \text{-a.s.}$$

with $\Pr\{X_A \mid X_B, X_C\}$ given by $\Pr\{X_B, X_C\}$ $\Pr_J\{X_A\}$ using $\Pr_J$ from above. The claim follows:

$$\Pr\{X_A \mid X_B, X_C\} = \Pr\{X_A \mid X_B = x_B, X_C = x_C\}.$$ 

Remark 3.3. 1. Lem. 3.2 shows that definition 3.7 generalizes the one from [26].
2. Thm. 4.4 in [2] shows that definition 3.7 also generalizes the one from [2].
3. In contrast with [2] or [26] definition 3.7 can accommodate any variable from $V$ or $J$ at any spot of the conditional independence statement.
4. $\perp \quad P$ satisfies the semi-graphoid/sepatorid axioms (see [3] or rules 1-5 in Lem. 2) for $\perp \quad P$ as these rules hold for any distribution and are preserved under conjunction.

4 σ-separation

In this section we will define σ-separation on directed mixed graphs (DMG) and present the generalized directed global Markov property stating that every iSCM will entail the conditional independencies that come from σ-separation in its induced DMG. We again will closely follow the work in [9].

Definition 4.1 (Directed mixed graph (DMG)). A directed mixed graph (DMG) $G$ consists of a set of nodes $V$ together with a set of directed edges (→) and bidirected edges (↔). In case $G$ contains no directed cycles it is called an acyclic directed mixed graph (ADMG).

Definition 4.2 (σ-Open path in a DMG). Let $G$ be a DMG with set of nodes $V$ and $C \subseteq V$ a subset. Consider a path $\pi$ in $G$ with $n \geq 1$ nodes:

$v_1 \leftrightarrow \cdots \leftrightarrow v_n$.

The path will be called C-σ-open if:

1. the endnodes $v_1, v_n \notin C$, and
2. every triple of adjacent nodes in $\pi$ that is of the form:
   
   (a) collider: $v_i \leftrightarrow v_i \leftrightarrow v_{i+1}$, satisfies $v_i \in C$,
   
   (b) left chain: $v_i \leftrightarrow v_i \leftrightarrow v_{i+1}$, satisfies $v_i \notin C$ or $v_i \in C \cap \Sc^C(v_i)$,
   
   (c) right chain: $v_i \leftrightarrow v_i \leftrightarrow v_{i+1}$, satisfies $v_i \notin C$ or $v_i \in C \cap \Sc^C(v_i)$,
   
   (d) fork: $v_i \leftrightarrow v_i \leftrightarrow v_{i+1}$, satisfies $v_i \notin C$ or $v_i \in C \cap \Sc^C(v_i)$.

Similar to d-separation we define σ-separation in a DMG.

Definition 4.3 (σ-Separation in a DMG). Let $G$ be a DMG with set of nodes $V$. Let $A, B, C \subseteq V$ be subsets.

1. We say that $A$ and $B$ are σ-connected by $C$ or not σ-separated by $C$ if there exists a path $\pi$ with some $n \geq 1$ nodes in $G$ with one endnode in $A$ and one endnode in $B$ that is C-σ-open. In symbols this statement will be written as follows:

   $$A \overset{\sigma}{\notin} B \mid C.$$ 

2. Otherwise, we will say that $A$ and $B$ are σ-separated by $C$ and write:

   $$A \overset{\sigma}{\perp} B \mid C.$$ 

Remark 4.4. 1. In any DMG we will always have that σ-separation implies d-separation, since every C-d-open path is also C-σ-open because $\{v\} \subseteq \Sc^C(v)$.
2. If a DMG $G$ is acyclic, i.e. an ADMG, then σ-separation coincides with d-separation (also called m- or m'-separation in this context).

