Structural Intervention Distance (SID) for Evaluating Causal Graphs

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Abstract

Causal inference relies on the structure of a graph, often a directed acyclic graph (DAG). Different graphs may result in different causal inference statements and different intervention distributions. To quantify such differences, we propose a (pre-)distance between DAGs, the structural intervention distance (SID). The SID is based on a graphical criterion only and quantifies the closeness between two DAGs in terms of their corresponding causal inference statements. It is therefore well-suited for evaluating graphs that are used for computing interventions. Instead of DAGs it is also possible to compare CPDAGs, completed partially directed acyclic graphs that represent Markov equivalence classes. Since it differs significantly from the popular Structural Hamming Distance (SHD), the SID constitutes a valuable additional measure. We discuss properties of this distance and provide an efficient implementation with software code available on the first author’s homepage (an R package is under construction).

1. Introduction

Given a true causal DAG \( \mathcal{G} \), we want to assess the goodness of an estimate \( \mathcal{H} \): more generally, we want to measure closeness between two DAGs \( \mathcal{G} \) and \( \mathcal{H} \). The Structural Hamming Distance (SHD, see Definition 1) counts the number of incorrect edges. Although this provides an intuitive distance between graphs, it does not reflect their capacity for causal inference. Instead, we propose to count the pairs of vertices \((i, j)\), for which the estimate \( \mathcal{H} \) correctly predicts intervention distributions within the class of distributions that are Markov with respect to \( \mathcal{G} \). This results in a new (pre-)distance between DAGs, the Structural Intervention Distance, which adds valuable additional information to the established SHD. We are not aware of any directly related idea.

Throughout this work we consider a finite family of random variables \( \mathbf{X} = (X_1, \ldots, X_p) \) with index set \( V := \{1, \ldots, p\} \) (we use capital letters for random variables and bold letters for sets or vectors). We denote their joint distribution by \( \mathcal{L}(\mathbf{X}) \) and denote corresponding densities of \( \mathcal{L}(\mathbf{X}) \) with respect to Lebesgue or the counting measure, by \( p(\cdot) \) (implicitly assuming their existence). We also denote conditional densities and the density of \( \mathcal{L}(\mathbf{Z}) \) with \( \mathbf{Z} \subset \mathbf{X} \) by \( p(\cdot) \). A graph \( \mathcal{G} = (V, \mathcal{E}) \) consists of nodes \( V \) and edges \( \mathcal{E} \subseteq V^2 \). With a slight abuse of notation we sometimes identify the nodes (or vertices) \( j \in V \) with the
variables $X_j$. In Appendix A we provide further terminology regarding directed acyclic graphs (DAGs) (e.g. Lauritzen, 1996; Spirtes et al., 2000; Koller and Friedman, 2009) which we require in our work.

The rest of this article is organized as follows: Sections 1.1 and 1.2 review the Structural Hamming Distance and the do calculus (e.g. Pearl, 2009), respectively. In Section 2 we introduce the new structural intervention distance, prove some of its properties and provide possible extensions. Section 3 contains experiments on synthetic data and Section 4 describes an efficient implementation of the SID.

1.1 Structural Hamming Distance

The Structural Hamming Distance (Acid and de Campos, 2003; Tsamardinos et al., 2006) considers two partially directed acyclic graphs (PDAGs, see appendix) and counts how many edges do not coincide.

**Definition 1 (Structural Hamming Distance)** Let $P$ be the space of PDAGs over $p$ variables. The Structural Hamming Distance (SHD) is defined as

$$\text{SHD} : P \times P \to \mathbb{N}$$

$$(G, H) \mapsto \# \left\{ (i, j) \in V^2 \mid G \text{ and } H \text{ do not have the same type of edge between } i \text{ and } j \right\},$$

where edge types are defined in Appendix A.

Equivalently, we count pairs $(i, j)$, such that $((i, j) \in E_G \Delta E_H)$ or $((j, i) \in E_G \Delta E_H)$, where $A \Delta B := (A \setminus B) \cup (B \setminus A)$ is the symmetric difference. Definition 1 includes a distance between two DAGs since these are special cases of PDAGs. In this work, the SHD is primarily used as a measure of reference when comparing with our new structural intervention distance. A comparison to other but similar structural distances (e.g. counting only missing edges) can be found in de Jongh and Druzdzel (2009); all distances they consider are of similar type as SHD.

1.2 Intervention Distributions

Assume that $\mathcal{L}(X)$ is absolutely continuous with respect to a product measure. Then, $\mathcal{L}(X)$ is Markov with respect to $G$ if and only if the joint density factorizes according to

$$p(x_1, \ldots, x_p) = \prod_{j=1}^{p} p(x_j \mid x_{pa_j}),$$

see for example Lauritzen (1996) Thm 3.27. The intervention distribution given $\text{do}(X_i = \hat{x}_i)$ is then defined as

$$p_G(x_1, \ldots, x_p \mid \text{do}(X_i = \hat{x}_i)) = \prod_{j \neq i} p(x_j \mid x_{pa_j}) \delta(x_i = \hat{x}_i).$$

This, again, is a probability distribution. We can therefore take expectations or marginalize over some of the variables. One can check (see proof of Proposition 6) that this definition
implies \( p_G(y \mid do(X = \hat{x})) = p(y) \) if \( Y \) is a parent (or non-descendant) of \( X \); intervening on \( X \) does not show any effect on the distribution of \( Y \). If \( Y \) is not a parent of \( X \), we can compute (marginalized) intervention distributions by taking into account only a subset of variables from the graph \( \text{(Pearl 2009 Thm 3.2.2)} \).

**Proposition 2 (Adjustment Formula for Parents)** Let \( X \neq Y \) be two different nodes in \( G \). If \( Y \) is a parent of \( X \) then

\[
p_G(y \mid do(X = \hat{x})) = p(y).
\] (1)

If \( Y \) is not a parent of \( X \) then

\[
p_G(y \mid do(X = \hat{x})) = \sum_{\text{pa}_X} p(y \mid \hat{x}, \text{pa}_X) p(\text{pa}_X).
\] (2)

Whenever we can compute the marginalized intervention distribution \( p(y \mid do(X = \hat{x})) \) by a summation \( \sum_z p(y \mid \hat{x}, z) p(z) \) as in (2), we call the set \( Z \) a valid adjustment set for the intervention \( Y \mid do(X) \). Proposition 2 states that \( Z = \text{PA}_X^G \) is a valid adjustment set for \( Y \mid do(X) \) (for any \( Y \)). Figure 1 shows that for a given graph there may be other possible adjustment sets.

\[ \begin{array}{c}
\text{Q} \\
\text{X} \\
\text{B} \\
\text{Y} \\
\text{A} \\
\text{W} \\
\end{array} \]

Figure 1: The sets \( Z = \{P, Q\} \) and \( Z = \{P, A\} \) are valid adjustment sets for \( Y \mid do(X) \); \( Z = \{P\} \) is the smallest adjustment set. Any set containing \( W \), however, cannot be a valid adjustment set (see Lemma 5 below).

## 2. Structural Intervention Distance

### 2.1 Motivation and Definition

We propose a new graph-based (pre-)metric, the Structural Intervention Distance (SID). When comparing graphs (or DAGs in particular), there are many (pre-)metrics one could consider: an appropriate choice should depend on the further usage and purpose of the graphs. Often one is interested in a causal interpretation of a graph that enables us to predict the result of interventions. We then require a distance that takes this important goal into account. From now on we implicitly assume that an intervention distribution is computed using adjustment for parents as in Proposition 2; we discuss other choices of adjustment

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1. We sometimes use different letters for the variables in order to avoid subscripts.
sets in Section 2.4.5. The following Example 1 shows that the SHD (Definition 1) is not well suited for capturing aspects of the graph that are related to intervention distributions.

Example 1 Figure 2 shows a true graph \( G \) (left) and two different graphs (e.g. estimates) \( \mathcal{H}_1 \) (center) and \( \mathcal{H}_2 \) (right). The only difference between \( \mathcal{H}_1 \) and \( G \) is the additional edge

\[
\begin{array}{c}
X_1 \rightarrow X_2 \rightarrow Y_2 \\
| X_3 \end{array}
\]

true graph \( G \)

\[
\begin{array}{c}
X_1 \rightarrow X_2 \rightarrow Y_2 \\
\rightarrow Y_1
\end{array}
\]

graph \( \mathcal{H}_1 \)

\[
\begin{array}{c}
X_1 \leftarrow X_2 \rightarrow Y_2 \\
\rightarrow Y_1
\end{array}
\]

graph \( \mathcal{H}_2 \)

Figure 2: Two graphs (center and right) that have the same SHD to the true graph (left), but differ in the SID.

