



HAL
open science

Latent Instrumental Variables as Priors in Causal Inference based on Independence of Cause and Mechanism

Nataliya Sokolovska, Pierre-Henri Wuillemin

► **To cite this version:**

Nataliya Sokolovska, Pierre-Henri Wuillemin. Latent Instrumental Variables as Priors in Causal Inference based on Independence of Cause and Mechanism. 2020. hal-02897093

HAL Id: hal-02897093

<https://hal.science/hal-02897093v1>

Preprint submitted on 16 Jul 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Latent Instrumental Variables as Priors in Causal Inference based on Independence of Cause and Mechanism

Nataliya Sokolovska

NutriOmics, Sorbonne University
Paris, France

nataliya.sokolovska@sorbonne-universite.fr

Pierre-Henri Wuillemin

LIP6, Sorbonne University
Paris, France

pierre-henri.wuillemin@lip6.fr

Abstract

Causal inference methods based on conditional independence construct Markov equivalent graphs, and cannot be applied to bivariate cases. The approaches based on independence of cause and mechanism state, on the contrary, that causal discovery can be inferred for two observations. In our contribution, we challenge to *reconcile* these two research directions. We study the role of latent variables such as latent instrumental variables and hidden common causes in the causal graphical structures. We show that the methods based on the independence of cause and mechanism, *indirectly contain traces of the existence of the hidden instrumental variables*. We derive a novel algorithm to infer causal relationships between two variables, and we validate the proposed method on simulated data and on a benchmark of cause-effect pairs. We illustrate by our experiments that the proposed approach is simple and extremely competitive in terms of empirical accuracy compared to the state-of-the-art methods.

1 Introduction

Causal inference purely from non-temporal observational data is challenging. Instead of learning causal structure of an entire dataset, some researchers focus on analysis of causal relations between two variables only. The state-of-the-art conditional independence-based causal discovery methods (see, e.g., [16, 24]) construct graphs that are Markov equivalent, but these methods are not applicable in the case of two variables, since $X \rightarrow Y$ and $Y \rightarrow X$ are Markov equivalent.

The statistical and probabilistic causal inference methods based on assumptions of independence of cause and mechanism (see [17] for general overview) appeared relatively recently, and achieve very reasonable empirical results. The main idea behind these methods is as follows: if a simple function that fits data exists, then it is likely that it also describes a causal relation in the data.

The main goal of our paper is to try to reconcile these two modern viewpoints on causal inference: the research direction initiated by [24, 16] which is based on the assumption of conditional independencies, and the more recent research avenue where the main claim is that causal inference between two observations only is feasible [21, 15, 4, 20, 22, 12] and whose theory relies on the independence of cause and mechanism.

To illustrate the intuition behind our approach, let us consider an example from [17] with altitude and temperature, where A is altitude, T is temperature, $P(A)$ are cities locations, $P(T|A)$ is the physical mechanism of temperature given altitude, and it can be shown that changing the cities locations $P(A)$, the conditional probability $P(T|A)$ does not change. The postulate of independence of cause and mechanism allows to infer the causal direction $A \rightarrow T$. Any latent variables are ignored in this case. However, the cities locations depend on a country, since each country has different urban policy, population density, etc. Thus, in this example $P(A)$ has at least one latent variable which is county C . However, no matter what country is chosen, the physical mechanism $P(T|A)$ holds, and the true underlying causal structure is $C \rightarrow A \rightarrow T$. A country defines distribution of cities. Having two or more countries leads to a family of distributions. This *mixture of probability distributions is independent* from $P(T|A)$. Thus, this example also explains what is meant under the *independence between probability distributions*.

Our contribution is multi-fold:

- Our main theoretical result is an alternative viewpoint on the recently appeared causal inference algorithms that are based on the independence of cause and mechanism¹.
- Assuming the existence of the hidden instrumental variables, we propose a novel method of causal inference. Since we consider a bivariate causal inference case where only X and Y are observed, we also propose an approach to estimate the latent instrumental variables for cases where the cluster assumption for X and Y holds.
- We investigate the role of latent common causes, and we propose a method to identify them.
- We validate our method on a synthetic data set on which we perform extensive numerical experiments, and on the Cause-Effect benchmark which is actively used by the causal inference community.

The paper is organized as follows. Section 2 discusses the state-of-the-art methods of bivariate causal inference. Preliminaries on the instrumental variables are provided in Section 3. We consider the role of the instrumental variables for causal inference, and we introduce our approach in Section 4. In Section 5, we discuss the results of our numerical experiments on synthetic, as well as on standard challenges. Concluding remarks and perspectives close the paper.