It was shown in [8] that σ-separation satisfies the graphoid/sepatorid axioms (see [3] or [2]):

Lemma 4.5 (Graphoid and separoid axioms). Let $G$ be a DMG with set of nodes $V$ and $A, B, C, D \subseteq V$ subsets. Then we have the following rules for σ-separation in $G$ (with $\perp$ standing for $\perp^G$):

1. Redundancy: $A \perp B \mid B$ always holds.
2. Symmetry: $A \perp B \mid D \implies B \perp A \mid D$.
3. Decomposition: $A \perp B \cup C \mid D \implies A \perp B \mid D$.
4. Weak Union: $A \perp B \cup C \mid D \implies A \perp B \mid C \cup D$.
5. Contraction: $\left( A \perp B \mid C \cup D \right) \wedge \left( A \perp C \mid D \right)$

   $$\implies A \perp B \cup C \mid D.$$
6. Intersection: $\left( A \perp B \mid C \cup D \right) \wedge \left( A \perp C \mid B \cup D \right)$

   $$\implies A \perp B \cup C \mid D.$$ 

whenever $A, B, C, D$ are pairwise disjoint.
7. Composition: $\left( A \perp B \mid D \right) \wedge \left( A \perp C \mid D \right)$

   $$\implies A \perp B \cup C \mid D.$$
It was also shown that $\sigma$-separation is stable under marginalisation (see [8][9]):

**Theorem 4.6** ($\sigma$-Separation under marginalisation, see [8][2]). Let $G$ be a DMG with set of nodes $V$. Then for any sets $A, B, C \subseteq V$ and $L \subseteq V \setminus (A \cup B \cup C)$ we have the equivalence:

$$A \leadsto_G B \mid C \iff A \leadsto_{G \setminus L} B \mid C,$$

where $G \setminus L$ is the DMG that arises from $G$ by marginalising out the variables from $L$.

5 A GLOBAL MARKOV PROPERTY

The most important ingredient for our results is a generalized directed global Markov property that relates the graphical structure of any iSCM $M$ to the conditional independencies of the observed random variables via a $\sigma$-separation criterion. Since we have no access to the latent nodes $u \in U$ of an iSCM with graph $G^+$ we need to marginalize them out. This will give us an induced directed mixed graph (DMG) $G$.

**Definition 5.1** (Induced DMG of an iSCM). Let $M = (G^+, X, P_U, g)$ be an iSCM with $G^+ = (V \cup U \cup J, E^+)$.

The induced directed mixed graph (DMG) $G$ of $M$ is defined as follows:

1. $G$ contains all nodes from $V \cup J$.
2. $G$ contains all the directed edges of $G^+$ whose endnodes are both in $V \cup J$.
3. $G$ contains the bidirected edge $v \leftrightarrow w$ with $v, w \in V$ if and only if $v \neq w$ and there exists an $u \in U$ with $v, w \in Ch^-_{G^+}(u)$, i.e. $v$ and $w$ have a common latent confounder.

The following generalized directed global Markov property directly generalizes from mSCMs (see [8][9]) to iSCMs.

**Theorem 5.2** ($\sigma$-Separation criterion). Let $M$ be an iSCM with induced DMG $G$. Then for all subsets $A, B, C \subseteq V \cup J$ we have the implication:

$$A \leadsto_G B \mid C \implies X_A \perp \!
\perp_{\text{w}} X_B \mid X_C.$$

In words, if $A$ and $B$ are $\sigma$-separated by $C$ in $G$ then the corresponding variables $X_A$ and $X_B$ are conditional independent given $X_C$ under $P$, i.e. under the joint distribution $P_U(X_V, do(X_J))P_J(X_J)$ for any product distribution $P_J = \otimes_{j \in J} P_J$.

**Proof.** As mentioned, after specifying the product distribution $P_J$ the iSCM $M$ constitutes a well-defined mSCM with the same induced DMG $G$. So the $\sigma$-separation criterion for iSCMs directly follows from the mSCM-version proven in [8][9].

**Remark 5.3.** Note that, since $\sigma$-separation is stable under marginalisation (see [8][9]) also the $\sigma$-separation criterion is stable under marginalisation.