\( Y_1 \rightarrow Y_2 \), the only difference between \( \mathcal{H}_2 \) and \( G \) is the reversed edge between \( X_1 \) and \( X_2 \). The SHD between the true DAG and the others is therefore one in both cases:

\[
\text{SHD}(G, \mathcal{H}_1) = 1 = \text{SHD}(G, \mathcal{H}_2).
\]

We now consider a distribution \( p(.) \) that is Markov with respect to \( G \) and compute all intervention distributions using parent adjustment [2]. We will see that these two “mistakes” have different impact on the correctness of those intervention distributions.

First, we consider the DAG \( \mathcal{H}_1 \). All nodes except for \( Y_2 \) have the same parent sets in \( G \) and \( \mathcal{H}_1 \) and thus, the parent adjustment implies exactly the same formula. Since \( X_1 \) and \( X_2 \) are parents of \( Y_2 \) in both graphs, also the intervention distributions from \( Y_2 \) to \( X_1 \) and \( X_2 \) are correct. We will now argue why \( G \) and \( \mathcal{H}_1 \) agree on the intervention distribution from \( Y_2 \) to \( Y_3 \) and from \( Y_2 \) to \( Y_1 \). When computing the intervention distribution from \( Y_2 \) to \( Y_3 \) in \( \mathcal{H}_1 \), we adjust not only for \( \{X_1, X_2\} \) as done in \( G \) but also for the additional parent \( Y_1 \). We thus have to check whether \( \{X_1, X_2, Y_1\} \) is a valid adjustment set for \( Y_3 \mid \text{do}(Y_2) \). Indeed, since \( Y_2 \perp Y_1 \mid \{X_1, X_2\} \) (the distribution is Markov with respect to \( G \)) we have:

\[
p_{\mathcal{H}_1}(y_3 \mid \text{do}(Y_2 = \hat{y}_2)) = \sum_{x_1,x_2,y_1} p(y_3 \mid x_1, x_2, y_1, \hat{y}_2)p(x_1, x_2, y_1) = \sum_{x_1,x_2,y_1} p(x_1, x_2, y_1, y_3)p(\hat{y}_2 \mid x_1, x_2) = p(y_3 \mid \text{do}(Y_2 = \hat{y}_2))
\]

It remains to show that \( p_{\mathcal{G}}(y_1 \mid \text{do}(Y_2 = \hat{y}_2)) = p(y_1) = p_{\mathcal{H}_1}(y_1 \mid \text{do}(Y_2 = \hat{y}_2)) \), where the last equality is given by [1]. But since \( Y_1 \perp X_1, X_2 \) it follows from the parent adjustment [2] that \( p_{\mathcal{G}}(y_1 \mid \text{do}(Y_2 = \hat{y}_2)) = p(y_1) \). Thus, all intervention distributions computed in \( \mathcal{H}_1 \) agree with those computed in \( G \). Proposition 7 shows that this is not a coincidence. It proves
that all estimates for which the true DAG is a subgraph correctly predict the intervention distributions.

The “mistake” in graph $H_2$, namely the reversed edge, is more severe. For computing the correct intervention distribution from $X_2$ to $Y_1$, for example, we need to adjust for the confounder $X_1$, as suggested by the parent adjustment (2) applied to $G$. In $H_2$, however, $X_2$ does not have any parent, so there is no variable adjusted for. In general, $H_2$ therefore leads to a wrong intervention distribution $p_{H_2}(y_1 \mid \text{do}(X_2 = \hat{x}_2)) \neq p_{G}(y_1 \mid \text{do}(X_2 = \hat{x}_2))$. Also, when computing the intervention distribution from $X_1$ to $Y_i$, $i = 1, 2, 3$, we are adjusting for $X_2$, which is now a parent of $X_1$ in $H_2$. Again, this may lead to $p_{H_2}(y_i \mid \text{do}(X_1 = \hat{x}_1)) \neq p_{G}(y_i \mid \text{do}(X_1 = \hat{x}_1))$. Further, the intervention distributions from $X_1$ to $X_2$ and from $X_2$ to $X_1$ may not be correct, either. In fact, $H_2$ makes eight erroneous predictions for many observational distributions $p(.)$.

The preceding deliberations are reflected by the structural intervention distance we propose below (Definition 4). We will see that

$$\text{SID}(G, H_1) = 0 \neq 8 = \text{SID}(G, H_2).$$

Furthermore, Proposition 6 below shows us how to read off the SID from the graph structures.

The following argumentation motivates the formal definition of the SID. Given a true DAG $G$ and an estimate $H$, we would like to count the number of intervention distributions, which are computed using the structure of $H$, that coincide with the “true” intervention distributions inferred from $G$. This number, however, depends on the observational distribution over all variables. Since we regard $G$ as the ground truth we assume that the observational distribution is Markov with respect to $G$. Consider now a specific distribution that factorizes over all nodes, i.e. all variables are independent (this distribution is certainly Markov with respect to $G$). Then, $G$ and $H$ agree on all intervention distributions, even though their structure can be arbitrarily different. We therefore consider all distributions that are Markov with respect to $G$ instead of only one: we count all pairs of nodes, for which the predicted interventions agree for all observational distributions that are Markov with respect to $G$. Those pairs are said to “correctly estimate” the intervention distribution.

**Definition 3** Let $G$ and $H$ be DAGs over variables $X = (X_1, \ldots, X_p)$. For $i \neq j$ we say that the intervention distribution from $i$ to $j$ is correctly inferred by $H$ with respect to $G$ if

$$p_G(x_j \mid \text{do}(X_i = \hat{x}_i)) = p_H(x_j \mid \text{do}(X_i = \hat{x}_i)) \quad \forall \mathcal{L}(X) \text{ Markov wrt } G \text{ and } \forall \hat{x}_i$$

Otherwise, that is if

$$\exists \mathcal{L}(X) \text{ Markov wrt } G \text{ and } \hat{x}_i \text{ with } p_G(x_j \mid \text{do}(X_i = \hat{x}_i)) \neq p_H(x_j \mid \text{do}(X_i = \hat{x}_i))$$

we call the intervention distribution from $i$ to $j$ falsely inferred by $H$ with respect to $G$.

Here, $p_G$ and $p_H$ are computed using parent adjustment as in Proposition 3 (Section 2.4.5 discusses an alternative to parent adjustment).

The SID counts the number of falsely inferred intervention distributions. The definition is independent of any distribution which is crucial to allow for a purely graphical characterization.
**Definition 4 (Structural Intervention Distance)** Let $G$ be the space of DAGs over $p$ variables. We then define $\text{SID} : G \times G \to \mathbb{N}$

$$(G, \mathcal{H}) \mapsto \#\{(i, j), i \neq j \mid \text{the intervention distribution from } i \text{ to } j \text{ is falsely estimated by } \mathcal{H} \text{ with respect to } G\}$$

as the structural intervention distance (SID).

Although the SID is a (pre-)metric, see Section 2.3, it does not satisfy all properties of a metric, in particular it is not symmetric (see Section 2.4.4 for a symmetrized version).

### 2.2 An Equivalent Formulation

The SID as defined in (3) is difficult to compute. We now provide an equivalent formulation that is based on graphical criteria only. We will see that for each pair $(i, j)$ the question becomes whether $\text{PA}^G_{X_i}$ is a valid adjustment set for the intervention $X_j \mid \text{do}(X_i)$ in graph $G$. Shpitser et al. (2010) prove the following characterization of adjustment sets. The reader may think of $Z = \text{PA}^G_X$, which is always a valid adjustment set, as stated in Proposition 2.

**Lemma 5 (Characterization of valid Adjustment Sets)** Consider a DAG $G = (V, E)$, variables $X, Y \in V$ and a subset $Z \subset V \setminus \{X, Y\}$. Consider the property of $Z$ w.r.t. $(G, X, Y)$

$$\begin{align*}
(*) \quad & \text{In } G, \text{ no } Z \in Z \text{ is a descendant of any } W \text{ which lies on a directed } \\
& \text{path from } X \text{ to } Y \text{ and } Z \text{ blocks all non-directed paths from } X \text{ to } Y.
\end{align*}$$

We then have the following two statements:

(i) Let $L(X)$ be Markov with respect to $G$. If $Z$ satisfies $(*)$ w.r.t. $(G, X, Y)$, then $Z$ is a valid adjustment set for $Y \mid \text{do}(X)$.

