Variable Definition and Independent Components

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Abstract

In the causal modelling literature, it is well known that "ill-defined" variables may give rise to "ambiguous manipulations" (Spirtes and Scheines, 2004). Here, we illustrate how ill-defined variables may also induce mistakes in causal inference when standard causal search methods are applied (Spirtes et al., 2000; Pearl, 2009). To address the problem, we introduce a representation framework, which exploits an *independent component representation* of the data, and demonstrate its potential for detecting ill-defined variables and avoiding mistaken causal inferences.
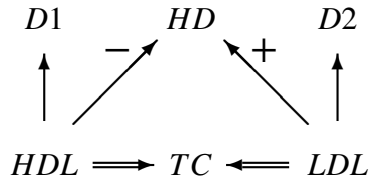
$$D1 \qquad HD \qquad D2$$

$$HDL \Longrightarrow TC \Longleftarrow LDL$$

Figure 1: A structure where the manipulation on TC with respect to HD is "ambiguous".

1 The Problem of Variable Definition

Some choices of variables may lead to less informative, or even false, causal claims. This problem was pointed out by, among others, Spirtes and Scheines (2004), Eberhardt (2016), and Woodward (2016). Here is a classic example by Spirtes and Scheines (2004). Consider the following hypothetical data generating process (Figure 1). Total cholesterol (TC) is a deterministic function (e.g., the sum) of two variables, viz. low-density lipoproteins (LDL) and high-density lipoproteins (HDL), respectively known as "bad" and "good" cholesterol. The two cholesterols, in fact, have different causal roles: LDL causes heart disease (HD), while HDL prevents it. Moreover, assume that HDL and LDL cause, respectively, a disease called "disease 1" ($D1$) and a disease called "disease 2" ($D2$). Spirtes and Scheins point out that, if only TC, but neither HDL nor LDL is observed, a manipulation of TC with respect to HD is "ambiguous", because it leaves underdetermined the values of TC's underlying determinants, such that the effect on HD is unpredictable.

More generally, in applied causal inference, often the variables under study are, like TC, functions of other variables with heterogeneous causal roles. For example, in macroeconomics a researcher deals with aggregate variables such as gross domestic product, foreign sales, total imports, etc., which are sums or averages of other variables, whose individual causal roles may be multifarious and opaque to the researcher. Often, the researcher is unable to observe the

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underlying micro-behaviours simply because statistical agencies provide aggregate data, but do not reveal information on the single units. In other cases, collecting micro data may be too complex or costly. Treating aggregate variables as if they had a homogeneous causal role, however, may lead to less informative or false causal claims, as shown by the TC example. We shall refer to an aggregate variable incurring such problems as *ill-defined*. Notice, thus, that whether a variable is ill-defined is relative to a variable set. That is, it may be ill-defined in a set but well-defined in another.

The problem of variable definition is often underestimated by the wider public. For instance, not sufficient attention has been paid to its consequences for causal inference by constraint-based discovery methods (Spirtes et al., 2000; Pearl, 2009). We shall return to this point in the next section, by showing how the presence of TC in a variable set may lead to wrong causal inferences. To address the problem, we introduce a representation framework—the "independent component" representation—for modelling structures containing two kinds of dependencies, namely traditional causal dependencies between well-defined variables, and dependencies between ill-defined variables and their determinants (see, e.g., Figure 1). Next, we demonstrate the potential of this framework for identifying ill-defined variables and reducing the risk of mistaken causal inferences.

2 Causal Search with Ill-defined Variables

The last decades have witnessed the development and popularization of constraint-based discovery methods for causal inference (Spirtes et al., 2000; Pearl, 2009). In this framework, a causal structure is represented as a triple $\langle \mathbf{V}, \mathcal{E}, \Pr \rangle$, where $\langle \mathbf{V}, \mathcal{E} \rangle$ is a directed acyclic graph (DAG) consisting of a set $\mathbf{V}$ of variables and a set $\mathcal{E}$ of edges among them, and $\Pr$ is the

probability distribution over **V** associated to the DAG. Pr is assumed to comply with the Causal Markov Condition (CMC) and, typically, the Causal Faithfulness Condition (CFC). CMC says that

(CMC) For any $V_i \in \mathbf{V} = \{V_1, \ldots, V_n\}$, $V_i \perp\!\!\!\perp \mathbf{Non_i} | \mathbf{Par_i}$,

where $\mathbf{Par_i}$ denotes the set of parents (direct causes) of V_i, and $\mathbf{Non_i}$ denotes the set of non-descendants (non-effects) of V_i. In words, each variable is probabilistically independent of its non-effects, conditional on its direct causes. CMC presupposes that for every pair of variables in **V**, every common direct cause of the pair is in **V** or has the same value for all units in the population (causal sufficiency). CFC says:

(CFC) $\langle \mathbf{V}, \mathcal{E}, \text{Pr} \rangle$ is such that every conditional independence relation true in Pr is entailed by CMC applied to the true DAG $\langle \mathbf{V}, \mathcal{E} \rangle$.