**Remark 5.4** (Causal calculus for mechanism change). The $\sigma$-separation criterion [5,2] can be viewed as the causal calculus for mechanism change (also sometimes called “soft” interventions, see [8][1][6][2][4]). As an example consider $A, B \subseteq V$, $I \subseteq J$ and $x'_I \in X_I$, $x_J \in X_J$. Then we have:

$$A \leadsto_G I \mid B \cup (J \setminus I) \implies \mathbb{P}_U(X_A|X_B, do(X_I = x'_I)) = \mathbb{P}_U(X_A|X_B, do(X_I = x_J), do(X_{J\setminus I} = x_{J\setminus I})).$$

So the graphical independence of the intervention nodes implies that the conditional probability is independent of the actual intervention on $I$.

6 CAUSAL CALCULUS FOR PERFECT INTERVENTIONS

6.1 The extended iSCM

In this section we want to consider (perfect) interventions onto the observed nodes and improve upon the general rules mentioned in [5,2]. For an elegant treatment of this we need to gather for a given iSCM $M$ all interventional iSCMs $M_{do(W)}$, where $W$ runs through all subsets of observed variables, and glue them all together into one big extended iSCM $\hat{M}$. To consider all interventions at once we will need to introduce additional intervention variables $I_v$ to the graph $G^+$, $v \in V$, which indicate which interventional mechanisms to use. Such techniques were already used in the acyclic case in [18][19][21]. The definition will be made in such a way that $\hat{M}$ will still be a well-defined iSCM. So all the results for iSCMs will apply to $\hat{M}$, most importantly the $\sigma$-separation criterion (Thm 5.2).

**Definition 6.1.** Let $M = (G^+, X, P_U, g)$ be an iSCM with $G^+ = (V \cup U \cup J, E^+)$. The extended iSCM $\hat{M} = (\hat{G}^+, \hat{X}, \hat{P}_U, \hat{g})$ will be defined as follows:

1. For every $v \in V$ define the interventional domain $I_v := X_v \cup \{\varnothing_v\}$, where $\varnothing_v$ is a new symbol corresponding to the observational (non-interventional) regime. For a set $A \subseteq V$ we put $I_A := \prod_{v \in A} I_v$ and $\varnothing_A := (\varnothing_v)_{v \in A}$.
2. Let $\hat{G}^+$ be the graph $G^+$ with the additional interventional nodes $I_v$ and directed edges $I_v \rightarrow v$ for every $v \in V$. For a uniform notation we sometimes write $I_j$ instead of $J$ for $j \in J$. So we have:
3. For every $A \subseteq V$ we define the mechanism:

$$\hat{g}_A : \hat{X}_{Pa^+(A)\setminus A} \rightarrow \hat{X}_A.$$
Consider the subgraph of $G^+$:

$$H(x_A) := \left( P^+_{A} \cup A \right)_{do(I(x_A))}. $$

Then define recursively for $v \in A$:

$$\hat{g}_A, v(x_A, x_{P^+_{A}(A)\setminus A}) := \begin{cases} x_v & \text{if } v \in I(x_A), \\ g_{S, v}(x_{P^+_{A}(A)(S), S}) & \text{if } v \notin I(x_A), \end{cases}$$

where $S := Sc^{H(x_A)}(v)$ is also a loop in $G^+$.

4. These functions then are again globally compatible and $M$ constitutes a well-defined iSCM.

5. All the distributions in $M$ then are given by the general procedure of iSCMs (see Def. 2.6). We introduce the notation for $C \subseteq V$ and $(x_C, x_J) \in \mathcal{X}_C \times \mathcal{X}_J$:

$$\mathbb{P}_U(X_V | I_C = x_C, X_J = x_J) := \mathbb{P}_U(X_V | do((I_C, I_V \setminus C, X_J) = (x_C, \emptyset_V \cup C, x_J)).$$

6. The extended DMG $\hat{G}$ of $G^+$ is then the induced DMG of $\hat{G}^+$, i.e. the induced DMG $G$ with the additional edges $I_v \rightarrow v$ for every $v \in V$.

The following result now relates the interventional distributions of the iSCM $M$ with the ones from the extended iSCM $\hat{M}$. These relations will be used in the following.