2 Related Work

In this section, we discuss the state-of-the-art methods of bivariate causal inference and the corresponding assumptions. In the current work, we focus on a family of causal inference methods which are based on a postulate telling that if $X \rightarrow Y$, then the marginal distribution $P(X)$ and the conditional distribution $P(Y|X)$ are independent [10, 9, 22]. These approaches provide causal directions based on the estimated conditional and marginal distributions from observed non-temporal data. Probably one of the oldest and well-studied models describing causal relations that are necessary to mention, are Structural Causal Models (SCM). A SCM where $X \rightarrow Y$ is defined as follows:

$$X = N_X, \quad Y = f_Y(X, N_Y), \tag{1}$$

where N_X and N_Y are independent. Given f_Y and the noise distributions P_{N_Y} and P_{N_X} , we can sample data following a SCM.

A recently proposed but already often used *Postulate of Independence of Cause and Mechanism* is formulated as follows (see, e.g., [10, 9, 22]). If X causes Y , then $P(X)$ and $P(Y|X)$ estimated from observational data contain no information about each other. Looking for a parallel between the postulate and the SCM, we assume that in a SCM, f_Y and P_{N_Y} contain no information about P_X and visa versa. The postulate describes the independence of mechanisms, and tells that a causal direction can be inferred from estimated marginal and conditional probabilities of random variables from a data set. In the following, we investigate this research direction.

It is not obvious how to formalise the independence of the marginal and conditional probabilities. A reasonable claim [17] is that an optimal measure of dependence is the algorithmic mutual information that relies on the description length in the sense of Kolmogorov complexity. Since the exact

¹Here, we follow the simplification used by [17], however, we are aware that the independence of our interest is between the *prior* of the cause and the mechanism.

computations are not feasible, there is a need for a practical and reliable approximation encoding that in a causal direction $P(X)$ and $P(Y|X)$ would require more compact model classes than in an anticausal direction.

Two families of methods of causal inference dealing with bivariate relations are often discussed. For a more general overview of causal structure learning see [6, 17]. Additive noise models (ANM) introduced by [7] and [18] is an attempt to describe causal relations between two variables. The ANM assume that if there is a function f and some noise E such that $Y = f(X) + E$, where E and X are independent, then the direction is inferred to $X \rightarrow Y$. A generalised extension of the ANM, called post-nonlinear models, was introduced by [26]. However, the known drawback of the ANM is that the model is not always suitable for inference on discrete tasks [3].

Another research avenue exploiting the asymmetry between cause and effect are the linear trace (LTr) method [27] and information-geometric causal inference (IGCI) [9]. If the true model is $X \rightarrow Y$, and if $P(X)$ is independent from $P(Y|X)$, then the trace condition is fulfilled in the causal direction, and violated in the anticausal one. The IGCI method exploits the fact that the density of the cause and the log slope of the function-transforming cause to effect are uncorrelated. However, for the opposite direction, the density of the effect and the log slope of the inverse of the function are positively correlated. The trace condition is proved under the assumption that the covariance matrix is drawn from a rotation invariant prior [10]. The method was generalized for non-linear cases [13], and it was shown that the covariance matrix of the mean embedding of the cause in reproducing kernel Hilbert space is free independent with the covariance matrix of the conditional embedding of the effect given cause. The case of high-dimensional variables is considered in [8] and [27], where the IGCI is considered. Here, the independence between probability distributions is based on the trace condition. The identifiability via the trace condition is proved [8, 17] for deterministic relations, and no theory exists for noisy cases which are much more relevant for real-life applications.

Origo [2] is a causal discovery method based on the Kolmogorov complexity. The Minimum Description Length (MDL) principle can be used to approximate the Kolmogorov complexity for real tasks. Namely, from algorithmic information viewpoint, if $X \rightarrow Y$, then the shortest program that computes Y from X will be more simple, or compact, than the shortest program computing X from Y . The obvious weakness of methods based on the Kolmogorov complexity, and also of Origo, is that the MDL only approximates Kolmogorov complexity, and involves unknown metric errors that are difficult to control. The empirical performance is highly dependent on a dataset, and Origo was reported to reach the state-of-the-art performance on the multivariate benchmarks (Acute inflammation, ICDM abstracts, Adult data set), however, it performs less accurately than the ANM on the univariate benchmark of cause-effect pairs with known ground truth (the Tübingen data set) [14]. We also use this benchmark for our experiments.