CFC ensures that there is no causal dependence without probabilistic dependence, that is, all probabilistic independencies in the DAG correspond to causal independencies.

Based on these assumptions, constraint-based discovery methods are designed to recover the causal structure from data, by identifying conditional independencies among variables and then causally connecting variables not found to be independent. We shall now consider examples of simple data generating processes including one ill-defined variable, TC, and show how using constraint-based methods based on conditional independencies—whilst ignoring that TC is ill-defined—may lead to mistakes. To anticipate, such mistakes involve apparent violations of CMC or CFC, which the search methods presuppose. Notice, however, that our interest here is not in providing novel counterexamples to CMC and CFC. These violations, in fact, could be avoided by choosing a "more suitable" variable set for causal inference—in this case, one

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featuring *HDL* and *LDL* instead of *TC*. And indeed, a formulation of CMC requiring that variables be independent of their non-effects conditional on their *well-defined* direct causes would not incur any violation. In this paper, however, we do not want to presuppose what counts as an ill-defined variable or a suitable variable set. Our goal is to avoid mistaken causal inferences *in virtue of detecting ill-defined variables*.

Suppose that, in $\mathbf{V} = \{X, Y, Z\}$, Y is the non-deterministic cause of both X and Z, viz. the true structure is $X \longleftarrow Y \longrightarrow Z$. If all variables are well-defined, one can infer some properties of the causal structure by testing conditional independencies and applying a constraint-based discovery method. In particular, the independence $X \perp\!\!\!\perp Z \mid Y$ and CFC allow one to exclude $X \longrightarrow Y \longleftarrow Z$ from the set of possible structures. Now, let the set of observed variables be $\mathbf{V}' = \{TC, D1, D2\}$. That is, suppose again that one does not observe or measure *LDL* and *HDL*, but only *TC*. In this case, too, the true structure is not a collider. Assuming that the dependencies over $\mathbf{V}'$ are causally interpretable, the most plausible structure—the one we wish to rationalize in this paper—would be a common cause, viz. $D1 \longleftarrow TC \longrightarrow D2$. However, since *HDL* and *LDL* are independent, $LDL \perp\!\!\!\perp HDL$, it follows that $D1$ and $D2$ are independent, too, viz. $D1 \perp\!\!\!\perp D2$. If the true structure is a common cause, this contradicts CFC, which would entail a dependence between the effects of the common cause. Moreover, being $D1$ and $D2$ dependent on (respectively) *LDL* and *HDL*, $D1$ and $D2$ become dependent upon conditioning on TC, viz. $D1 \not\perp\!\!\!\perp D2 \mid TC$. For example, suppose one knows that one patient's total cholesterol has increased. Then, knowing that disease 1 is absent gives one relevant information to predict that disease 2 is present. If the true structure is a common cause, this conditional dependence would violate CMC, which would entail the independence of $D1$ and $D2$ given their common cause. Based on $D1 \perp\!\!\!\perp D2$ and $D1 \not\perp\!\!\!\perp D2 \mid TC$, as well as $TC \not\perp\!\!\!\perp D1$ and $TC \not\perp\!\!\!\perp D2$, a constraint-based algorithm (e.g., PC, FCI; Spirtes et al. 2000) will infer an unshielded collider

on TC, viz. $D1 \longrightarrow TC \longleftarrow D2$. A researcher applying the algorithm without knowing that TC is the sum of HDL and LDL (which are causes of, respectively, $D1$ and $D2$) will thus infer the wrong structure. The reason, ultimately, is that TC is ill-defined in $\mathbf{V}'$.

Similarly, assume that all variables in $\mathbf{V}$ are well-defined, but now X causes Y, and Y causes Z, viz. the true structure is $X \longrightarrow Y \longrightarrow Z$. Under CMC, it holds $Z \perp\!\!\!\perp X \mid Y$, and under CFC, it holds $X \not\perp\!\!\!\perp Z$. Now, consider the set of observed variables $\mathbf{V}'' = \{Da, TC, D1\}$, where Da (not represented in Figure 1), denoting dairies, is a cause of LDL but not of HDL. Again, suppose that one observes TC but neither HDL nor LDL. Here, too, the true structure is not a collider. The most plausible causal interpretation of the dependencies over $\mathbf{V}''$ is a directed path, viz. $Da \longrightarrow TC \longrightarrow D1$. However, since Da is a cause of LDL, which is independent of the cause HDL of $D1$, it holds $Da \perp\!\!\!\perp D1$, which violates CFC. Moreover, it holds $Da \not\perp\!\!\!\perp D1 \mid TC$, which violates CMC. From this, one may again wrongly infer a collider on TC, viz. $Da \longrightarrow TC \longleftarrow D1$. Ultimately, the reason is that TC ill-defined in $\mathbf{V}''$.

These simple examples show how conditional independencies are sensitive to the presence of ill-defined variables in fork and chain structures[1] but ill-defined variables are undetectable from conditional independencies only. This may lead to mistaken inferences (viz. the inference of colliders) if one unreflectively applies constraint-based algorithms.