**Proposition 6.2.** Let $M = (G^+, \mathcal{X}, \mathbb{P}_U, g)$ be an iSCM with $G^+ = (V \cup U \cup J, E^+)$ and $\hat{M}$ the extended iSCM. Let $A, B, C \subseteq V$ be pairwise disjoint set of nodes and $x_{C \cup J} \in \mathcal{X}_{C \cup J}$. Then we have the equations:

$$\mathbb{P}_U(X_A | X_B, do(x_{C \cup J} = x_{C \cup J})) = \mathbb{P}_U(X_A | X_B, I_C = x_C, X_J = x_J) = \mathbb{P}_U(X_A | X_B, I_C = x_C, X_C = x_C, X_J = x_J).$$

**Proof.** Consider the first equality. For any subset $D \subseteq V$ the variable $X_D^{do(x_{C \cup J} = x_{C \cup J})}$ was recursively defined in $M_{do(C)}$ via $g$ using $G_{do(C)}$. The variable $X_D^{do(I(x_C, I_V \setminus C, X_J) = (x_C, \emptyset_V \cup C, x_J))}$ was recursively defined in $M$ via the same $g$ but using $I(x_C, \emptyset_V \setminus C)$ and $G_{do(C)}$. Since $x_C \in \mathcal{X}_C$ we have that $I(x_C, \emptyset_V \setminus C) = C$ and thus $G_{do(C)} = G_{do(C)}$. It directly follows that:

$$X_D^{do(x_{C \cup J} = x_{C \cup J})} = X_D^{do(I(x_C, I_V \setminus C, X_J) = (x_C, \emptyset_V \cup C, x_J))}.$$

This shows the equality of top and middle line. For the equality between the middle and bottom line note that:

$$I_C = x_C \quad \forall x_C \in \mathcal{X}_C \quad X_C = x_C.$$

6.2 The three main rules of causal calculus

**Notation 6.3.** Since everything has been defined in detail in the last section we now want to make use of a simplified and more suggestive notation for a better readability.

1. We identify variables $X_A$ with the set of nodes $A$.
2. We omit values $x_V$ and the subscript in $\mathbb{P}_U$. E.g. we write $P(Y | IT, T, Z, do(W))$ instead of $P(U(X_Y | IT = x_T, X_T = x_T, X_Z, do(W) = x_W).$

where the latter comes from the extended iSCM of the intervened iSCM $M_{do(W)} := M_{do(W \setminus J)}$ of $M$.

3. We write $Y \perp\!\!\!\!\perp_{G^+} Z, do(W)$ for $X_Y \perp\!\!\!\!\perp_{G_{do(W)}} X_T | X_Z, do(W)$ etc.

4. We write $Y \perp\!\!\!\!\perp_{G_{do(W)}} I_X | X, Z, do(W)$ to mean $Y \perp\!\!\!\!\perp_{G_{do(W)}} I_X | X, Z,$ where $G_{do(W)}$ is the extended DMG of the intervened graph $G_{do(W)}$.

**Theorem 6.4 (The three main rules of causal calculus).** Let $M$ be an iSCM with set of observed nodes $V$ and intervention nodes $J$ and induced DMG $G$. Let $X, Y, Z \subseteq V$ and $J \subseteq W \subseteq V \cup J$ be subsets.

1. **Insertion/deletion of observation:**

   If $Y \sigma_{G} X | Z, do(W)$ then:

   $$P(Y | X, Z, do(W)) = P(Y | Z, do(W)).$$

2. **Action/observation exchange:**

   If $Y \sigma_{G} I_X | X, Z, do(W)$ then:

   $$P(Y | do(X), Z, do(W)) = P(Y | X, Z, do(W)).$$

3. **Insertion/deletion of actions:**

   If $Y \sigma_{G} I_X | Z, do(W)$ then:

   $$P(Y | do(X), Z, do(W)) = P(Y | Z, do(W)).$$

**Proof.** 1. Thm. 2.6 applied to $G_{do(W)}$ gives:

$$Y \sigma_{G} X | Z, do(W) \quad \Huge{[\text{2}] \quad \Huge{\Rightarrow}} \quad Y \perp\!\!\!\!\perp_{G} X | Z, do(W).$$