(ii) If $Z$ does not satisfy $(*)$ w.r.t. $(G, X, Y)$, then there exists $L(X)$ that is Markov with respect to $G$ that leads to $p_G(y \mid \text{do}(X = \hat{x})) \neq \sum_z p(y \mid \hat{x}, z)p(z)$, meaning $Z$ is not a valid adjustment set.

If $Y \notin \text{PA}^G_X$, then $Z = \text{PA}^G_X$ satisfies condition $(*)$ and statement (i) reduces to Proposition 2. In fact, condition $(*)$ is a slight extension of the backdoor criterion (Pearl, 2009). It is not surprising that other sets than the parent set work, too. We may adjust for children of $X$, for example, as long as they are not part of a directed path, see Figure 1 above. Similarly, we do not have to adjust for parents of $X$ for which all unblocked paths to $Y$ lead through $X$.

Using Lemma 5 we obtain the following equivalent definition of the SID, which is entirely graph-based and will later be exploited for computation.

**Proposition 6** The SID has the following equivalent definition.

$$\text{SID}(G, \mathcal{H}) = \#\{(i, j), i \neq j \mid \begin{cases} j \in \text{DE}^G_i & \text{if } j \in \text{PA}^H_i \\ \text{PA}^H_i \text{ does not satisfy } (*) \text{ for } (G, i, j) & \text{if } j \notin \text{PA}^H_i \end{cases}\}$$

The proof is provided in Appendix B; it is based on Lemma 5.
2.3 Properties

We first investigate metric properties of the SID. Let us denote the number of nodes in a graph by \( p \) (this is overloading notation but does not lead to any ambiguity). We then have that

\[
0 \leq \text{SID}(G, H) \leq p \cdot (p - 1)
\]

and

\[
G = H \Rightarrow \text{SID}(G, H) = 0.
\]

The SID therefore satisfies the properties of what is sometimes called a pre-metric.

The SID is not symmetric: e.g., for a non-empty graph \( G \) and an empty graph \( H \), we have that \( \text{SID}(G, H) \neq 0 = \text{SID}(H, G) \) (if \( G \) is the empty DAG, all sets of nodes satisfy (*) and are therefore valid adjustment sets).

If \( \text{SID}(G, H) = 0 \) parent adjustment leads to the same intervention distributions in \( G \) and \( H \) but it does not necessarily hold that \( G = H \). Example 1 shows graphs \( G \neq H_1 \) with \( \text{SID}(G, H_1) = 0 \). Using Proposition 6 we can characterize the set of DAGs that have structural intervention distance zero to a given true DAG \( G \):

**Proposition 7** Consider two DAGs \( G \) and \( H \). We then have

\[
\text{SID}(G, H) = 0 \iff G \leq H
\]

Here, \( G \leq H \) means that \( G \) is a subgraph of \( H \) (see Appendix A). The proof is provided in Appendix C; it works for any type of adjustment set, not just the parent set (see Section 2.4.5). Proposition 7 states that \( H \) can contain many more (additional) edges than \( G \) and still receives an SID of zero. Intuitively, the SID counts the number of pairs \((i, j)\), such that the intervention distribution inferred from the graph \( H \) is wrong; the latter happens if the estimated set of parents \( \text{PA}_H^X_i \) is not a valid adjustment set in \( G \). If an estimate \( H \) contains strictly too many edges, i.e. \( G \leq H \) and \( \text{pa}_G^X_i \subseteq \text{pa}_H^X_i \) for all \( i \), the intervention distributions are correct; this follows from \( p(x_j | x_i, \text{pa}_H^X_i) = p(x_j | x_i, \text{pa}_G^X_i) \), see also Lemma 5. For computing intervention distributions in practice, we have to estimate \( p(x_j | x_i, \text{pa}_H^X_i) \) based on finitely many samples. This can be seen as a regression task, a well-understood problem in statistics. It is therefore a question of the regression or feature selection technique, whether we see this equality (at least approximately) in practice as well. Section 2.4.3 shows a simple way to combine the SID with another measure in order to obtain zero distance if and only if the two graphs coincide.

The following proposition provides loose and sharp bounds when relating SID to the SHD: they underline the difference between these two measures. The proof is provided in Appendix D.

**Proposition 8 (Relating SID and SHD)** Consider two DAGs \( G \) and \( H \).

(1a) When the SHD is zero, the SID is zero, too:

\[
\text{SHD}(G, H) = 0 \implies \text{SID}(G, H) = 0
\]

2. A function \( d: G \times G \to \mathbb{R} \) is called a premetric if \( d(a, b) \geq 0 \) and \( d(a, a) = 0 \).
(1b) We have
\[ \text{SHD}(\mathcal{G}, \mathcal{H}) = 1 \implies \text{SID}(\mathcal{G}, \mathcal{H}) \leq 2 \cdot (p - 1). \]
This bound is sharp.

(2) There exists \( \mathcal{G} \) and \( \mathcal{H} \) such that \( \text{SID}(\mathcal{G}, \mathcal{H}) = 0 \) but \( \text{SHD}(\mathcal{G}, \mathcal{H}) = p(p - 1)/2 \) which achieves the maximal possible value. Therefore we cannot bound SHD from SID.

2.4 Extensions

2.4.1 SID between a DAG and a CPDAG

Let \( \mathcal{C} \) denote the space of CPDAGs (completed partially directed acyclic graphs) over \( p \) variables. Some causal inference methods like the PC-algorithm (Spirtes et al., 2000) or Greedy Equivalence Search (Chickering, 2002) do not output a single DAG, but rather a completed PDAG \( \mathcal{C} \in \mathcal{C} \) representing a Markov equivalence class of DAGs. In order to compute the SID between a (true) DAG \( \mathcal{G} \) and an (estimated) PDAG, we can in principle enumerate all DAGs in the Markov equivalence class and compute the SID for each single DAG. This way, we obtain a vector of distances, instead of a single number, and we can compute lower and upper bounds for these distances.

Since the enumeration becomes computationally infeasible with large graph size, we propose to extend the CPDAG locally. Especially for sparse graphs, this provides a considerable computational speed-up. We make use of the fact that the PDAG \( \mathcal{C} \) represents a Markov equivalence class of DAGs only if each chain component is chordal (Andersson et al., 1997). We extend each chordal chain component \( c \) (see Section A) locally to all possible DAGs \( \mathcal{C}_{c,1}, \ldots, \mathcal{C}_{c,k} \), leaving the other chain components undirected (Meek, 1995).

For each extension \( \mathcal{C}_{c,h} \) (\( 1 \leq h \leq k \)) and for each vertex \( i \) within the chain component \( c \), we consider
\[
I(\mathcal{G}, \mathcal{C}_{c,h})_i := \# \left\{ j \neq i \mid \begin{array}{l}
X_j \in \text{DE}^\mathcal{G}_{X_i} \\
\text{PA}^\mathcal{C}_{c,h}_{X_i} \text{ does not satisfy \((*)\) for graph } \mathcal{G} \text{ if } X_j \notin \text{PA}^\mathcal{C}_{c,h}_{X_i}
\end{array} \right\}.
\]
For each chain component \( c \), we thus obtain \( k \) vectors \( I(\mathcal{G}, \mathcal{C}_{c,1}), \ldots, I(\mathcal{G}, \mathcal{C}_{c,k}) \) each having \#\( c \) entries. We then represent each vector with its sum
\[
S(\mathcal{G}, \mathcal{C}_{c,h}) = \sum_{i \in c} I(\mathcal{G}, \mathcal{C}_{c,h})_i \quad (h = 1, \ldots, k)
\]
and save the minimum and the maximum over the \( k \) values
\[
\min_h S(\mathcal{G}, \mathcal{C}_{c,h}), \quad \max_h S(\mathcal{G}, \mathcal{C}_{c,h}).
\]
These values correspond to the “best” and “worst” DAG extensions. We then report the sum over all minima and the sum over all maxima as lower and upper bound, respectively
\[
\text{SID}_{\text{lower}}(\mathcal{G}, \mathcal{C}) = \sum_c \min_h S(\mathcal{G}, \mathcal{C}_{c,h}), \quad \text{SID}_{\text{upper}}(\mathcal{G}, \mathcal{C}) = \sum_c \max_h S(\mathcal{G}, \mathcal{C}_{c,h}).
\]

This leads to the extended definition
\[
\text{SID} : \mathcal{G} \times \mathcal{C} \rightarrow \mathbb{N} \times \mathbb{N} \quad (\mathcal{G}, \mathcal{C}) \mapsto (\text{SID}_{\text{lower}}(\mathcal{G}, \mathcal{C}), \text{SID}_{\text{upper}}(\mathcal{G}, \mathcal{C}))
\]
The definition guarantees that the neighborhood orientation of two nodes do not contradict each other. Both the lower and upper bounds are therefore met by a DAG member in the equivalence class of $C$.