3 Independence of Probability Distributions and Instrumental Variables

Let X and Y be two correlated variables. In the settings considered by [17], in order to decide whether $X \rightarrow Y$ or $Y \rightarrow X$, it is proposed to check if the distributions $P(X)$ and $P(Y|X)$ are independent. As far as we know, this independence between distributions (and not between random variables) does not have any formal definition. However, some useful properties can be derived, and various criteria were constructed for different cases [21, 15, 4, 20, 22, 12]. In this paper, we adopt the following definition. Let $P(X, Y)$ be the joint distribution of X, Y in a population \mathcal{P} ; let $Q(X, Y)$ be the joint distribution of X, Y in another population \mathcal{Q} . If X is the cause of Y , the causal mechanism should be the same in the two distributions:

$$P(X, Y) = P(X) \cdot P(Y|X) \text{ and } Q(X, Y) = Q(X) \cdot P(Y|X),$$

i.e. $P(Y|X) = Q(Y|X)$, on the contrary, $P(X|Y) \neq Q(X|Y)$. More generally, for all mixed populations between \mathcal{P} and \mathcal{Q} , and then, for all mixtures $Q_\lambda = \lambda P + (1 - \lambda)Q$ with $\lambda \in [0, 1]$,

$$\forall \lambda \in [0, 1], Q_\lambda(X) \perp\!\!\!\perp Q_\lambda(Y|X) \iff Q_\lambda(Y|X) = P(Y|X).$$

Now we consider λ as a hyper-parameter for a (latent) prior I_X that allows to select the population ($P(X|I_X = 0) = P(X)$, $P(X|I_X = 1) = Q(X)$). In this meta-model, I_X and X are dependent, X and Y are dependent. But I_X and Y are independent conditionally to X . On the contrary, if we consider λ as a hyper-parameter for a (latent) prior I_Y , that allows to select the population

($P(Y|I_Y = 0) = P(Y)$, $P(Y|I_Y = 1) = Q(Y)$). In this meta-model, I_Y and Y are dependent, X and Y are dependent. But since, $P(X|Y) \neq Q(X|Y)$, I_Y and X are not independent, even conditionally to Y .

To provide some intuition behind such a mixture model: let $P(X)$ and $Q(X)$ be the distributions of cities locations in two different countries, and $P(Y|X)$ be a physical mechanism predicting weather given location. Then λ is the hyper-parameter controlling the proportion of observations in each country, and note that λ , $P(X)$, and also $Q(X)$ are independent from $P(Y|X)$.

Such a representation of the problem as a mixture model with latent priors, motivates our proposition to use models with instrumental latent variables.

The aim of models with *instrumental variables* [25, 5, 1] where X , Y , and I_X are observed, and U is an unobserved confounder, is to identify the causal effect of X on Y . Assuming that the relationships are linear, and applying a linear Gaussian structural causal model, one can write:

$$X = \alpha_0 + \alpha I_X + \delta U + \epsilon_X, \quad Y = \beta_0 + \beta X + \gamma U + \epsilon_Y, \quad (2)$$

where ϵ_X and ϵ_Y are noise terms, independent of each other. It is assumed, without loss of generality that U , ϵ_X , and ϵ_Y have mean zero. *Note that the common cause U can be absent*, and we are not going to assume that U exists when modelling dependencies between X and Y . The instrumental variable I_X is uncorrelated with ancestors of X and Y . The instrumental variable is a source of variation for X , and it only influences Y through X . Studying how X and Y respond to perturbations of I_X can help to deduce how X influences Y . A two-stage least squares [19] can be used to solve the problem.

Probability Distributions as Random Variables. Similarly to [8, 17], we consider probability distributions as random variables. $P(X)$ is a function of $X \in [0, 1]$, and, thus, they are random variables distributed in $[0, 1]$. Note that a model where a probability is randomly generated is an example of a hierarchical model, or of a model with priors, where some parameters are treated as random variables.

4 Latent Instrumental Variables for Causal Discovery

In this section, we show that the methods based on the independence of cause and mechanism, introduced by [21, 15, 4, 20, 22, 12], also *indirectly contain traces of the existence of the hidden instrumental variable*. It can be seen as follows. $P(X)$ generates X in the approaches proposed and investigated by the scientists mentioned above. In our method, we assume that X are generated by I_X . Therefore, there is a strong parallel between $P(X)$ and I_X which are both *priors for the observations*. So, our method also provides some intuition and interpretation of the recently proposed algorithms based on the independence between the “cause and the mechanism”. We provide some theoretical results on the independence of the causal mechanisms in terms of probability distributions and information theory. These results allow us to derive a novel algorithm of causal inference which is presented in this section below.

Our observations are X and Y , two one-dimensional vectors of the same length, and these variables are correlated. Here, we suppose that either causality between these variables exists, and either $X \rightarrow Y$, or $Y \rightarrow X$, or a common latent cause $X \leftarrow U \rightarrow Y$ can be identified, where U is a hidden variable that can impact X and/or Y . Let I_X and I_Y denote latent instrumental variables of X and Y respectively. In the current contribution, *we do not observe the instrumental variables, we assume that they exist*, and can be approximated. *We do not assume that U exists, however, we show how its existence can be deduced*, if it is the case.