The latter directly gives the claim:

$$P(Y | X, Z, do(W)) = P(Y | Z, do(W)).$$

2. The $\sigma$-separation criterion 2.6 w.r.t. to $G_{do(W)}$ gives:

$$Y \sigma_{G} I_X | X, Z, do(W) \quad \Huge{[\text{2}] \quad \Huge{\Rightarrow}} \quad Y \perp\!\!\!\!\perp_{p} I_X | X, Z, do(W).$$

Together with Prp. 2.6 (applied to $M_{do(W)}$) we have:

$$P(Y | do(X), Z, do(W)) = P(Y | do(X), Z, do(W)).$$

$$Y \perp\!\!\!\!\perp_{p} I_X | X, Z, do(W) \quad \Huge{[\text{2}] \quad \Huge{\Rightarrow}} \quad P(Y | X, Z, do(W)).$$
3. As before we have:
\[ Y \perp_{G} I_{X} \mid Z, \text{do}(W) \]
\[ \Rightarrow \quad Y \perp_{P} I_{X} \mid Z, \text{do}(W). \]
And again:
\[ \mathbb{P}(Y \mid \text{do}(X), Z, \text{do}(W)) \]
\[ \mathbb{P}(Y \mid I_{X}, Z, \text{do}(W)) \]
\[ \mathbb{P}(Y \mid Z, \text{do}(W)). \]

\[ \mathbb{P}(Y \mid I_{X}, Z, \text{do}(W)) \]
\[ \mathbb{P}(Y \mid Z, \text{do}(W)). \]

Remark 6.5. The conditions for aboves rules are usually phrased in terms of further graph transformations. E.g. for rule 3 in the acyclic setting one requires \( Y \perp_{G} X \mid Z, W \) in the graph \( G_{\text{do}(W)} \) that is further mutilated on the set \( X(Z) \), the set of all \( X \)-nodes that are not ancestors of any \( Z \)-node in \( G_{\text{do}(W)} \) (see [18, 19, 21]). When reduced to those acyclic settings they will be equivalent to the our formulation via \( \sigma \)-separation including the intervention nodes.

We presented the above only in terms of \( \sigma \)-separation in the extended iSCM because in this form it was clear how to generalize to arbitrary iSCMs. We also believe that the formulaic expressions in terms of \( \sigma \)-separation will be easier to parse and to remember as their relations to the claims and implications are directly visible.

6.3 The general adjustment criterion

Notation 6.6. Let \( M = (G^+, X, \mathbb{P}, g) \) be an iSCM with \( G^+ = (V \cup U \cup J, E^+) \). The following set of nodes/variables will play the described roles:

1. \( Y \): the outcome variables,
2. \( X \): the treatment or intervention variables,
3. \( Z_0 \): the core set of adjustment variables,
4. \( Z_+ \): additional adjustment variables,
5. \( L \): “latent adjustment variables”,
6. \( Z := Z_0 \cup Z_+ \): all actual adjustment variables,
7. \( C \): context variables,
8. \( W \): default intervention variables containing \( J \),
9. \( S \): variables inducing selection bias when \( S = s \).

We are interested in finding a “do(\( X \))-free” expression for the (conditional) causal effect \( \mathbb{P}(Y \mid \text{do}(X), \text{do}(W)) \) only using data for \( C, X, Y, Z \) that was organized under selection bias \( S = s \) and intervention do(\( W \)) and additional unbiased observational data for \( C, Z \) given do(\( W \)). The task can be achieved via the following criterion, which is a generalization of the acyclic case of the selection-backdoor criterion (see [1]), the backdoor criterion (see [18, 19, 21]) and its extensions (also see [3, 22, 24, 28]) to general iSCMs.