The differences between lower and upper bounds can be quite large. If the true DAG is a (Markov) chain $X_1 \rightarrow \ldots \rightarrow X_p$ of length $p$, the corresponding equivalence class contains the correct DAG resulting in an SID of zero (lower bound); it also includes the reversed chain $X_1 \leftarrow \ldots \leftarrow X_p$ resulting in a maximal SID of $p \cdot (p - 1)$.

In order to provide a better intuition for these lower and upper bounds we relate them to “strictly identifiable” intervention distributions in the Markov equivalence class.

**Definition 9** Consider a completed partially directed graph $C$ and let $C_1, \ldots, C_k$ be the DAGs contained in the Markov equivalence class represented by $C$. We say that the intervention distribution from $i$ to $j$ is

- identifiable in $C$ if $p_{C_g}(x_j \mid \text{do}(X_i = x_i))$ is the same for all $C_g \in \{C_1, \ldots, C_k\}$ and for all distributions $p(.)$ that are Markov with respect to $C$.

- strictly identifiable in $C$ if $p_{C_g}(x_j \mid \text{do}(X_i = x_i))$ is the same for all $C_g \in \{C_1, \ldots, C_k\}$ and for all distributions $p(.)$.

- identifiable in $C$ w.r.t. $G$ if $p_{C_g}(x_j \mid \text{do}(X_i = x_i))$ is the same for all $C_g \in \{C_1, \ldots, C_k\}$ and for all distributions $p(.)$ that are Markov w.r.t. $G$.

Definition 3 further calls a (strictly) identifiable intervention distribution from $i$ to $j$ estimated correctly if $p_G(x_j \mid \text{do}(X_i = \hat{x}_i)) = p_C(x_j \mid \text{do}(X_i = \hat{x}_i))$ for all $L(X)$ that are Markov with respect to $G$. With this notation we have the following remark, which is visualized by Figure 3.

**Remark 10** Given a true DAG $G$ and an estimated CPDAG $C$. It then holds (see Figure 3) that

$$\# \left\{ \text{interv. distr. that are identifiable in } C \text{ w.r.t. } G \text{ and inferred falsely by } C \text{ w.r.t. } G \right\} = \text{SID}_{\text{lower}}(G, C)$$

$$\# \left\{ \text{interv. distr. that are identifiable in } C \text{ w.r.t. } G \text{ and inferred correctly by } C \text{ w.r.t. } G \right\} = p \cdot (p - 1) - \text{SID}_{\text{upper}}(G, C)$$

$$\# \left\{ \text{interv. distr. that are strictly identifiable in } C \text{ and inferred falsely by } C \text{ w.r.t. } G \right\} \leq \text{SID}_{\text{lower}}(G, C)$$

$$\# \left\{ \text{interv. distr. that are strictly identifiable in } C \text{ and inferred correctly by } C \text{ w.r.t. } G \right\} \leq p \cdot (p - 1) - \text{SID}_{\text{upper}}(G, C).$$

Choosing the lower and upper bound to match intervention distributions that are identifiable w.r.t. $G$ (rather than being strictly identifiable) is a conservative choice. If we use the estimated CPDAGs to provide us with candidate experiments that could reveal nodes with a strong causal effect, we do not want to miss good candidates.

The procedure above fails if $C$ is not a completed PDAG and therefore does not represent a Markov equivalence class. This may happen for some versions of the PC algorithm, when they are based on finitely many data or in the existence of hidden variables. For each node
i, we can then consider all subsets of undirected neighbors as possible parent sets and again report lower and upper bounds. The same is done if the chain component is too large (with more than eight nodes). These modifications are implemented in our R-code that is available on the first author’s homepage.

2.4.2 SID between a CPDAG and a DAG or CPDAG

If we simulate from a linear Gaussian SEM with different error variances, for example, we cannot hope to recover the correct DAG from the joint distribution. If we assume faithfulness, however, it is possible to identify the correct Markov equivalence class. In such situations, one may want to compare the estimated structure with the correct Markov equivalence class (represented by a CPDAG) rather than with the correct DAG. Again, we denote the space of CPDAGs by $C$. We have defined the SID on $G \times G$ (Definition 4) and on $G \times C$ (Section 2.4.1). We now want to extend the definition to $C \times G$ and $C \times C$, where we compare an estimated structure with a true CPDAG $C$. The CPDAG $C$ represents a Markov equivalence class that includes many different DAGs $G_1, \ldots, G_k$. These different DAGs lead to different intervention distributions. The main idea is therefore to consider only those $(i, j)$ for which the intervention distribution from $i$ to $j$ is identifiable in $C$ (Definition 9). Maathuis and Colombo (2013) introduce a generalized backdoor criterion that can be used to characterize identifiability of intervention distributions. Lemma 11 is a direct implication of their Corollary 4.2 and provides a graphical criterion in order to decide whether an intervention distribution is identifiable in a CPDAG. To formulate the result, we define that a path $X_{a_1}, \ldots, X_{a_s}$ in a partially directed graph is possibly directed if no edge between $X_{a_f}$ and $X_{a_{f+1}}$, $f \in \{1, \ldots, s-1\}$, is pointing towards $X_{a_f}$.

**Lemma 11** Let $X_i$ and $X_j$ be two nodes in a CPDAG $G$. The intervention distribution from $i$ to $j$ is not identifiable if and only if there is a possibly directed path from $X_i$ to $X_j$ starting with an undirected edge.
We then define
\[
\text{SID} : \mathbb{C} \times \mathbb{G} \rightarrow \mathbb{N} \\
(C, H) \mapsto \#\{(i, j), i \neq j | \text{the interv.
\text{distr from } i \text{ to } j \text{ is identif. in } C \\
\text{and } \exists \mathcal{L}(X) \text{ that is Markov wrt } C_1 \in \mathcal{C} \text{ such that} \\
p_{C_1}(x_j | \text{do}(X_i = \hat{x}_i)) \neq p_{H}(x_j | \text{do}(X_i = \hat{x}_i))\}
\]

In a DAG, all effects are identifiable. The definitions then reduce to the case of DAGs and \ref{sid-dag}. The extension to \text{SID}: \mathbb{C} \times \mathbb{C} \rightarrow \mathbb{N} \times \mathbb{N} is completely analogous to \ref{sid-dag} in Section \ref{sid-dag} with lower and upper bounds of the SID score \ref{sid-dag} between a true CPDAG and all DAGs in the estimated Markov equivalence class.

\subsection{2.4.3 Penalizing additional edges}

The estimated DAG may have strictly more edges than the true DAG and still receives an SID of zero (Proposition \ref{sid-dag}). We have argued in Section \ref{sid-dag} that for computing causal inference this fact only introduces statistical problems that can be dealt with if the sample size increases. In some practical situations, however, it may nevertheless be seen as an unwanted side effect. This problem can be addressed by introducing an additional distance measuring the difference in number of edges between \(G\) and \(H\).

\[\text{DNE}(G, H) = |\#\text{edges in } G - \#\text{edges in } H| .\]

Here, a directed or undirected edge counts as one edge. For any DAG \(G\) and any DAG \(H\), it then follows directly from Proposition \ref{sid-dag} that
\[G = H \iff (\text{SID}(G, H) = 0 \text{ and DNE}(G, H) = 0) .\]

Analogously, we have for any DAG \(G\) and any CPDAG \(C\)
\[G \in C \iff (\text{SID}_{\text{lower}}(G, C) = 0 \text{ and DNE}(G, C) = 0) .\]

\subsection{2.4.4 Symmetrization}

We may also want to compare two DAGs \(G\) and \(H\), where neither of them can be seen as an estimate of the other. For these situations we suggest a symmetrized version of the SID:
\[
\text{SID}_{\text{symm}}(G, H) = \frac{\text{SID}(G, H) + \text{SID}(H, G)}{2} .
\]

Although we believe that this version fits most purposes in practice, there are other possibilities to construct symmetric versions of SID. As a slight modification of Definition \ref{sid-dag} we may also count all pairs \((i, j)\), such that the intervention distributions coincide for all distributions that are Markov with respect to both graphs. Note that this would result in a distance that is always zero if one of its arguments is the empty graph, for example.