Assumption 1. In case of observational non-temporal data, if I_X exists such that $I_X \rightarrow X$, and if I_Y exists such that $I_Y \rightarrow Y$, and if the random variables X and Y are correlated, then we assume that it is impossible that both $I_X \perp\!\!\!\perp Y|X$ and $I_Y \perp\!\!\!\perp X|Y$ hold.

Theorem 1. *Let X and Y be two correlated random variables, and they do not have any common cause. We assume that either X causes Y or visa versa. If there exists a random variable I_X such that $I_X \rightarrow X$, and if $I_X \perp\!\!\!\perp Y|X$, then we are able to infer causality and decide that $X \rightarrow Y$.*

Proof. Several directed acyclic graphs (DAGs) may be Markov equivalent [16, 24]. We assume that once an essential graph is found, the directed arcs of this graph are interpreted causally. Then, the only DAG which is interpreted causally, is the causal graph.

Under the assumption that $I_X \rightarrow X$, and if $I_X \perp\!\!\!\perp Y|X$, then the only possible directed graph is $I_X \rightarrow X \rightarrow Y$. In case where $I_X \not\perp\!\!\!\perp Y|X$, we get $I_X \rightarrow X \leftarrow Y$.

□

Theorem 2. *If the true causal structure is $I_X \rightarrow X \rightarrow Y$, and X and Y do not have any common cause, then $P(Y|X)$ does not contain any information about $P(X)$ and vice versa, however, $P(X|Y)$ and $P(Y)$ are not independent.*

Proof. Assume that $I_X \perp\!\!\!\perp Y|X$. Let us consider the relation between $P(Y|X)$ and $P(X)$. In the following, we treat $P(Y|X)$, $P(X|Y)$, $P(X)$, and $P(Y)$ as random variables. We can write:

$$P(Y|I_X, X) = P(Y|X). \quad (3)$$

Note that we do not have $P(X)$ in eq. (3) when we express $P(Y|X)$ for $I_X \rightarrow X \rightarrow Y$. Let us consider the relation between $P(X|Y)$ and $P(Y)$ for the same graphical structure. We get:

$$P(X|Y) = \frac{P(Y|X)P(X|I_X)}{P(Y)}, \quad (4)$$

where the form of the nominator is due to the fixed dependencies $I_X \perp\!\!\!\perp Y|X$. From eq. (4), we clearly see that $P(X|Y)$ is not independent from $P(Y)$ for this graphical structure. □

4.1 Construction of the Instrumental Variables

Assumption 2. (Cluster assumption.) For X and Y , the cluster assumption holds: data belonging to the same cluster share similar properties.

In some tasks the instrumental variables (IV) are observed, and their application is straightforward. In a number of applications, they are not provided. Here, we discuss how they can be approximated, and we draft a procedure to estimate the instrumental variables. In our experiments, in Section 5 we apply the proposed method for the IV construction. Note that the identification and characterisation of latent variables is a challenge in itself. Our work is slightly similar to [11, 23] in that we apply clustering methods to create the latent variables. Taking into account that only X and Y are observed, the instrumental variables can be constructed using either X , Y , or both, and an optimal choice of the variables that influence an IV is related to a graphical structure we try to identify and to orient. So, for a structure $I_X \rightarrow X \rightarrow Y$, I_X does not contain information about Y , and I_X has to be constructed from X only. On the contrary, in case of $X \rightarrow Y \leftarrow I_Y$, I_Y is not independent from X , and I_Y has to contain information about both X and Y .

We propose that the decision whether I_X and I_Y are to be constructed from one or two variables is taken by Algorithm 2. The proposed algorithm constructs the instrumental variables separately from X , Y (I_{X_X} , I_{Y_Y}), and from both ($I_{X_{XY}}$, $I_{Y_{YX}}$), and tests which instrumental variables are more relevant. We rely on clustering methods for the instrumental variables estimation, in our experiments, we apply the k-means clustering approach, however, other clustering approaches can be used. Algorithm 1 drafts the procedures to approximate the candidates for the IV.