Theorem 6.7 (General adjustment criterion and formula). Let the setting be like in 6.6 Assume that data was collected under selection bias, \( \mathbb{P}(V \mid S = s, \text{do}(W)) \) (or under \( \mathbb{P}(V \mid \text{do}(W)) \)) and \( S = \emptyset \), but there are unbiased samples from \( \mathbb{P}(Z \mid C, \text{do}(W)) \). Further assume that the variables satisfy:

1. \( (Z_0, L) \perp_{G} I_{X} \mid C, \text{do}(W), \) and
2. \( Y \perp_{G} (I_{X}, Z_+) \mid C, X, Z_0, L, \text{do}(W), \) and
3. \( Y \perp_{G} S \mid C, X, Z, \text{do}(W), \) and
4. \( L \perp_{G} X \mid C, Z, \text{do}(W). \)

Then one can estimate the conditional causal effect \( \mathbb{P}(Y \mid C, \text{do}(X), \text{do}(W)) \) via the adjustment formula:

\[ \mathbb{P}(Y \mid C, \text{do}(X), \text{do}(W)) \]
\[ = \quad \int \mathbb{P}(Y \mid X, Z, C, S = s, \text{do}(W)) \, d\mathbb{P}(Z \mid C, \text{do}(W)) \]

Proof. Since \( C, \text{do}(W) \) occur everywhere as a conditioning set, we will suppress \( C, \text{do}(W) \) in the following everywhere. Then note that the \( \sigma \)-separation criterion [22] implies the corresponding conditional independencies in following when indicated. The adjustment formula then derives from the following computations:

\[ \mathbb{P}(Y \mid \text{do}(X)) \]
\[ = \quad \int \mathbb{P}(Y \mid Z_0, L, \text{do}(X)) \, d\mathbb{P}(Z_0, L \mid \text{do}(X)) \]
\[ \mathbb{P}(Y \mid Z_0, L, \text{do}(X)) \]
\[ = \quad \int \int \mathbb{P}(Y \mid X, Z_0, L) \, d\mathbb{P}(Z_0, L \mid I_{X}) \]
\[ \mathbb{P}(Y \mid X, Z_0, L) \]
\[ = \quad \int \int \int \mathbb{P}(Y \mid X, Z_0, L) \, d\mathbb{P}(Z_0, L \mid I_{X}) \]
\[ \mathbb{P}(Y \mid X, Z_0, L) \]
\[ = \quad \int \int \int \int \mathbb{P}(Y \mid X, Z_0, L) \, d\mathbb{P}(Z_0, L \mid I_{X}) \]

Remark 6.8. Note that the adjustment formula in theorem 6.7 does not depend on \( L \). This thus allows us to even choose variables for \( L \) that come from an iSCM \( M' \) that marginalizes to \( M \), e.g. \( L \subseteq U \) or by extending directed edges \( v \rightarrow w \) by \( v \rightarrow \ell \rightarrow w \) with \( \ell \in L \). This technique was used in [22] to find all adjustment sets in the acyclic case with \( S = C = \emptyset \), see below.
Causal calculus in the presence of cycles, latent confounders and selection bias

Figure 1: An induced DMG $G$ with intervention node $I_X$ (the others are left out for readability). The variables satisfy the general adjustment criterion for $P(Y|C, do(X))$ with $L = \{L_1, L_2\}$ and $Z_+ = \{Z_1, Z_2\}$. Note that $L_2$ could also have been a latent variable.

Corollary 6.9. Let the notations be like in 6.6 and 6.7 and $W = J = \emptyset$. We have the following special cases, which in the acyclic case will reduce to the ones given by the indicated references:

1. General selection-backdoor (see [3]): $C = \emptyset$, and
   (a) $(Z_0, L) \perp \perp I_X$,
   (b) $Y \perp \perp (I_X, Z_+) | X, Z_0, L$, and
   (c) $Y \perp \perp S | X, Z$, and
   (d) $L \perp \perp X | Z$, implies:
   $$P(Y|do(X)) = \int P(Y|X, Z, S = s) dP(Z).$$

2. Selection-backdoor (see [17]): $C = L = \emptyset$, and
   (a) $Z_0 \perp \perp I_X$,
   (b) $Y \perp \perp (I_X, Z_+, S) | X, Z_0$, and
   (c) $L \perp \perp X | Z$, implies:
   $$P(Y|do(X)) = \int P(Y|X, Z, S = s) dP(Z).$$

