ETHzürich

AI Center Projects in Machine Learning

Causal Discovery via Conditional Divergence

Soel Micheletti, Yunshu Ouyang, Alexander Hägele Department of Computer Science, ETH Zurich

1 Introduction

4 Results & Discussion

Distinguishing cause and effect is a fundamental problem in science. The most elementary bivariate case, however, is already highly challenging using solely observational data [5].

Formally, given two random variables X and Y, we want to distinguish between three cases:

1. X causes Y (noted $X \rightarrow Y$).

 $2. X \leftarrow Y.$

Novel Divergence Measures

AUROC of divergence measures for different datasets

| CCS | 0.744 | 0.905 | 0.960 | 0.897 | 0.613 | 0.685 | 0.566 | 0.584 |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|
| CHD | 0.750 | 0.914 | 0.976 | 0.905 | 0.627 | 0.676 | 0.580 | 0.574 |
| CKL | 0.744 | 0.910 | 0.955 | 0.893 | 0.604 | 0.687 | 0.575 | 0.584 |

3. X and Y are not causally related (either because they are independent or because of confounding phenomena).

The central actor of our analysis is CDCI [1], a novel algorithm that achieves stateof-the-art performance. Our contributions include the proposal of two extensions, and an empirical performance analysis in the presence of hidden confounders. We release an open source package available on PyPI [4].

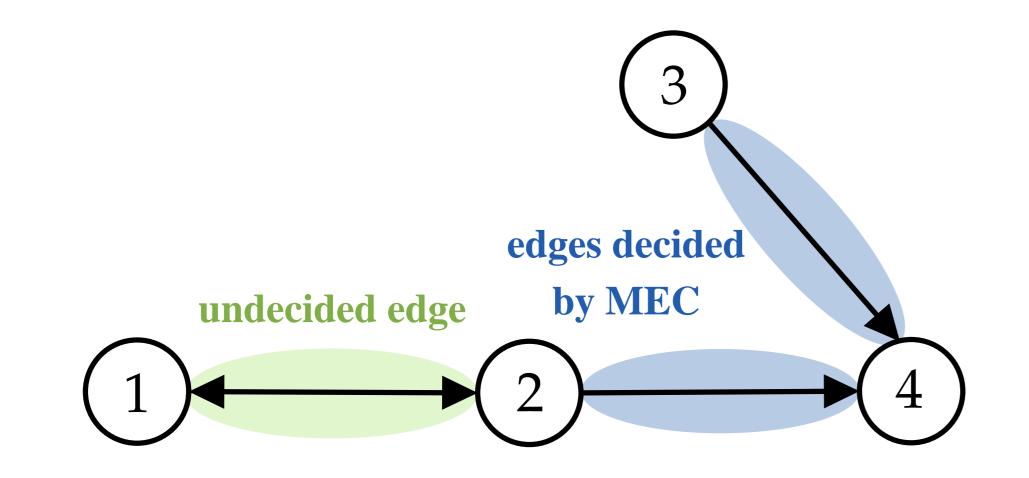


Figure 1: An example graph with one undecided edge in the MEC. CDCI can help distinguish the edge direction based on conditional divergence of variables.

2 Method Overview

CDCI relies on the fundamental assumption that if $X \rightarrow Y$, then the conditional distribution Pr[Y|X = x] is invariant for different values of x [2, 3, 6]. Define the

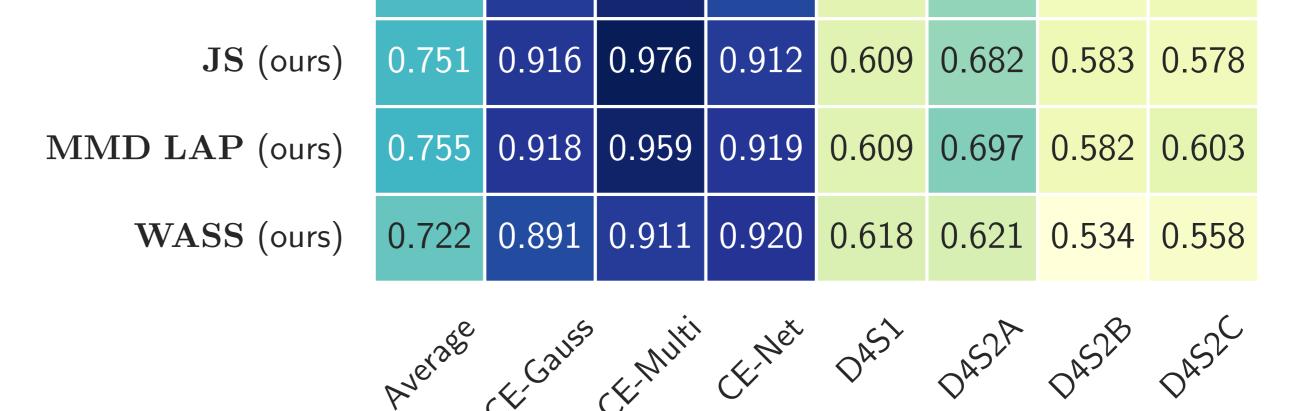
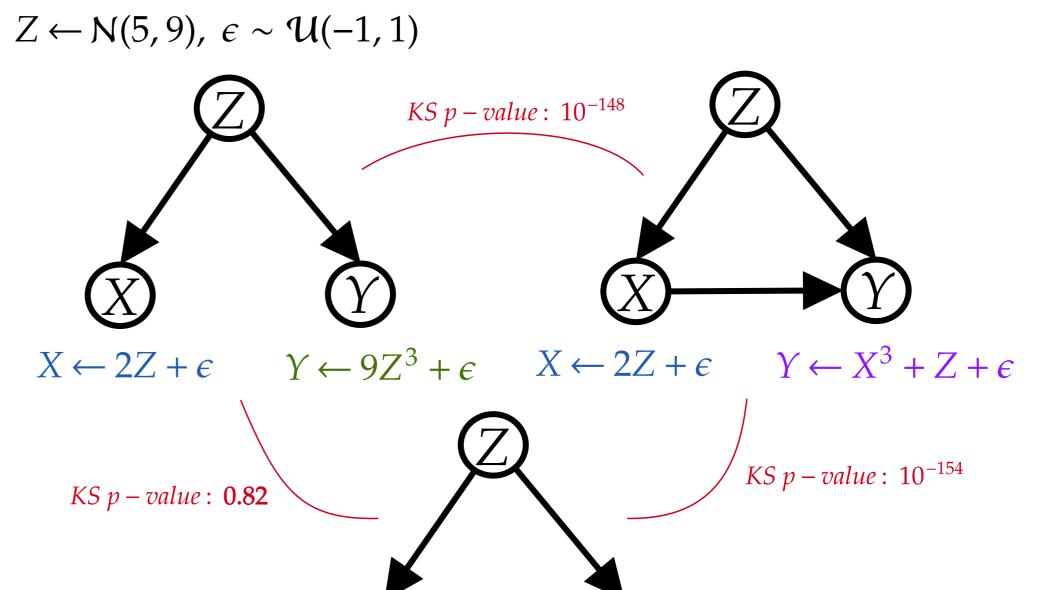