Algorithm 2 compares the distance (we considered the Euclidean distance in our experiments but another measure, e.g., the Kullback-Leibler can be used) between I_{X_X} and $I_{X_{XY}}$, and between I_{Y_Y} and $I_{Y_{YX}}$. The intuition behind this criterion is as follows. If Y influences clustering of X less, than X impacts clustering of Y (the condition *if* ($\text{dist}(I_{X_X}, I_{X_{XY}}) < \text{dist}(I_{Y_Y}, I_{Y_{YX}})$) in the algorithm), then we apply I_X constructed from X only, and I_Y is constructed from X and Y . And visa versa. An important remark is that this criterion has a lot in common with the causal discovery methods based on the *Kolmogorov complexity* and the *MDL*: to infer causality, our criterion choses a simpler model.

4.2 A Symmetric Causal Inference Algorithm

Once the instrumental variables are fixed, e.g., as it is proposed in the previous section, we apply a symmetric algorithm sketched as a decision tree on Figure 1 based on the conditional (in)dependence tests. It takes I_X , I_Y , X , and Y , and returns a causal direction. Precisely, if a conditional independence test tells that $Y \perp\!\!\!\perp I_X|X$ is true, then $X \rightarrow Y$ inferred, otherwise we test whether $X \perp\!\!\!\perp I_Y|Y$, and if it is true, then Y causes X . The last case where X and Y are correlated but both $Y \perp\!\!\!\perp I_X|X$ and $X \perp\!\!\!\perp I_Y|Y$ are false, let us conclude that there is a common hidden cause $Y \leftarrow U \rightarrow X$.

5 Experiments

In this section, we illustrate the predictive efficiency of the proposed method on both artificial and real data sets.

Algorithm 1 Construction of IV Candidates

I_{X_X} (IV variable of X from X)
 Fix a number of clusters K
 Cluster $\{X_i\}_{i=1}^N$ into K clusters
for $i = 1 : N$ **do**
 I_{i,X_X} is the center of the cluster where
 X_i belongs
end for
 $I_{X_{XY}}$ (IV variable of X from X and Y)
 Fix a number of clusters K
 Cluster $\{X_i, Y_i\}_{i=1}^N$ into K clusters
for $i = 1 : N$ **do**
 $I_{i,X_{XY}}$ is the 1st coordinate (corresponding to X) of the clusters centres where
 (X_i, Y_i) belongs
end for
 I_{Y_Y} (IV variable of Y from Y)
 is constructed similarly to the IV variable of X from X
 $I_{Y_{YX}}$ (IV variable of Y from X and Y)
 is constructed similarly to the IV variable of X from (X, Y) (Take the 2nd coordinate of the clusters centres)

Algorithm 2 Approximation of the Instrumental Variables (IV) I_X and I_Y from X and Y .

Input: Observations X and Y , a clustering algorithm
Output: Instrumental variables I_X and I_Y
 // Construct instrumental variables to be tested
 Construct IV of X , I_{X_X} using X only
 Construct IV of X , $I_{X_{XY}}$ using X and Y
 Construct IV of Y , I_{Y_Y} using Y only
 Construct IV of Y , $I_{Y_{YX}}$ using X and Y
 // Take the decision which IV to use
if ($\text{dist}(I_{X_X}, I_{X_{XY}}) < \text{dist}(I_{Y_Y}, I_{Y_{YX}})$) **then**
 // the IV of X is constructed from X only
 $I_X = I_{X_X}$
 // the IV of Y is constructed from both X and Y
 $I_Y = I_{Y_{YX}}$
else
 // the IV of Y is constructed from Y
 $I_Y = I_{Y_Y}$
 // the IV of X is constructed from X and Y
 $I_X = I_{X_{XY}}$
end if

5.1 Simulated Data

We consider simple discrete and continuous scenarios. In the discrete case, we fix the structures and the probability distributions on the graphs, and generate binary variables. In the continuous case, we use a Gaussian distribution. We generate the instrumental variables I_X and I_Y , X and Y , and the hidden variable U . We use the `bnlearn` R package to construct the synthetic data sets, we also use the conditional independence tests from the same package. For our discrete setting with binary variables, we apply an asymptotic mutual information independence test `ci.test(test='mi')`, and for the continuous setting with Gaussian variables, the exact t-test for Pearson's correlation `ci.test(test='cor')`. Note that the above mentioned conditional independence tests from the `bnlearn` R package return "big" p-values if variables are conditionally independent, and the p-values are small (with an arbitrary threshold 0.05) for dependent variables.