3. Extended backdoor (see [23][28]): $C = S = \emptyset$,
   (a) $(Z_0, L) \perp \perp I_X$,
   (b) $Y \perp \perp (I_X, Z_+) | X, Z_0, L$, and
   (c) $L \perp \perp X | Z$, implies:
   $$P(Y|do(X)) = \int P(Y|X, Z) dP(Z).$$

4. Backdoor (see [18][19][21]): $C = S = L = Z_+ = \emptyset$,
   (a) $Z \perp \perp I_X$,
   (b) $Y \perp \perp I_X | X, Z$, implies:
   $$P(Y|do(X)) = \int P(Y|X, Z) dP(Z).$$

A generalization of the criterion for selection without (or only partial) external data of $\emptyset$ is given in the appendix.

Remark 6.10. The conditions in theorem 6.7 and corollary 6.9 are in the acyclic setting usually phrased in terms of sub-structures of the graph $G$ (see [18][19][21]). E.g. for the backdoor criterion for a DAG $G$ instead of $L \perp \perp I_X$ we could have written that $L$ does not contain any descendent of $X$, and for $Y \perp \perp I_X | X, Z$ that $Z$ blocks all “backdoor paths” from $X$ to $Y$. As before, we presented the results only in terms of $\sigma$-separation because the relations to their use is directly indicated (e.g. in the proofs). Furthermore, the formulaic framework of $\sigma$-separation makes the generalization to arbitrary iSCMs possible.

7 TWIN NETWORKS AND COUNTERFACTUALS

We shortly want to mention that with iSCMs one can do counterfactual reasoning as well. Given an iSCM $M$ with graph $G^+ = (V \cup U \cup J, E^+)$, a set $W \subseteq V \cup J$ and $x_W \in X_W$ the corresponding intervened iSCM $M_{do(W)}$ with graph $G^+_{do(W)}$ and distribution $\delta_{x_W}$ on $W$ one can construct a (merged) twin iSCM $M_{twin}$ similarly to the acyclic case (see [21]). This is done by identifying/merging the nodes, mechanisms and variables from the non-descendents of $W$, NonDesc$^+ (W)$ and NonDesc$^+_{do(W)} (W)$, which are unchanged by the action do$ (x_W)$. Then one has the two different branches Desc$^+ (W)$ and Desc$^+_{do(W)} (W)$ in the network. This construction then allows one to formulate counterfactual statements like in the acyclic case (see [21]), but now for general iSCMs. E.g. one could state the assumption of strong ignorability (see [21][24]) as:

$$\left( y_{do(x=W)} \right) \sigma_{\text{G}_{\text{twin}}} X | Z.$$

All the causal reasoning rules derived so far can thus also be applied to reason about counterfactuals.

8 CONCLUSION

We proved the three main rules of causal calculus and general adjustment criteria with corresponding formulas to recover from interventions and selection bias for general iSCMs, which allow for arbitrary probability distributions, non-/linear functional relations, latent confounders, external non-/probabilistic parameter/action/intervention nodes and cycles. This generalizes all the corresponding results of acyclic causal models (see [1][18][19][21][23][24][28]) to general iSCMs. Future work might address completeness
questions (see [12,21,29]) and extensions of Tian’s algorithm for identifiability (see [10,12,13,21,26,30,32]) to general iSCMs.

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References


SUPPLEMENTARY MATERIAL

A  MORE ON ADJUSTMENT CRITERIA

The following generalizes the adjustment criterion of type I in \cite{3}.

**Theorem A.1** (General adjustment without external data). Let the setting be like in \cite{6,6}. Assume that data was collected under selection bias, $\mathbb{P}(V|S = s)$. Further assume that the variables satisfy:

1. $Y \perp S \mid do(X)$,
2. $Z_0 \perp I_X \mid S$,
3. $Y \perp Z_+ \mid Z_0, S, do(X)$,
4. $Y \perp I_X \mid X, Z, S$.