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[1]By contrast, no mistake occurs if TC is truly a collider. For instance, the inferred structure over $\mathbf{V}''' = \{Da, TC, Ol\}$, where Ol (olive oil) causes HDL but not LDL, is $Da \longrightarrow TC \longleftarrow Ol$, as it should be.

3 A Novel Representation Framework

We now introduce a series of definitions, which will allow us to precisely define the notion of ill-defined variable. First, we introduce a class of data generating mechanisms inducing the problem of ill-defined variables. We call them "augmented" structural causal models, by which we extend the traditional notion of structural causal models (Pearl, 2009; Peters et al., 2017) to structures including deterministic assignments.

Augmented structural causal model   An *augmented structural causal model* $\mathfrak{C} := (\mathbf{A}_W, \mathbf{A}_I, \mathrm{Pr})$ consists of a collection $\mathbf{A}_W$ of m assignments, a collection $\mathbf{A}_I$ of k assignments, and a probability distribution Pr such that:

(i) the collection of $\mathbf{A}_W$ consists of assignments

$$W_i := f_i(\mathbf{Par_i}, S_i), \quad \text{for } i = 1, \ldots, m,$$

where $\mathbf{Par_i} \subseteq \mathbf{W} \backslash \{W_i\}$ are called the parents of W_i, and S_i are called *noises*, or *shocks*;

(ii) Pr over $\mathbf{S} = \{S_1, \ldots, S_m\}$ is such that the shocks are mutually independent, viz. $\mathrm{Pr}(\mathbf{S}) = \mathrm{Pr}(S_1) \cdot \ldots \cdot \mathrm{Pr}(S_m)$; hence, the S_i are also called *independent components*;

(iii) the collection of $\mathbf{A}_I$ consists of assignments

$$I_i := f_i(\mathbf{Det_i}), \quad \text{for } i = 1, \ldots, k,$$

where $\mathbf{Det_i} \subset \mathbf{V}$ are called *determinants* of I_i.

$\mathfrak{C}$ is defined over a set of variables $\mathbf{V} = \mathbf{W} \cup \mathbf{I}$ with cardinality $n = m + k$. We associate to $\mathfrak{C}$ a graph $\mathcal{G}_V$ (see, e.g. the graph in Figure 1, where TC is the only variable with a deterministic assignment). $\mathcal{G}_V$ is obtained by creating a node for each element of $\mathbf{V}$, and by drawing a directed edge $\longrightarrow$ from each parent in $\mathbf{Par_i}$ (if not empty) to W_i, and a *modified* directed edge $\Longrightarrow$ from each determinant in $\mathbf{Det_i}$ to I_i. Henceforth, we restrict our attention to acyclic structures, such that $\mathcal{G}_V$ is a *modified* DAG, to cases where $\mathbf{Det_i}$ has at least two elements, and to assignments $\mathbf{A}_W$ in which the shocks are additive. For simplicity, we also assume that no pair of variables I_i, I_j in $\mathbf{I}$, $I_i \neq I_j$, are linked in $\mathcal{G}_V$ by a bidirected modified "active" (i.e., without colliders) path $I_i \Longleftarrow \cdots \Longrightarrow I_j$.

By replacing all modified directed edges $\Longrightarrow$ with standard edges $\longrightarrow$, $\mathcal{G}_V$ becomes a standard DAG, labelled $\widetilde{\mathcal{G}}_V$. By removing from $\mathcal{G}_V$ the nodes in $\mathbf{I}$ and the edges connecting $\mathbf{I}$ to $\mathbf{W}$, we obtain a subgraph of $\mathcal{G}_V$, which we denote $\mathcal{G}_W$.

Let us now introduce a particular graph associated with $\mathfrak{C}$, which we call independent component (IC) representation, or $\mathcal{G}^{IC}$. $\mathcal{G}^{IC}$ contains edges between shocks and endogenous variables but not among endogenous variables themselves. Despite this apparent limitation, the information in $\mathcal{G}^{IC}$ shall be key to the purpose of our paper. Although here we are not concerned with how $\mathcal{G}^{IC}$ is recovered, we should mention that there exist powerful statistical learning techniques, such as Independent Component Analysis (ICA) (Hyvärinen et al., 2001), which under certain assumptions (viz., non-Gaussianity) infer the dependence coefficients, and thus identify the absence of dependencies, between shocks and endogenous variables in $\mathfrak{C}$, and thereby recover the edges in $\mathcal{G}^{IC}$.