We consider and simulate discrete and continuous data for two following scenarios: 1) $X \rightarrow Y$, and $X \leftarrow U \rightarrow Y$. We test a various number of observations, from 10 to 10,000, and we observe that in the discrete case, even for such a simple problem as one with variables taking binary values, a big number of observations is needed to obtain a reasonable performance. Figure 2 illustrates the p-values of the conditional independence tests for the discrete (two left plots) and continuous (two right plots) settings. We show the results for both cases $X \perp\!\!\!\perp I_Y|Y$ and $Y \perp\!\!\!\perp I_X|X$. We observe

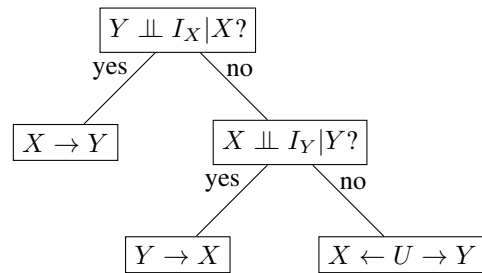


Figure 1: A Symmetric Causal Inference Algorithm

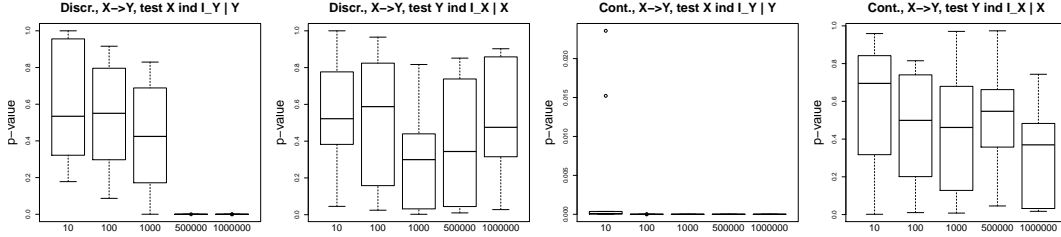


Figure 2: Simulated data. Ground truth: $X \rightarrow Y$. Two plots on the left: discrete data; two plots of the right: continuous data. The p-values of an asymptotic mutual information test (for the discrete case) and an exact t-test for Pearson’s correlation (the continuous case) as a function of the number of observations (x-axis).

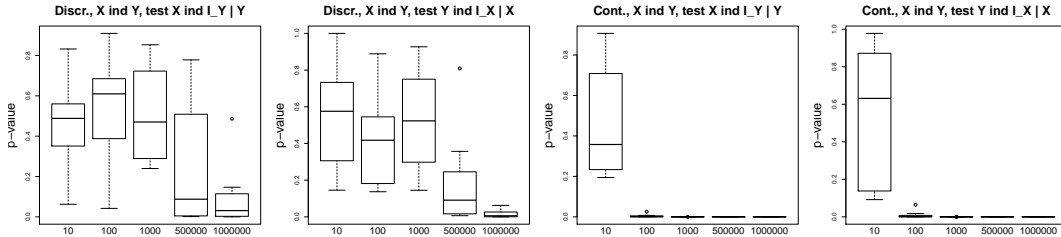


Figure 3: Simulated data. Ground truth: $X \perp\!\!\!\perp Y|U$. On the left: two plots for the discrete setting; on the right: two plots for the continuous setting. The p-values as a function of the number of observations (x-axis).

that for the ground truth $X \rightarrow Y$, $X \perp\!\!\!\perp I_Y|Y$ asymptotically converges to small p-values (close to 0), and $Y \perp\!\!\!\perp I_X|X$ returns big p-values even for big number of observations.

Figure 3 shows our results for the scenario $X \leftarrow U \rightarrow Y$. For the discrete and continuous experiments, we test whether $Y \perp\!\!\!\perp I_X|X$ and whether $X \perp\!\!\!\perp I_Y|Y$. We see that the variables are not independent. On Figure 4, we demonstrate the p-values of the conditional independence test $Y \perp\!\!\!\perp X|U$, what is more a sanity check, and we observe that in this case where the ground truth is $X \leftarrow U \rightarrow Y$, the p-values are far from 0 for both continuous and discrete scenarios.

5.2 Cause-Effect Pairs

We have tested the proposed algorithm on the benchmark collection of the cause-effect pairs, obtained from <http://webdav.tuebingen.mpg.de/cause-effect>, version 1.0. The data set contains 100 pairs from different domains, and the ground truth is provided. The goal is to infer which variable is the cause and which is the effect.

The pairs 52 – 55, 70 – 71, and 81 – 83 are excluded from the analysis, since they are multivariate problems. Note that each pair has an associated weight, provided with the data set, since several cause-effect pairs can come from the same scientific problem, and in a number of publications reporting results on this data set, the accuracy is a weighted average. We apply the proposed method, described in Section 4, to infer causality on the benchmark data. On Figure 5, we show the standard

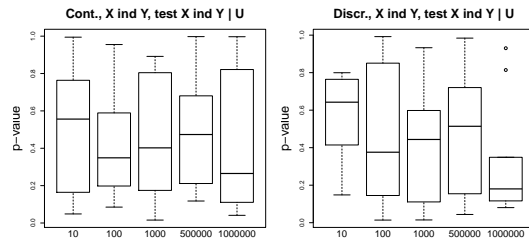


Figure 4: Simulated data. Ground truth: $X \perp\!\!\!\perp Y|U$. The results of the conditional independence tests for $X \perp\!\!\!\perp Y|U$ for continuous (on the left) and discrete (on the right) data. On the x-axis: the number of observations.