\subsection{2.4.5 Alternative Adjustment Sets}

In this work we use the parent set for adjustment. Since it is easy to compute and depends only on the neighbourhood of the intervened nodes it is widely used in practice. Any other
method to compute adjustment sets in graphs can be used, too, of course. Choosing an adjustment set of minimal size (see Figure 1) is more difficult to compute but has the advantage of a small conditioning set: Textor and Liskiewicz (2011) discuss recent advances in efficient computation. In contrast to the parent set, it depends on the whole graph. Using the experimental setup from Section 3.1 below, we compare the SID computed with parent adjustment with the SID computed with the minimal adjustment set for randomly generated dense graphs of size \( p = 5 \). Since the minimal adjustment set need not be unique, we decided to choose the smallest set that is found first by the computational algorithm. Figure 4 shows that the differences between the two values of SID, once computed with parent sets and once computed with minimal adjustment sets, are rather small (especially compared to the differences between SID and SHD, see Section 3.1). In about 70% of the cases, they are exactly the same.

2.4.6 Hidden Variables (future work)

If some of the variables are unobserved, not all of the intervention distributions are identifiable from the true DAG. We provide a “road map” on how this case can be included in the framework of the SID. As it was done for CPDAGs (Section 2.4.2) we can exclude the non-identifiable pairs from the structural intervention distance. In the presence of hidden variables, the true structure can be represented by an acyclic directed mixed graph (ADMG), for which Shpitser and Pearl (2006) address the characterization of identifiable intervention distributions. Alternatively, we can regard a maximal ancestral graph (MAG) (Richardson and Spirtes, 2002) as the ground truth, for which the characterization becomes more difficult. Methods like FCI (Spirtes et al., 2000) and its successors (Colombo et al., 2012; Claassen et al., 2013) output an equivalence class of MAGs that are called partial ancestral graphs (PAGs) (Richardson and Spirtes, 2002). To compare an estimated PAG to the true MAG, we would again go through all MAGs represented by the PAG (see Section 2.4.1) and provide lower and upper bounds (as in Section 2.4.1). Future work might show that this can be done efficiently.
2.4.7 Multiple Interventions (future work)

The structural intervention distance compares the two graph’s predictions of intervention distributions. Until now, we have only considered interventions on single nodes. Instead, one may also consider multiple interventions. A slightly modified version of Lemma 5 still holds, but the (union of the) parent sets do not necessarily provide a valid adjustment set, even for the true causal graph. Instead, one needs to define a “canonical” choice of a valid adjustment set. Furthermore, given a method that computes a valid adjustment set in the correct graph, one needs to handle the computational complexity that arises from the large number of possible interventions: for each number \( k \) of multiplicity of interventions there are \( 2^k \) possible intervention sets and \( p - k \) possible target nodes \( j \). In total we thus have \( \sum_{k=1}^{p-1} \binom{p}{k} (p - k) = p(2^{p-1} - 1) \) intervention distributions. In practice, one may first address the case of intervening on two nodes, where the number of possible intervention distributions is \( p(p - 1)(p - 2)/2 \).

3. Simulations

3.1 SID versus SHD

For \( p = 5 \) and for \( p = 20 \) we sample 10,000 pairs of random DAGs and compute both the SID and the SHD between them. We consider two probabilities for iid sampling of edges, namely \( p_{\text{connect}} = 1.5/(p - 1) \) (resulting in an expected number of 0.75\(p \) edges) for a sparse setting and \( p_{\text{connect}} = 0.3 \) for a dense setting. Furthermore, the order of the variables is chosen from a uniformly distributed permutation among the vertices. The left panels in Figure 5 show two-dimensional histograms with SID and SHD. It is apparent that the SHD and SID constitute very different distance measures. For example, for SHD equal to a low number such as one or two (see \( p = 5 \) in the dense case), the SID can take on very different values. This indicates, that compared to the SHD, the SID provides additional information that are appropriate for causal inference. The observations are in par with the bounds provided in Proposition 8.

For each pair \( \mathcal{G} \) and \( \mathcal{H} \) of graphs we also generate a distribution by defining a linear structural equation model

\[
X_j = \sum_{k \in \text{pa}_G^j} \beta_{jk} X_k + N_j, \quad j = 1, \ldots, p,
\]

whose graph is identical to \( \mathcal{G} \). We sample the coefficients \( \beta_{jk} \) uniformly from \([-1.0; -0.1] \cup [0.1; 1.0]\). The noise variables are normally distributed with mean zero and variance one. Due to the assumption of equal error variances for the error terms, the DAG is identifiable from the distribution \([\text{Peters and Bühlmann, 2014}]\). With the linear Gaussian choice we can characterize the true intervention distribution \( p(x_j | \hat{x}_i) \) by one number, namely the derivative of the expectation with respect to \( \hat{x}_i \) (which is also called the total causal effect of \( X_i \) on \( X_j \)). Its derivation can be found in Appendix E. We can then compare the intervention distributions from \( \mathcal{G} \) and \( \mathcal{H} \) and report the number of pairs \((i, j)\), for which these two numbers differ. For numerical reasons we regard two numbers as different if their absolute difference is larger than \( 10^{-8} \). The right panels in Figure 5 show the comparison.
to the SID. In all of the 20,000 cases, the SID counts exactly the number of those “wrong” causal effects. A priori this is not obvious since Definition 4 only requires that there exists a distribution that discriminates between the intervention distributions. The result shown in Figure 5 suggests that the intervention distributions differ for most distributions. Two possible reasons for inequality have indeed small probability: (1) a non-detectable difference that is smaller than $10^{-8}$ and (2) vanishing coefficients that would violate faithfulness (Spirtes et al., 2000, Thm 3.2). We are not aware of a characterization of the distributions that do not allow to discriminate between the intervention distributions.

Figure 5: We generate 10,000 pairs of random small dense graphs (top) and larger sparse graphs (bottom). For each pair of graphs $(G, H)$ we also generate a distribution which is Markov w.r.t $G$. The two-dimensional histograms compare SID$(G, H)$ with SHD$(G, H)$ (left) and SID$(G, H)$ with the number of pairs $(i,j)$, for which the calculated causal effects differ (right). The SID measures exactly the number of wrongly estimated causal effects and thus provides additional and very different information as the SHD.

3.2 Comparing Causal Inference Methods

As in Section 3.1 we simulate sparse random DAGs as ground truth (100 times for each value of $p$ and $n$). We again sample $n$ data points from the corresponding linear Gaussian structural equation model with equal error variances (as above coefficients are uniformly chosen from $[-1; -0.1] \cup [0.1; 1]$) and apply different inference methods. This setting allows
us to use the PC algorithm (Spirtes et al. 2000), conservative PC (Ramsey et al. 2006),
greedy equivalent search (GES) (Chickering 2002) and greedy DAG search based on the
assumption of equal error variances (GDS_{EEV}) (Peters and Bühlmann 2014). Table 1 reports the average SID between the true DAG and the estimated ones. GDS_{EEV} is the
only method that outputs a DAG. All other methods output a Markov equivalence class for
which we apply the extension suggested in Section 2.4.1. Additionally, we report the results
for a random estimator RAND that does not take into account any of the data: we sample
a DAG as in Section 3.1 but with $p_{\text{connect}}$ uniformly chosen between 0 and 1. Section 2.4.1
provides an example, for which the SID can be very different for two DAGs within the same
Markov equivalence class. Table 1 shows that this difference can be quite significant even on
average. While the lower bound often corresponds to a reasonably good estimate, the upper
bound may not be better than random guessing for small sample sizes. In fact, for $p = 5$ and
$n = 100$, the distance to the RAND estimate was less than the upper bound for PC in 77 out
of the 100 experiments (not directly readable from the aggregated numbers in the table).
For the SHD, however, the PC algorithm outperforms random guessing; e.g., for $p = 5$ and
$n = 100$, RAND is better than PC in 8 out of 100 experiments. This supports the idea
that the PC algorithm estimates the skeleton of a DAG more reliably than the directions
of its edges. The results also show how much can be gained when additional assumptions
are appropriate; all methods exploit that the data come from a linear Gaussian SEM while
only GDS_{EEV} makes use of the additional constraint of equal error variances, which leads
to identifiability of the DAG from the distribution (Peters and Bühlmann 2014). We draw
different conclusions if we consider the SHD (see Table 2). For $p = 40$ and $n = 100$, for
example, PC performs best with respect to SHD while it is worst with respect to SID.