IC representation   Consider $\mathfrak{C} := (\mathbf{A}_W, \mathbf{A}_I, \mathrm{Pr})$, with $\mathbf{V} = \mathbf{W} \cup \mathbf{I}$, *card*$(\mathbf{V}) = n = m + k$. An *IC representation* of $\mathfrak{C}$ is a DAG $\mathcal{G}_V^{IC} = \langle \mathbf{V} \cup \mathbf{S}, \mathcal{E}^{IC} \rangle$ such that $\mathcal{E}^{IC}$ consists of the following
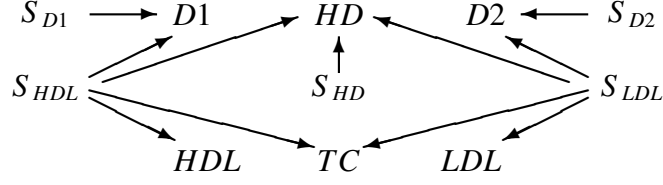
Figure 2: $\mathcal{G}_V^{IC}$ corresponding to the DAG $\mathcal{G}_V$ in Figure 1.

edges: (i) $S_i \longrightarrow W_i$, for any $i = 1, \ldots, m$; (ii) $S_i \longrightarrow W_j$, for any $i \neq j$ such that there is a directed standard path $W_i \longrightarrow \cdots \longrightarrow W_j$ in $\mathcal{G}_V$; (iii) $S_i \longrightarrow I_h$, for any $S_i \in \mathbf{S}$ and any $I_h \in \mathbf{I}$ such that there is a directed modified path $W_i \Longrightarrow \cdots \Longrightarrow I_h$ in $\mathcal{G}_V$; (iv) $S_i \longrightarrow I_h$, for any $S_i \in \mathbf{S}$ and any $I_h \in \mathbf{I}$ such that from W_i to I_h in $\mathcal{G}_V$ there is a directed standard path followed by a directed modified path with the same orientation, $W_i \longrightarrow \cdots \Longrightarrow I_h$.

Let us illustrate this definition relative to Figure 2, where $\mathbf{W} = \{HDL, LDL, D1, D2, HD\}$ and $\mathbf{I} = \{TC\}$. (i) There is a shock for each variable in $\mathbf{W}$. Some shocks (e.g., S_{D1}) only hit one variable ($D1$). Other are common to multiple variables. (ii) For any variable (e.g., HDL), its shock (S_{HDL}) also hits all of its descendants, if any ($D1, HD$). (iii) Any shock to a determinant of a variable I_i in $\mathbf{I}$ (e.g., S_{HDL}) also hits I_i (TC). (iv) If $\mathbf{V}$ contained a cause of a determinant of I_i (e.g., dairies, Da, which causes LDL), its shock (S_{Da}) would also hit I_i (TC).

One may also define $\mathcal{G}^{IC}$ relative to any subset $\mathbf{O}$ of variables in $\mathbf{V}$, namely $\mathcal{G}_O^{IC} = \langle \mathbf{O} \cup \mathbf{S}_O, \mathcal{E}_O^{IC} \rangle$. $\mathbf{S}_O$ is obtained by removing from $\mathbf{S}$ those shocks, which $\mathfrak{C}$ assigns to variables in $\mathbf{W}$ that are not in $\mathbf{O}$, and by adding those shocks, which $\mathfrak{C}$ assigns to variables in $\mathbf{W}$ that are determinants of variables in $\mathbf{I} \cap \mathbf{O}$. $\mathcal{E}_O^{IC}$ is obtained by removing from $\mathcal{E}^{IC}$ all of those edges, whose tails are not in $\mathbf{S}_O$. For any variable set $\mathbf{O}$, we call "idiosyncratic" a shock to a variable X in $\mathcal{G}_{\mathbf{O}}^{IC}$ that is a parent of X and of no other variable. We may now define *ill*- and *well*-defined variables:

Ill- and well-defined variables   Let $\mathfrak{C}$ over $\mathbf{V} = \mathbf{W} \cup \mathbf{I}$ contain the assignment $I := f(\mathbf{Det}_I)$, $card(\mathbf{Det}_I) \geq 2$. Let $\mathbf{Des}_I$ denote the set of all descendants of determinants of I in $\mathcal{G}_V$.[2] Assume $I \in \mathbf{O} \subseteq \mathbf{V}$. Then, I is *ill-defined* in $\mathbf{O}$ if and only if, for some $Des_j \in \mathbf{Des}_I$, there exists a variable Y such that (i) $Y \in \mathbf{O}$, (ii) $Y \neq I$, (iii) Y belongs to a (possibly empty) active path from Det_i to Des_j in $\mathcal{G}_V$ (viz. $Det_i \longrightarrow \cdots \longrightarrow Des_j$ or $Det_i \longrightarrow \cdots \Longrightarrow Des_j$), and (iv) $\mathcal{G}^{IC}_{\{I,Y\}}$ contains no shock S_Y common to I, Y, for which $S_Y \perp\!\!\!\perp Y|I$ in $\mathfrak{C}$. Any variable in $\mathbf{O}$ that is not ill-defined in $\mathbf{O}$ is *well-defined* in $\mathbf{O}$.