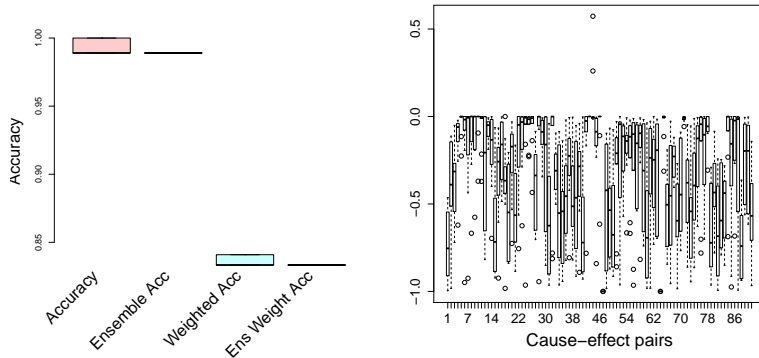


Figure 5: On the left: accuracy on the Cause-Effect Benchmark. On the right: the difference between the test statistics $X \perp\!\!\!\perp I_Y|Y$ and $Y \perp\!\!\!\perp I_X|X$.

(unweighted) accuracy and the weighted accuracy where the weights for each observation pair are given in the data set. To increase the stability and accuracy, we also propose a scenario where we split the data into k -folds, carry out causal inference on each fold separately, and take an ensemble decision on the causal direction. The accuracy for such an ensemble approach is also shown on Figure 5 for weighted accuracy using the ensemble method and the unweighted ensemble result. The number of folds in our experiments is 10. In our experiments, we show both the weighted and unweighted accuracy. Speaking about the state-of-the-art results on the Cause-Effect pairs, it was reported that Origo [2] achieves 58% accuracy, and the Additive Noise models (ANM) [18] reach $72 \pm 6\%$. Figure 5 illustrates that the proposed method outperforms the state-of-the-art algorithms: the weighted accuracy which is compared to the above mentioned methods is 83.2%. Note that the ensemble method reduced the variance significantly.

Figure 5 shows our results for the case where the number of clusters, i.e., modalities of the hidden instrumental variables is set to 15 both for I_X and I_Y . We tested different numbers of clusters for the instrumental variables construction (see Section 4.1 for details). For the current task, we did not notice any important impact on the result, however, taking extremely small (2-3) and big (70 - 100) numbers of clusters degrades the performance.

What is central and what is interesting to look at, are the p-values of the conditional independence tests (here the exact t-test for Pearson’s correlation from `bnlearn` R package) $X \perp\!\!\!\perp I_Y|Y$ and $Y \perp\!\!\!\perp I_X|X$. On Figure 5 on the right we show their difference. If the p-values of the test $X \perp\!\!\!\perp I_Y|Y$ are small (that is X and I_Y are not independent given Y) and the results of $Y \perp\!\!\!\perp I_X|X$ are relatively big (or bigger than ones of $X \perp\!\!\!\perp I_Y|Y$) telling that Y and I_X are independent given X , then the plotted difference is negative. It is exactly what is observed for almost all cause-effect pairs.

6 Conclusions

We challenged to bring together two principle research avenues on causal inference, i.e. causal inference using conditional independence and methods based on the postulate of independence of cause and mechanism. The causal inference methods based on the independence of cause and mechanism, or, to be precise, between the prior and the mechanism, and that consider probability distributions as random variables, appear more and more often in the machine learning community. In this contribution, we provide some theoretical foundations for this family of algorithms. Our main message is that the role of the hidden instrumental variables can not be neglected.

We propose an algorithm to estimate the latent instrumental variables efficiently. We also introduce a simple (and symmetric) algorithm to perform causal inference for the case of only two observed variables, where the corresponding instrumental variables are approximated. Our original approach is simple to implement, since it is based on a clustering algorithm (we used the k -means clustering, but any other clustering method can be tested) and on conditional independence tests. It can be applied to both discrete and continuous data, and we have shown that it is extremely competitive compared to the state-of-the-art methods on a real benchmark, where a cluster assumption holds.

Currently, we consider an extension of the proposed algorithm to more complex graphs, and potentially huge applications such as modelling gene interactions. Another avenue of research are novel metrics to measure the conditional independence of variables.