3.3 Scalability of the SID

For different values of $p$ we report here the processor time needed for computing the SID
between two random graphs with $p$ nodes. We choose the same setting for sparse and
dense graphs as in Section 3.1. Figure 6 shows box plots for 100 pairs of graphs for each
value of $p$ ranging between 5 and 50. The figure suggests that the time complexity scales
approximately quadratic and cubic in the number of nodes for sparse and dense graphs,
respectively.²

4. Implementation

We sketch here the implementation of the Structural Intervention Distance while details
are presented in Algorithms 1 and 2 in Appendix F using pseudo code. The key idea of
our algorithm is based on Proposition 6. Condition (*) contains two parts that need to be
checked. Part (1) addressed the issue whether any node from the conditioning set is a
descendant of any node on a directed path (see line 28 in Algorithm 1). Here, we make use
of the $p \times p$ PathMatrix: its entry $(i,j)$ is one if and only if there is a directed path from
$i$ to $j$. This can be computed efficiently by squaring the matrix $(\text{Id} + G)^{\lceil \log_2(p) \rceil}$ times
since $G$ is idempotent; here we denote by $G$ the adjacency matrix the DAG $G$. For part (2)

² The experiments were performed on a 64bit Ubuntu machine using one core of the Intel Core2 Duo CPU
P8600 at 2.40GHz.
Table 1: Average SID to true DAG for 100 simulation experiments with standard deviation, for different \( n \) and \( p \). For the methods that output a Markov equivalence class (CPC, PC and GES), two rows are shown: they represent DAGs from the equivalence class with the smallest and with the largest distance, i.e. the lower and upper bounds in (4) in Section 2.4.1. Smallest averages are highlighted.

| \( p \) | \( GDS_{EEV} \) | CPC | PC | GES | RAND |
|---|---|---|---|---|---|
| 5 | 1.7 ± 2.2 | 2.9 ± 3.2 | 4.3 ± 4.7 | 3.3 ± 4.2 | 6.1 ± 4.0 |
| 20 | 14.1 ± 10.5 | 22.8 ± 17.1 | 37.0 ± 26.8 | 24.4 ± 17.4 | 47.7 ± 28.8 |
| 40 | 37.2 ± 27.2 | 56.7 ± 36.3 | 91.3 ± 58.3 | 58.9 ± 34.6 | 119.1 ± 63.8 |

| \( p \) | \( GDS_{EEV} \) | CPC | PC | GES | RAND |
|---|---|---|---|---|---|
| 5 | 0.6 ± 1.6 | 1.7 ± 3.4 | 3.0 ± 4.7 | 1.9 ± 3.7 | 6.3 ± 5.0 |
| 20 | 3.0 ± 6.7 | 7.4 ± 10.3 | 26.4 ± 28.7 | 8.3 ± 10.2 | 53.1 ± 36.6 |
| 40 | 7.8 ± 10.2 | 13.8 ± 12.6 | 62.1 ± 45.5 | 19.7 ± 18.7 | 132.2 ± 79.8 |

Table 2: Same experiment as in Table 1, this time reporting the average SHD to the true DAG. Smallest averages are highlighted.

| \( p \) | \( GDS_{EEV} \) | CPC | PC | GES | RAND |
|---|---|---|---|---|---|
| 5 | 1.0 ± 1.1 | 3.1 ± 1.4 | 2.6 ± 1.4 | 2.7 ± 1.5 | 6.2 ± 2.2 |
| 20 | 11.3 ± 3.1 | 13.4 ± 3.7 | 11.3 ± 3.1 | 15.0 ± 3.3 | 96.7 ± 47.8 |
| 40 | 43.7 ± 6.6 | 27.2 ± 4.9 | 22.6 ± 4.6 | 45.4 ± 6.1 | 377.9 ± 195.8 |

| \( p \) | \( GDS_{EEV} \) | CPC | PC | GES | RAND |
|---|---|---|---|---|---|
| 5 | 0.3 ± 0.6 | 2.6 ± 1.5 | 2.3 ± 1.4 | 2.5 ± 1.5 | 6.0 ± 2.0 |
| 20 | 2.8 ± 1.9 | 8.6 ± 2.7 | 7.7 ± 2.6 | 7.8 ± 2.7 | 98.4 ± 50.7 |
| 40 | 10.6 ± 3.6 | 17.0 ± 3.5 | 15.3 ± 3.4 | 17.8 ± 4.0 | 393.5 ± 189.8 |

of \((*)\) we check whether the conditioning set blocks all non-directed paths from \( i \) to \( j \) (see line 31 in Algorithm 1). It is the purpose of the function rondp (line 9 in Algorithm 1) to compute all nodes that can be reached on a non-directed path.
Figure 6: Box plots for the processor time needed to compute the SID for one pair of random graphs (averaged over 100 pairs), for varying $p$ and sparse (left) and dense graphs (right). The computational complexity roughly scales quadratic or cubic in $p$ for sparse or dense graphs, respectively.

Algorithm \[2\] also presented in the appendix, describes the function `rondp` that computes all nodes reachable on non-directed paths. In a breadth-first search we go through all node-orientation combinations and compute the $2p \times 2p$ `reachabilityMatrix`. Afterwards we compute the corresponding `PathMatrix` (line 24 in Algorithm \[2\]). We then start with a vector `reachableNodes` (consisting of parents and children of node $i$) and read off all reachable nodes from the `reachabilityPathMatrix`. We then filter out the nodes that are reachable on a non-directed path.

Note that in the whole procedure computing the `PathMatrix` is computationally the most expensive part. Making sure that this computation is done only once for all $j$ is one reason why we do not use any existing implementation (e.g. for $d$-separation). The worst case computational complexity for computing the SID between dense matrices is $O(p \cdot \log_2(p) \cdot f(p))$, where squaring a matrix requires $O(f(p))$; a naive implementation yields $f(p) = p^3$ while Coppersmith and Winograd \[1987\] report $f(p) = O(p^{2.375477})$, for example. Sparse matrices lead to improved computational complexities, of course (see also Section 3.3).

We also implemented the steps required for computing the SID between a DAG and a completed PDAG (both options from Section 2.4.1) using a function that enumerates all DAGs from partially directed graph. Those steps, however, are not shown in the pseudo code in order to ensure readability.

Our software code for SID is provided as R-code on the first author’s homepage.

5. Conclusions

We have proposed a new (pre-) distance, the Structural Intervention Distance (SID), between directed acyclic graphs and completed partially directed acyclic graphs. Since the SID is a one-dimensional measure of distances between high-dimensional objects it does not
capture all aspects of the difference. The SID measures “closeness” between graphs in terms of their capacities for causal effects (intervention distributions). It is therefore well suited for evaluating different estimates of causal graphs. The distance differs significantly from the widely used Structural Hamming Distance (SHD) and can therefore provide a useful complement to existing measures. Based on known results for graphical characterization of adjustment sets we have provided a representation of the SID that enabled us to develop an efficient algorithm for its computation. Simulations indicate that in order to draw reliable causal conclusions from an estimated DAG (i.e. to obtain a small SID), we require more samples than what is suggested by the SHD.

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Appendix A. Terminology for Directed Acyclic Graphs

We summarize here some well known facts about graphs, essentially taken from Peters [2012]. Let \( \mathcal{G} = (V, E) \) be a graph with \( V := \{1, \ldots, p\} \), \( E \subset V^2 \) and corresponding random variables \( X = (X_1, \ldots, X_p) \). A graph \( \mathcal{G}_1 = (V_1, \mathcal{E}_1) \) is called a subgraph of \( \mathcal{G} \) if \( V_1 = V \) and \( \mathcal{E}_1 \subseteq \mathcal{E} \); we then write \( \mathcal{G}_1 \subseteq \mathcal{G} \). If additionally, \( \mathcal{E}_1 \neq \emptyset \), we call \( \mathcal{G}_1 \) a proper subgraph of \( \mathcal{G} \). A node \( i \) is called a parent of \( j \) if \( (i, j) \in E \) and a child if \( (j, i) \in E \). The set of parents of \( j \) is denoted by \( \text{PA}_j^\mathcal{G} \), the set of its children by \( \text{CH}_j^\mathcal{G} \). Two nodes \( i \) and \( j \) are adjacent if either \( (i, j) \in E \) or \( (j, i) \in E \). We call \( \mathcal{G} \) fully connected if all pairs of nodes are adjacent. We say that there is an undirected edge between two adjacent nodes \( i \) and \( j \) if \( (i, j) \in E \) and \( (j, i) \in E \); we denote this edge by \( i \rightarrow j \). An edge between two adjacent nodes is directed if it is not undirected; if \( (i, j) \in E \), we denote it by \( i \rightarrow j \). The skeleton of \( \mathcal{G} \) is the set of all edges without taking the direction into account, that is all \( (i, j) \), such that \( (i, j) \in E \) or \( (j, i) \in E \). The number of edges in a graph is the size of the skeleton, i.e. undirected edges count as one.