For instance, TC is well-defined in $\{Da, TC\}$ because Da is neither a determinant of TC nor a descendant of a determinant of TC, and vice versa. By contrast, TC is ill-defined in $\{HDL, TC\}$ because HDL is a determinant of TC, and $S_{HDL} \not\perp\!\!\!\perp HDL|TC$; also, TC is ill-defined in $\{TC, D1\}$ and $\{TC, HD\}$ because $D1$ and HD are effects of determinants of TC, and (respectively) $S_{D1} \not\perp\!\!\!\perp D1|TC$ and $S_{HD} \not\perp\!\!\!\perp HD|TC$. More generally, a variable I is ill-defined in $\mathbf{O}$ if and only if $\mathbf{O}$ also contains a variable Y among I's determinants or their descendants, and $\mathcal{G}^{IC}_{\{I,Y\}}$ contains no shock S_Y on I, Y, such that I screens off S_Y from Y in $\mathfrak{C}$. This lack of screening off intuitively captures the idea that a manipulation of I with respect to Y is ambiguous. In turn, to explain the lack of screening off, we need the following Proposition (proof in Appendix):

Proposition 1   Let $\mathfrak{C}$ over $\mathbf{V} = \mathbf{W} \cup \mathbf{I}$ contain the assignment $I := f(\mathbf{Det}_I)$, $card(\mathbf{Det}_I) \geq 2$. Assume CMC and CFC in $\mathcal{G}_W$. Then, for any Det_i, Des_i, Anc_i, where Des_i is a descendant of Det_i, and Anc_i is an ancestor of Det_i, it holds $Anc_i \not\perp\!\!\!\perp Des_i|I$, except for a parameter set Θ

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[2]Notice that $\mathbf{Det}_I \subseteq \mathbf{Des}_I$ by definition of "descendant".

(characterizing the assignments in $\mathfrak{C}$) that violates CFC in $\widetilde{\mathcal{G}}_V$.[3]

We can also define a graph $\mathcal{G}_O = \langle \mathbf{O}, \mathcal{E}_O \rangle$ representing the structure over $\mathbf{O}$, where $\mathcal{E}_O$ consists of the following edges. First, $\mathcal{G}_O$ has a modified edge $X \Longrightarrow Y$ if and only if there is a directed path $X \Longrightarrow \cdots \Longrightarrow Y$ in $\mathcal{G}_V$, and no variable between X and Y is in $\mathbf{O}$. Next, let the tail $\diamond$ of the arrow $X \diamond\!\!\longrightarrow Y$ indicate that X is ill-defined in $\{X, Y\}$. Then, $\mathcal{G}_O$ has an edge $X \diamond\!\!\longrightarrow Y$ for any $\langle X, Y, Z \rangle$ for which $X, Y \in \mathbf{O}$, $Z \in \mathbf{V}$, $Z \notin \mathbf{O}$, and $\mathcal{G}_V$ features a path $X \Longleftarrow Z \longrightarrow Y$, *unless* $\mathcal{G}_O^{IC}$ has a shock S common to X, Y for which $S \perp\!\!\!\perp Y | X$ in $\mathfrak{C}$, in which case $X \longrightarrow Y$ is in $\mathcal{G}_O$. Furthermore, $\mathcal{G}_O$ has a standard edge $X \longrightarrow Y$ if $\mathcal{G}_V$ has a directed path from X to Y featuring standard edges $\longrightarrow$ and/or modified edges $\Longrightarrow$, and no variable between X and Y is in $\mathbf{O}$. Finally, $\mathcal{G}_O$ has a bidirected edge $X \longleftrightarrow Y$ if and only if $\mathcal{G}_V$ has an active path $X \longleftarrow \cdots \longleftarrow Z \longrightarrow \cdots \longrightarrow Y$ featuring standard or modified edges, and only X, Y on that path are in $\mathbf{O}$. No further edges are in $\mathcal{G}_O$.

Illustrated in relation to Figure 1, $\mathcal{G}_{\{HDL,TC,LDL\}}$ is $HDL \Longrightarrow TC \Longleftarrow LDL$, and $\mathcal{G}_{\{HDL,LDL,HD\}}$ is $HDL \longrightarrow HD \longleftarrow LDL$. The two problematic structures with ill-defined variables from §2, namely $\mathcal{G}_{\{TC,D1,D2\}}$ and $\mathcal{G}_{\{Da,TC,D1\}}$, are represented as, respectively, $D1 \longleftrightarrow\!\!\diamond TC \diamond\!\!\longrightarrow D2$ and $Da \longrightarrow TC \diamond\!\!\longrightarrow D1$. Finally, let us define the notions of ill- and well-defined *causes*:

Ill- and well-defined causes   For any $X, Y \in \mathbf{O}$, X is an *ill-defined cause* of Y in $\mathbf{O}$ if and only if $\mathcal{G}_{\{X,Y\}}$ contains the edge $X \diamond\!\!\longrightarrow Y$. For any $X, Y \in \mathbf{O}$, X is a *well-defined cause* of Y in $\mathbf{O}$ if and only if Y is well-defined in $\{X, Y\}$, and $\mathcal{G}_{\{X,Y\}}$ contains the edge $X \longrightarrow Y$.

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[3]We do *not* assume CFC in $\widetilde{\mathcal{G}}_V$. For such a Θ, I counts as well-defined in our framework, as the manipulation of I with respect to Des_i is not ambiguous.

For instance, *HDL* is a well-defined cause of *HD* in $\{HDL, HD\}$.[4] By contrast, *TC* is an ill-defined cause of *HD* in $\{TC, HD\}$.