Then one can estimate the causal effect $\mathbb{P}(Y|do(X))$ via the following adjustment formula from the biased data:

$$\mathbb{P}(Y|do(X)) = \int \mathbb{P}(Y|X, Z, S = s) \, d\mathbb{P}(Z|S = s).$$

**Proof.** First note that the $\sigma$-separation criterion \cite{2} implies the corresponding conditional independencies in following when indicated. We implicitly make use of proposition \cite{2} when needed. The adjustment formula then derives from the following computations:

$$Y \perp S \mid do(X) \quad \implies \quad \mathbb{P}(Y|do(X)) = \mathbb{P}(Y|S, do(X))$$

chain rule

$$Z_0 \perp I_X \mid S \quad \implies \quad \int \mathbb{P}(Y|Z_0, S, do(X)) \, d\mathbb{P}(Z_0|S, do(X))$$

\cite{2}

$$Y \perp Z_+ \mid Z_0, S, do(X) \quad \implies \quad \int \mathbb{P}(Y|Z_+, Z_0, S, do(X)) \, d\mathbb{P}(Z_+, Z_0|S)$$

\cite{2}

$$Y \perp I_X \mid X, Z, S \quad \implies \quad \int \mathbb{P}(Y|Z, S, X) \, d\mathbb{P}(Z|S).$$

The following theorem generalizes the adjustment criterion of type III in \cite{4}. For this we have to introduce even more adjustment sets: $Z_0^A, Z_0^B, Z_1^A, Z_1^B, Z_2, Z_3$ and $L_0, L_1$.

**Theorem A.2** (General adjustment with partial external data). Assume that data was collected under selection bias, $\mathbb{P}(V|S = s)$, but we have unbiased data from $\mathbb{P}(Z_{\leq 1}^B)$.

Further assume the conditions that are indicated on the equality signs in the proof. Then we have the adjustment formula:

$$\mathbb{P}(Y|do(X)) = \int \int \mathbb{P}(Y|S = s, Z, X) \, d\mathbb{P}(Z\setminus Z_{\leq 1}^B|S = s, Z_{\leq 1}^B) \, d\mathbb{P}(Z_{\leq 1}^B).$$

Note that this formula does not depend on $L_1$ and $L_2$. So $L_1$ and $L_2$ can be chosen in a graph $G'$ that marginalizes to $G$.

**Proof.**
\[ Z_{\leq 2} = Z_{\leq 1} \cup Z_2 \]

\[
\int P(Y|L_1, S, Z_{\leq 2}, \text{do}(X)) d(P(L_1, Z_2|S, Z_{\leq 1}, \text{do}(X)))
\]

\[
dP(Z^A|S, Z_{\leq 1}) dP(Z^B
\]

\[
Z = Z_{\leq 1} \cup Z_3
\]

\[
\int P(Y|L_1, S, Z, \text{do}(X)) dP(L_1|S, Z)
\]

\[
dP(Z \setminus Z^B_{\leq 1}|S, Z^B_{\leq 1}) dP(Z^B_{\leq 1})
\]

\[
Y \perp I_X \mid S, Z_{\leq 1}
\]

\[
\int P(Y|L_1, S, Z_{\leq 2}, \text{do}(X)) dP(L_1, Z_2|S, Z_{\leq 1})
\]

\[
dP(Z^A|S, Z_{\leq 1}) dP(Z^B|Z_{\leq 1})
\]

\[
\text{chain rule}
\]

\[
\int P(Y|L_1, S, Z, \text{do}(X)) dP(L_1|S, Z, \text{do}(X))
\]

\[
dP(Z \setminus Z^B_{\leq 1}|S, Z^B_{\leq 1}) dP(Z^B_{\leq 1})
\]

\[
\text{chain rule}
\]

\[
\int P(Y|S, Z, \text{do}(X)) dP(Z \setminus Z^B_{\leq 1}|S, Z^B_{\leq 1}) dP(Z^B_{\leq 1})
\]

\[
Y \perp I_X \mid X, S, Z
\]

\[
\int P(Y|S, Z, X) dP(Z \setminus Z^B_{\leq 1}|S, Z^B_{\leq 1}) dP(Z^B_{\leq 1})
\]

\[\square\]