A path \( \langle i_1, \ldots, i_n \rangle \) in \( \mathcal{G} \) is a sequence of (at least two) distinct vertices \( i_1, \ldots, i_n \), such that there is an edge between \( i_k \) and \( i_{k+1} \) for all \( k = 1, \ldots, n-1 \). If \( (i_k, i_{k+1}) \in E \) and \( (i_{k+1}, i_k) \notin E \) for all \( k \) we speak of a directed path between \( i_1 \) and \( i_n \) and call \( i_n \) a descendant of \( i_1 \). We denote all descendants of \( i \) by \( \text{DE}_i^\mathcal{G} \) and all non-descendants of \( i \) by \( \text{ND}_i^\mathcal{G} \). We call all a node \( j \) such that \( i \) is a descendant of \( j \) an ancestor of \( i \) and denote the set by \( \text{AN}_i^\mathcal{G} \). A path \( \langle i_1, \ldots, i_n \rangle \) is called a semi-directed cycle if \( (i_j, i_{j+1}) \in E \) for \( j = 1, \ldots, n \) with \( i_{n+1} = i_1 \) and at least one of the edges is oriented as \( i_j \rightarrow i_{j+1} \). If \( (i_{k-1}, i_k) \in E \) and \( (i_{k+1}, i_k) \in E \), as well as \( (i_k, i_{k-1}) \notin E \) and \( (i_k, i_{k+1}) \notin E \), \( i_k \) is called a collider on this path. \( \mathcal{G} \) is called a partially directed acyclic graph (PDAG) if there is no directed cycle, i.e. no pair \( (j, k) \), such that there are directed paths from \( j \) to \( k \) and from \( k \) to \( j \). \( \mathcal{G} \) is called a chain graph if there is no semi-directed cycle between any pair of nodes. Two nodes \( j \) and \( k \) in a chain graph are called equivalent if there exists a path
between \(j\) and \(k\) consisting only of undirected edges. A corresponding equivalence class of nodes (i.e. a (maximal) set of nodes that is connected by undirected edges) is called a **chain component**. \(\mathcal{G}\) is called a **directed acyclic graph** (DAG) if it is a PDAG and all edges are directed. A path in a DAG between \(i_1\) and \(i_n\) is **blocked by a set** \(S\) (with neither \(i_1\) nor \(i_n\) in this set) whenever there is a node \(i_k\), such that one of the following two possibilities hold: 1. \(i_k \in S\) and \(i_{k-1} \rightarrow i_k \rightarrow i_{k+1}\) or \(i_k \leftarrow i_{k-1} \leftarrow i_{k+1}\) or \(i_k \leftarrow i_{k-1} \leftarrow i_k\); or 2., \(i_{k-1} \rightarrow i_k \leftarrow i_{k+1}\) and neither \(i_k\) nor any of its descendants is in \(S\). We say that two disjoint subsets of vertices \(A\) and \(B\) are **d-separated** by a third (also disjoint) subset \(S\) if every path between nodes in \(A\) and \(B\) is blocked by \(S\). The joint distribution \(\mathcal{L}(X)\) is said to be **Markov with respect to the DAG** \(\mathcal{G}\) if

\[
A, B \text{ d-sep. by } C \Rightarrow X_A \perp X_B \mid X_C
\]

for all disjoint sets \(A, B, C\). \(\mathcal{L}(X)\) is said to be **faithful to the DAG** \(\mathcal{G}\) if

\[
A, B \text{ d-sep. by } C \Leftarrow X_A \perp X_B \mid X_C
\]

for all disjoint sets \(A, B, C\). Throughout this work, \(\perp\) denotes (conditional) independence.

We denote by \(\mathcal{M}(\mathcal{G})\) the set of distributions that are Markov with respect to \(\mathcal{G}\):

\[
\mathcal{M}(\mathcal{G}) := \{\mathcal{L}(X) : \mathcal{L}(X) \text{ is Markov wrt } \mathcal{G}\}.
\]

Two DAGs \(\mathcal{G}_1\) and \(\mathcal{G}_2\) are **Markov equivalent** if \(\mathcal{M}(\mathcal{G}_1) = \mathcal{M}(\mathcal{G}_2)\). This is the case if and only if \(\mathcal{G}_1\) and \(\mathcal{G}_2\) satisfy the same set of \(d\)-separations, that means the Markov condition entails the same set of (conditional) independence conditions. A set of Markov equivalent DAGs (so-called Markov equivalence class) can be represented by a completed PDAG which can be characterized in terms of a chain graph with undirected and directed edges (Andersson et al., 1997): this graph has a directed edge if all members of the Markov equivalence class have such a directed edge, it has an undirected edge if some members of the Markov equivalence class have an edge in the same direction and some members have an edge in the other direction, and it has no edge if all members in the Markov equivalence class have no corresponding edge.

**Appendix B. Proof of Proposition 6**

Let us denote by \(A\) the set of pairs \((i, j)\) appearing in Definition 4 and by \(B\) the corresponding set of pairs in Proposition 6. We will show that \(A = B\).

\(A \subseteq B\): Consider \((i, j) \in A\).

Case (1): If \(X_j \in \text{PA}_{X_i}^H\), then \(p_H(x_j \mid \text{do}(X_i = \hat{x}_i)) = p(x_j)\). We will now show that \(p_G(x_j \mid \text{do}(X_i = \hat{x}_i)) = p(x_j)\) whenever \(X_i\) is not an ancestor of \(X_j\) in \(\mathcal{G}\) (and therefore \(X_i\) must be an ancestor of \(X_j\)).

\[
p_G(x_j \mid \text{do}(X_i = \hat{x}_i)) = \int_{\text{anc}(j)} \int_{\text{non-anc}(j)} p(x_1, \ldots, x_p \mid \hat{x}_i) \, dx_{\text{non-anc}(j)} \, dx_{\text{anc}(j)}
\]

\[
(1) = \int_{\text{anc}(j)} \prod_{k \in \text{anc}(j)} p(x_k \mid x_{\text{pa}(k)}) \, dx_{\text{anc}(j)}
\]

\[
= \int_{\text{anc}(j)} \int_{\text{non-anc}(j)} p(x_1, \ldots, x_p) \, dx_{\text{non-anc}(j)} \, dx_{\text{anc}(j)} = p(x_j)
\]
Equation (†) holds since parents of ancestors of \( j \) are ancestors of \( j \), too. One can therefore integrate out all non-ancestors (starting at the sink nodes).

Case (2): If, on the other hand, \( X_j \not\in \text{PA}^H_{X_i} \), then it follows by Lemma 5(i) that \( \text{PA}^H_{X_i} \) does not satisfy (*). In both cases we have \((i,j) \in B\).

\( A \supseteq B \): Now consider \((i,j) \in B\).

Case (1): If \( X_j \in \text{PA}^H_{X_i} \), then, again, \( p_H(x_j | \text{do}(X_i = \hat{x}_i)) = p(x_j) \) and \( X_j \in \text{DE}^G_{X_i} \).

Case (2): If \( X_j \not\in \text{PA}^H_{X_i} \), then \( \text{PA}^H_{X_i} \) does not satisfy (*) and Lemma 5(ii) implies \( p_G(x_j | \text{do}(X_i = \hat{x}_i)) \neq p_H(x_j | \text{do}(X_i = \hat{x}_i)) \). In both cases we have \((i,j) \in A\).

Appendix C. Proof of Proposition 7

\( \Leftarrow \): Assume that \( G \leq H \). We will use Proposition 6 to show that the SID is zero. If \( j \in \text{DE}^G_{X_i} \), then \( j \in \text{DE}^H_{X_i} \) which implies that \( j \not\in \text{PA}^H_{X_i} \). It therefore remains to show that any set \( Z \) that satisfies (*) for \((H,i,j)\) satisfies (*) for \((G,i,j)\), too. The first part of the condition is satisfied since any node that lies on a directed path in \( G \) lies on a directed path in \( H \). The second part holds because any non-directed path in \( G \) is also a path in \( H \) and must therefore be blocked by \( Z \). If a path is blocked in a DAG it is always blocked in the smaller DAG, too.