4 Identification

We now illustrate the applicability of our framework to detecting ill-defined variables and improving causal inference. We begin with a condition, under which one may unambiguously identify ill-defined variables.

Proposition 2: Sufficient condition for ill-definedness   Consider $\mathfrak{C}$ over $\mathbf{V}$, and $\mathbf{O} = \{X, Y, Z\} \subseteq \mathbf{V}$. Assume CMC and CFC in $\mathcal{G}_W$. Also assume (i) $X \perp\!\!\!\perp Z$, (ii) $X \not\!\perp\!\!\!\perp Y$, $Y \not\!\perp\!\!\!\perp Z$, $X \not\!\perp\!\!\!\perp Z|Y$, and (iii) $\mathcal{G}_O^{IC}$ has no idiosyncratic shock on Y. Then, Y is ill-defined in $\mathbf{O}$ with two determinants in $\mathbf{V}$, and $\mathcal{G}_O$ is $X \longleftrightarrow Y \diamond\!\!\longrightarrow Z$.

For instance, applied to $\mathbf{V}' = \{TC, D1, D2\}$, this condition establishes that TC is an ill-defined common cause of $D1$ and $D2$, viz. $D1 \longleftrightarrow TC \diamond\!\!\longrightarrow D2$, since $D1 \perp\!\!\!\perp D2$, $D1 \not\!\perp\!\!\!\perp TC$, $TC \not\!\perp\!\!\!\perp D2$, $D1 \not\!\perp\!\!\!\perp D2|TC$, and $\mathcal{G}_{V'}^{IC}$ has no idiosyncratic shock to TC. Proposition 2 is easily generalizable to cases with more than two determinants.

If one observes no effects of independent determinants of the ill-defined variable, for instance in $\mathbf{V}'' = \{Da, TC, D1\}$, the above condition is not applicable. Nonetheless, one may still reduce the ambiguity concerning ill-defined variables and partially recover the causal structure. To this end, let us assume that *d*eterminism induces *d*ependencies (DD):

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[4]At the same time, *HDL* is not a (well-defined) cause of TC in $\{HDL, TC\}$, because TC is not well-defined in that set.

(DD) For any I and any $Det_i \in \mathbf{Det}_I$ in $\mathfrak{C}$, it holds $I \not\perp\!\!\!\perp Det_i$.

In words, there are probabilistic dependencies between variables with deterministic assignments and their determinants. This assumption is only violated by cancelling paths from determinants to determined variables. Its satisfaction requires (similarly to CFC) the absence of special parameterizations. For simplicity, we also assume that $\mathbf{O}$ contains no determinants of variables in $\mathbf{O}$, such that $\mathcal{E}_O$ contains no modified edges $\Longrightarrow$.[5] Then, one may identify well-defined variables:

Proposition 3: Sufficient condition for well-definedness Consider $\mathfrak{C}$ over $\mathbf{V}$, and $\mathbf{O} \subseteq \mathbf{V}$. Assume DD. Assume CMC and CFC in $\mathcal{G}_W$. Assume that no determinant of ill-defined variables in $\mathbf{O}$ is in $\mathbf{O}$. Then, a variable X is well-defined in $\mathbf{O}$ if for any Y in $\mathbf{O}$, $X \neq Y$, one of (i)–(iv) holds: (i) $X \perp\!\!\!\perp Y$; (ii) in $\mathcal{G}^{IC}_{\{X,Y\}}$ X is not a child of an idiosyncratic shock, and X, Y are children of a common shock S, such that $S \perp\!\!\!\perp Y|X$; (iii) in $\mathcal{G}^{IC}_{\{X,Y\}}$ X is the only child of an idiosyncratic shock; (iv) in $\mathcal{G}^{IC}_{\{X,Y\}}$, X, Y are children of idiosyncratic shocks, and there is $\mathbf{Z} \subset \mathbf{O}$ such that $X \perp\!\!\!\perp Y|\mathbf{Z}$ and no $Z_i \in \mathbf{Z}$ is the child of an idiosyncratic shock in $\mathcal{G}^{IC}_{\{X,Z_i\}}$.

For instance, Da (which, to recall, causes LDL but not HDL) is well-defined in $\mathbf{V}''$, since (i) $Da \perp\!\!\!\perp D1$, and (ii) $\mathcal{G}^{IC}_{\{Da,TC\}}$ contains a shock S common to Da, TC, such that $S \perp\!\!\!\perp TC|Da$, and no idiosyncratic shock to Da, from which one may infer $Da \longrightarrow TC$. Next, one can identify putative ill-defined variables:

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[5]Of course, there is no a priori guarantee that $\mathbf{O}$ contains no determinants. Although one could easily relax this assumption, and thereby obtain a more general result, this would require a lengthier proof. For reasons of space, here we prioritize simplicity over generality.