References

- [1] J. Angrist and A. Krueger. Instrumental variables and the search for identification: From supply and demand to natural experiments. *Journal of Economic Perspectives*, 15(4):69–85, 2001.
- [2] K. Budhathoki and J. Vreeken. Causal inference by compression. In *ICDM*, 2016.
- [3] P. Bühlmann, J. Peters, and J. Ernest. Cam: Causal additive models, high-dimensional order search and penalized regression. *Annals of statistics*, 42:2526–2556, 2014.
- [4] P. Daniusis, D. Janzing, J.M. Mooij, J. Zscheischler, B. Steudel, K. Zhang, and B. Schölkopf. Inferring deterministic causal relations. In *UAI*, 2010.
- [5] J. Heckman. Instrumental variables: A study of implicit behavioral assumptions used in making program evaluations. *Journal of Human Resources*, 32(3):441–462, 1997.
- [6] C. Heinze-Deml, M. H. Maathuis, and N. Meinshausen. Causal structure learning. In *arXiv:1706.09141*, 2017.
- [7] P. Hoyer, D. Janzing, J. Mooij, J. Peters, and B. Schölkopf. Nonlinear causal discovery with additive noise models. In *NIPS*, 2009.
- [8] D. Janzing, P. O. Hoyer, and B. Schölkopf. Telling cause from effect based on high-dimensional observations. In *ICML*, 2010.
- [9] D. Janzing, J. Mooij, K. Zhang, J. Lemeire, J. Zscheischler, P. Daniusis, B. Steudel, and B. Schölkopf. Information-geometric approach to inferring causal directions. *Artificial Intelligence*, 2012.
- [10] D. Janzing and B. Schölkopf. Causal inference using the algorithmic Markov condition. *IEEE Transactions on Information Theory*, 56(10):5168–5194, 2010.
- [11] D. Janzing, E. Sgouritsa, O. Stegle, J. Peters, and B. Schölkopf. Detecting low-complexity unobserved causes. In *UAI*, 2011.
- [12] F. Liu and L. Chan. Causal inference on discrete data via estimating distance correlations. *Neural Computation*, 28, 2016.
- [13] F. Liu and L.-W. Chan. Causal inference on multidimensional data using free probability theory. *IEEE Transactions on Neural Networks and Learning Systems*, 2017.
- [14] J. M. Mooij, J. Peters, D. Janzing, J. Zscheischler, and B. Schölkopf. Distinguishing cause from effect using observational data: methods and benchmarks. *JMLR*, 17, 2016.
- [15] G. Parascandolo, N. Kilbertus, M. Rojas-Carulla, and B. Schölkopf. Learning independent causal mechanisms. In *ICML*, 2018.
- [16] J. Pearl. *Causality: Models, Reasoning and Inference*. Cambridge University Press, 2nd edition, 2009.
- [17] J. Peters, D. Janzing, and B. Schölkopf. *Elements of causal inference*. The MIT Press, 2017.
- [18] J. Peters, J. Mooij, D. Janzing, and B. Schölkopf. Causal discovery with continuous additive noise models. *JMLR*, 1(15):2009–2053, 2014.
- [19] T. Sawa. The exact sampling distribution of ordinary least squares and two-stage least squares estimators. *Journal of the American Statistical Association*, 64(327):923–937, 2012.
- [20] B. Schölkopf, Janzing D., J. Peters, E. Sgouritsa, and K. Zhang. On causal and anticausal learning. In *ICML*, 2012.
- [21] B. Schölkopf, D. Janzing, J. Peters, E. Sgouritsa, K. Zhang, and J.M. Mooij. Semi-supervised learning in causal and anticausal settings. *Empirical Inference*, pages 129–141, 2013.
- [22] E. Sgouritsa, D. Janzing, P. Hennig, and B. Schölkopf. Inference of cause and effect with unsupervised inverse regression. In *AISTATS*, 2015.
- [23] E. Sgouritsa, D. Janzing, J. Peters, and B. Schölkopf. Identifying finite mixtures of nonparametric product distributions and causal inference of confounders. In *UAI*, 2013.

- [24] P. Spirtes, C. Glymour, and R. Scheines. *Causation, Prediction, and Search*. MIT Press, 2000.
- [25] P. G. Wright. *The Tariff on animal and vegetable oils*. Investigations in international commercial policies. New York, The Macmillan Company, 1928.
- [26] K. Zhang and A. Hyvärinen. On the identifiability of the post-nonlinear causal models. In *UAI*, 2009.
- [27] J. Zscheischler, D. Janzing, and K. Zhang. Testing whether linear equations are causal: a free probability theory approach. In *UAI*, 2011.