\( \Rightarrow \): Suppose now that \( G \) contains an edge \( i \to j \) and that \( i \not\in \text{PA}^H_{X_j} \). We now construct an observational distribution \( p(.) \) according to \( X_k = N_k \) for all \( k \neq j \), \( X_j = \hat{x}_i + N_j \) and \( N_k \text{ iid } N(0,1) \) for all \( k \). This distribution is certainly Markov with respect to \( G \). We find for any \( \hat{x}_j \) that \( p_G(x_i | \text{do}(X_j = \hat{x}_j)) = p(x_i) \) and at the same time \( p_H(x_i | \text{do}(X_j = \hat{x}_j)) = p(x_i | \hat{x}_j) \neq p(x_i) \). Therefore, the SID is different from zero.

Appendix D. Proof of Proposition 8

The different statements can be proved as follows:

(1a) When the SHD is zero, each node has the same set of parents in \( G \) and \( H \). Therefore all adjustment sets are valid and the SID is zero, too.

(1b) The bound clearly holds since a SHD of one can change the set of parents of at most two nodes. Extending the example shown in Figure 2 from Example 1 to \( p-2 \) different \( Y \) nodes proves that the bound is sharp.

(2) Choosing \( G \) the empty graph and \( H \) (any) fully connected graph yields the result.

Appendix E. Computing causal effects for linear Gaussian structural equation models

Consider a linear Gaussian structural equation model with known parameters. The covariance matrix \( \Sigma_X \) of the \( p \) random variables can then be computed from the structural
coefficients and the noise variances. For a given graph we are also able to compute the causal effects analytically. Since the intervention distribution $L(X_j \mid \text{do}(X_i = \hat{x}_i))$ is again Gaussian with mean depending linearly on $\hat{x}_i$ and variance not depending on $\hat{x}_i$, we can summarize it by the so-called causal effect

\[ C_{ij} := \frac{\partial}{\partial \hat{x}_i} E [X_j \mid \text{do}(X_i = \hat{x}_i)]. \]

Let us denote by $\Sigma_2$ the submatrix of $\Sigma_X$ with rows and columns corresponding to $X_i, \text{PA}_{X_i}$, and by $\Sigma_1$ the $(1 \times (\#\text{PA}_{X_i} + 1))$-vector corresponding to the row from $X_j$ and columns from $X_i, \text{PA}_{X_i}$ of $\Sigma_X$. Then,

\[ C_{ij} = \Sigma_1 \cdot \Sigma_2^{-1} \cdot (1, 0 \ldots, 0)^T. \]
Appendix F. Algorithms

We present here pseudo code of two algorithms for computing the SID.

**Algorithm 1** Computing structural intervention distance

1: **input** two adjacency matrices $G$ and $H$ of size $p \times p$.
2: $\text{incorrectCausalEffects} \leftarrow \text{ZeroMatrix}(p,p)$
3: $\text{PathMatrix} \leftarrow \text{computePathMatrix}(G)$
4: **for** $i = 1$ to $p$ **do**
5: $\text{paG} \leftarrow \text{which}(G[i,i] == 1)$  \# parents of $i$ in $G$
6: $\text{paH} \leftarrow \text{which}(H[i,i] == 1)$  \# parents of $i$ in $H$
7: $\tilde{G} \leftarrow G$ without edges leaving $\text{paH}$ with a tail ($\text{paH} \rightarrow$)
8: $\text{PathMatrix2} \leftarrow \text{computePathMatrix}(\tilde{G})$
9: $\text{reachableOnNonDirectedPath} \leftarrow \text{rondp}(G,i,\text{paH},\text{PathMatrix},\text{PathMatrix2})$
10: **for** $j \neq i$ from 1 to $p$ **do**
11: $ijGNull, ijHNull, finished \leftarrow \text{false}$
12: **if** $\text{PathMatrix}[i,j] == 0$ **then**
13: $ijGNull \leftarrow \text{true}$  \# $G$ predicts the causal effect to be zero
14: **end if**
15: **if** $j$ is parent from $i$ in $H$ **then**
16: $ijHNull \leftarrow \text{true}$  \# $H$ predicts the causal effect to be zero
17: **end if**
18: **if** $\text{ijGNull and ijHNull}$ **then**
19: $\text{incorrectCausalEffects}[i,j] \leftarrow 1$
20: $\text{finished} \leftarrow \text{true}$  \# one mistake if only $H$ predicts zero
21: **end if**
22: **if** $\text{ijGNull and ijHNull or paG == paH}$ **then**
23: $\text{finished} \leftarrow \text{true}$  \# no mistakes if both predictions coincide
24: **end if**
25: **if** $\text{!finished}$ **then**
26: $\text{childrenOnDirectedPath} \leftarrow$ children of $i$ in $G$ that have $j$ as a descendant
27: **if** $\text{sum(PathMatrix[childrenOnDirectedPath,paH]) > 0}$ **then**
28: $\text{incorrectCausalEffects}[i,j] \leftarrow 1$  \# part (1)
29: **end if**
30: **if** $\text{reachableOnNonDirectedPath[j] == 1}$ **then**
31: $\text{incorrectCausalEffects}[i,j] \leftarrow 1$  \# part (2)
32: **end if**
33: **end if**
34: **end for**
35: **end for**
36: **output** $\text{sum(incorrectCausalEffects)}$
Algorithm 2 Finding all reachable nodes on non-directed paths (rondp)

1: **input** adjacency matrix $G$ of size $p \times p$, node $i$, PaH, PathMatrix, PathMatrix2.
2: $Pai \leftarrow \text{which}(G[i,\cdot] == 1)$  \ # parents of $i$ in $G$
3: $Chi \leftarrow \text{which}(G[\cdot,i] == 1)$  \ # children of $i$ in $G$
4: $toCheck \leftarrow Pai + p$ and $Chi$  \ # an index $> p$ indicates that this node is reached
   \ # with an outgoing edge, $\leq p$ with an incoming edge
5: $reachableNodes \leftarrow Pai$ and $Chi$
6: $reachableOnNonDirectedPath \leftarrow Pai + p \cdot \text{len}(Pai)$
7: $G[i,Chi] \leftarrow 0$
8: $G[i,Pai] \leftarrow 0$
9: **for all** $currentNode$ **in** $toCheck$ **do**
10: $PacN \leftarrow \text{which}(G[\cdot,currentNode] == 1)$
   \ # If one of the Pa of $currentNode$ (cN) is reachable and is not included in PaH,
   \ # then cN is reachable, too (i.e. $\exists$ path from $i$ that is not blocked by PaH).
11: $PacN2 \leftarrow PacN \setminus \text{PaH}$
12: $\text{reachabilityMatrix}[PacN2, currentNode] \leftarrow 1$  \ # same index rule as for $toCheck$
13: $\text{reachabilityMatrix}[PacN2 + p, currentNode] \leftarrow 1$
   \ # If $currentNode$ (cN) is reachable with $\rightarrow$ cN and cN is
   \ # an ancestor of PaH, then parents are reachable, too.
14: **if** $currentNode$ is an ancestor of PaH **then**
15: $\text{reachabilityMatrix}[currentNode, PacN + p] \leftarrow 1$
16: add $PacN$ to $toCheck$  \ # $toCheck$ is a set; it contains each index only once
17: **end if**
18: **if** $currentNode$ is not in PaH **then**
19: $\text{reachabilityMatrix}[currentNode + p, PacN + p] \leftarrow 1$
20: add $PacN$ to $toCheck$  \ # $toCheck$ is a set; it contains each index only once
21: **end if**
22: \ ...  \ # Apply analogous rules to the children ChcN of $currentNode$.
23: **end for**
24: $\text{reachabilityPathMatrix} \leftarrow \text{computePathMatrix}(\text{reachabilityMatrix})$
25: update $reachableNodes$ using $\text{reachabilityPathMatrix}$
26: update $reachableOnNonDirectedPath$ using $\text{reachabilityPathMatrix}$
   \ # We may have missed some nodes: if there is a directed (non-blocked) path
   \ # from $i$ to $k$, then all parents of $k$ are reachable from $i$ on a non-directed path.
27: add more nodes to $reachableOnNonDirectedPath$: Use PathMatrix2 to look for nodes
   \ $j$ as in $i \rightarrow \ldots \rightarrow k \leftarrow j$ ($k$ being a descendant of $i$ with no node from PaH in between)
28: remove all entries between $k$ and $j$ in $\text{computePathMatrix}$
29: update $reachableOnNonDirectedPath$ using $\text{reachabilityPathMatrix}$
30: $reachableOnNonDirectedPath \leftarrow \{j \mid j \text{ or } j + p \in reachableOnNonDirectedPath\}$
31: **output** $reachableOnNonDirectedPath$
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