Proposition 4: Necessary condition for ill-definedness Consider $\mathfrak{C}$ over $\mathbf{V}$ and its associated graph $\mathcal{G}_V$. Assume DD. Assume CMC and CFC in $\mathcal{G}_W$. Let X be ill-defined in $\mathbf{O} = \{X, Y\}$ with $\mathbf{Det}_X \cap \mathbf{O} = \emptyset$, $\mathbf{O} \subseteq \mathbf{V}$. Then: (i) $X \not\perp\!\!\!\perp Y$; (ii) in $\mathcal{G}_O^{IC}$ X, Y are children of a common shock; (iii.a) in $\mathcal{G}_O^{IC}$ X is child of an idiosyncratic shock, *or* (iii.b) in $\mathcal{G}_O^{IC}$ X is not a child of an idiosyncratic shock and there is a set of shocks $\mathbf{S}$ on X such that $X \perp\!\!\!\perp Y | \mathbf{S}$.

For instance, TC and $D1$ are such that (i) $TC \not\perp\!\!\!\perp D1$. Moreover, in $\mathcal{G}_{\{TC,D1\}}^{IC}$ they are (ii) children of a common shock and (iii.a) children of idiosyncratic shocks. Therefore, TC and $D1$ qualify as putatively ill-defined. Assuming the absence of bidirected modified paths, $\mathcal{G}_{\{TC,D1\}}$ cannot be $TC \Longleftarrow \cdots \Longrightarrow D1$. Therefore, only three structures are possible, namely $TC \diamond\!\!\!\longrightarrow D1$, $TC \longleftarrow\!\!\!\diamond D1$, and $TC \longleftrightarrow D1$. The ambiguity may be resolved by enlarging $\mathbf{V}''$ until a sufficient set $\mathbf{Z}$ of common causes of $TC, D1$ is found that screens them off, or (given $\mathbf{Z}$) the dependence between TC and $D1$ is oriented such that one is a well-defined cause of the other, viz. $TC \longrightarrow D1$ or $TC \longleftarrow D1$, or enough effects of determinants of TC or $D1$ are observed as to remove the idiosyncratic shock on TC or $D1$, such that either $TC \diamond\!\!\!\longrightarrow D1$ or $TC \longleftarrow\!\!\!\diamond D1$ holds.

5 Conclusion

The problem of variable definition is known to be responsible for ambiguous manipulations. Furthermore, we showed that it can lead to mistakes in causal inference by standard constraint-based causal search methods. To address the problem, we introduced a novel representation framework suitable for structures including ill-defined variables, viz. the independent component (IC) representation. We argued that recovering the IC representation can unambiguously identify ill-defined variables, under certain assumptions, or at least exclude

that certain variables are ill-defined, and consequently reduce the risk of mistaken causal inferences. Given recent advances in statistical techniques (e.g., Independent Componenent Analysis) by which one may recover the IC representation, our proposal holds great promise. Therefore, we strongly invite further research on the subject.

Appendix

Proof of Proposition 1. Assume *per absurdum* that there exist Anc_i, Des_i of Det_i, such that $Anc_i \perp\!\!\!\perp Des_i | I$ for any set of parameters Θ in $\mathfrak{C}$. This is possible only if one of (A)–(C) holds: **(A)** Det_i suffices to determine I, such that I renders Det_i irrelevant to Anc_i, Des_i. This requires $card(\mathbf{Det}_I) = 1$, contradicting $card(\mathbf{Det}_I) \geq 2$. **(B)** $card(\mathbf{Det}_I) \geq 2$ and for some $Det_j \in \mathbf{Det}_I$, there is no directed path $Det_j \longrightarrow \cdots \longrightarrow Des_i$. Then, Det_j would act as an exogenous noise on I, such that the edge $Det_i \Longrightarrow I$ would be observationally indistinguishable from a standard edge $Det_i \longrightarrow I$. Holding CFC in $\mathbf{W}$, and since I behaves like a child of Det_i, we would have $Anc_i \not\perp\!\!\!\perp Des_i | I$, contradicting our starting hypothesis. **(C)** $card(\mathbf{Det}_I) \geq 2$ and for any $Det_j \in \mathbf{Det}_I$, there is a directed path $Det_j \longrightarrow \cdots \longrightarrow Des_i$. Then, there exists a parameter set Θ such that $Anc_i \perp\!\!\!\perp Des_i | I$ and, necessarily, for any $Det_i, Det_j \in \mathbf{Det}_I$, $P_\Theta(I, Des_i | Det_i) = P_\Theta(I, Des_i | Det_j)$. For instance, assume $card(\mathbf{Det}_I) = 2$ and a generalized additive model such that $I = f(Det_i) + g(Det_j)$ and $D = f'(Det_i) + g'(Det_j) + S_D$. Then, $A \perp\!\!\!\perp D | I$ holds only if $f(Det_i) + f'(Det_i) = g(Det_i) + g'(Det_i)$. This point generalizes to larger cardinalities. Finally, since I is a parent of neither Anc_i nor Des_i in $\widetilde{\mathcal{G}}_V$, any parameter set Θ such that $Anc_i \perp\!\!\!\perp Des_i | I$ necessarily violates CFC in $\widetilde{\mathcal{G}}_V$. $\qquad\square$

Proof of Proposition 2. Let $\ast\!\!\longrightarrow$ denote one among $\longrightarrow$, $\longleftrightarrow$, and $\diamond\!\!\longrightarrow$. Assume *per absurdum* that (i)–(iii) are true but Y is well-defined. CMC and (ii) entail that $\mathcal{G}_V$ contains paths linking X, Y and Y, Z. CFC and (i) entail that $\mathcal{G}_V$ contains no path linking X, Z. Then, $\mathcal{G}_O$ contains only two edges, one connecting X, Y, and one connecting Y, Z. Among the possible structures in $\mathcal{G}_O$, $X\ast\!\!\longrightarrow Y \longrightarrow Z$, $X \longleftarrow Y \longleftarrow\!\ast Z$, $X \longleftarrow\!\ast Y \longrightarrow Z$, and $X \longleftarrow Y\ast\!\!\longrightarrow Z$ contradict (i), and $X\ast\!\!\longrightarrow Y \longleftarrow\!\ast Z$ contradicts (iii). In all other structures, viz. $X \longleftarrow\!\diamond Y \diamond\!\!\longrightarrow Z$, $X\ast\!\!\longrightarrow Y \diamond\!\!\longrightarrow Z$, and $X \longleftarrow\!\diamond Y \longleftarrow\!\ast Z$, Y is ill-defined. The latter two contradict (iii). Thus, $\mathcal{G}_O$ is

$X \longleftrightarrow Y \diamondsuit\!\!\longrightarrow Z$, and $\mathbf{Det}_Y$ has precisely two elements in $\mathbf{V}$ (one causing X and one causing Z); otherwise $\mathcal{G}_O^{IC}$ would contain an idiosyncratic shock on Y associated to its extra determinant(s), violating (iii). As a corollary, $\mathcal{G}_O^{IC}$ contains idiosyncratic shocks on X and Z. $\qquad\square$

Proof of Proposition 3. **(i)** From the definition of ill-defined variable, for any $I \in \mathbf{V}$, $\mathcal{G}_V$ contains a directed path from some $Det_i \in \mathbf{Det}_I$ to some descendant Des_j of Det_i. Under CFC and DD, I is ill-defined only if $\mathbf{O}$ contains some Y on that path, such that $I \not\perp\!\!\!\perp Y$. Hence, if $\mathbf{O} = \{X, Y\}$ and $X \perp\!\!\!\perp Y$, then X is well-defined. **(ii)** In $\mathcal{G}_{\{X,Y\}}^{IC}$, X is ill-defined and not a child of an idiosyncratic shock only if $\mathcal{G}_V$ contains directed paths from each $Det_i \in \mathbf{Det}_X$ to Y. Then, $\mathcal{G}_{\{X,Y\}}^{IC}$ contains no shock S common to X, Y, such that $S \perp\!\!\!\perp Y | X$. Since this contradicts (ii), X cannot be ill-defined. **(iii)** If X is the only child of an idiosyncratic shock in $\mathcal{G}_{\{X,Y\}}^{IC}$, then $\mathcal{G}_{\{X,Y\}}^{IC}$ contains a shock common to X, Y. Then, X is ill-defined in $\mathcal{G}_{\{X,Y\}}^{IC}$ only if $\mathbf{O}$ contains a node $Det_i \in \mathbf{Det}_X$, which is not a child of an idiosyncratic shock. This contradicts the assumption that $\mathbf{Det}_X \cap \mathbf{O} = \emptyset$. Hence, X is well-defined. **(iv)** Suppose *per absurdum* that X is ill-defined, entailing a directed path $Det_i \longrightarrow \cdots \longrightarrow Y$ in $\mathcal{G}_V$. Since $X \perp\!\!\!\perp Y | \mathbf{Z}$, some $Z_i \in \mathbf{Z} \subset \mathbf{O}$ is on that path. Then, Z_i is a child of an idiosyncratic shock in $\mathcal{G}_{\{X,Z_i\}}^{IC}$, contradicting (iv). Hence, X is well-defined. $\qquad\square$

Proof of Proposition 4. Preamble: From the definition of ill-defined variable, and from $\mathbf{Det}_X \cap \mathbf{O} = \emptyset$, it follows that $\mathcal{G}_{\{X,Y\}}$ is $X \diamondsuit\!\!\longrightarrow Y$. **(i)** Under CFC and DD, the preamble implies $X \not\perp\!\!\!\perp Y$. **(ii)** By definition of IC representation, $\mathcal{G}_{\{X,Y\}}^{IC}$ contains at least one common shock to X, Y due to a latent determinant of X. **(iii)** If $\mathcal{G}_V$ contains a determinant of X not linked to Y by a directed path, then X is a child of an idiosyncratic shock (iii.a). If, on the contrary, all determinants of X are linked to Y by directed paths in $\mathcal{G}_V$, then X is not a child of an idiosyncratic shock. Additionally, given $X \perp\!\!\!\perp Y | \mathbf{Det}_X$, it follows that there is a set $\mathbf{S}$ of shocks on

X's determinants, such that $X \perp\!\!\!\perp Y | \mathbf{S}$ (iii.b). $\qquad \square$

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