Figure 2: Performance of multiple divergence measures for CDCI on different datasets. Confounding Experiment



Normalized Conditional Divergence (NCD):

$$NCD_D(Y|X) := \mathbb{E}_{x \sim P[X]} \quad [D(P[\hat{Y}|X=x], P[\hat{Y}])]$$
(1)

where D is a valid probability distance measure and \hat{Y} is a standardized conditional distribution of Y given X = x.

Algorithm 1 The Conditional Divergence based Causal Inference (CDCI) algorithm for causal direction prediction based on conditional distribution divergence. **Input:** An i.i.d. bivariate joint distribution P(X, Y), and a probability distance D. **Output:** The causal score $C_{X \rightarrow Y}$ and direction. 1. Compute the conditional divergences for both directions using the probability distance D, as in Equation 1:

 $C_{X|Y} := NCD(X \mid Y) \text{ and } C_{Y|X} := NCD(Y \mid X)$

2. Compute the causal score:

$$C_{X \to Y} \coloneqq C_{X|Y} - C_{Y|X}$$

3. Output the causal score $C_{X \rightarrow Y}$ and

$$\begin{array}{ll} \text{direction} & \coloneqq \left\{ \begin{matrix} X \to Y & \quad \text{if } C_{X \to Y} > 0 \\ Y \to X & \quad \text{if } C_{X \to Y} < 0 \\ \text{Non-causal} & \quad \text{if } C_{X \to Y} = 0 \end{matrix} \right. \end{array}$$

$$X \leftarrow Y^{1/3} - (9^{1/3} - 2)Z + \epsilon \qquad Y \leftarrow 9Z^3 + \epsilon$$

Figure 3: Different confounding sets show that CDCDI cannot, as claimed, distinguish confounding from causation.

5 Conclusion

Strong points:

- No reliance on strong restricting assumptions
- Simple idea & implementation
- Nonetheless good performance

Weak points:

- No verified or provable theory
- False claims about confounding

Contributions: SM: implemented new divergence measures, PyPi package and investigated hidden confounder case; YO: performed kernel search for MMD, did ablation study with diff. binning strategies; AH: made plots and illustrations and prepared poster; all 3 were involved in reproduction of code and results.

References

3 Project Scope & Goals

- Reproduction of results and code
- Simple implementation & reproducible \checkmark
- Extension to novel divergence measures
- Jensen-Shannon (JS), Maximum-Mean (MMD), Wasserstein (+ others) 🗸
- Refuting claim: Distinguish between confounding and causation
- -Counter Example (see Fig. 3) \checkmark

• Ablation study: rationale of binning the conditionals \checkmark

[1] Bao Duong and Thin Nguyen. Bivariate causal discovery via conditional divergence. In *First Conference on Causal Learning and Reasoning*, 2022.

- [2] José AR Fonollosa. Conditional distribution variability measures for causality detection. In *Cause Effect Pairs in Machine Learning*, pages 339–347. Springer, 2019.
- [3] Dominik Janzing and Bernhard Schölkopf. Causal inference using the algorithmic markov condition. *IEEE Transactions on Information Theory*, 56(10):5168–5194, 2010.
- [4] Soel Micheletti. Conditional Divergence based Causal Inference. https://pypi.org/project/cdcicausality/, 2022. [Online; accessed 24th May 2022].
- [5] Joris M Mooij, Jonas Peters, Dominik Janzing, Jakob Zscheischler, and Bernhard Schölkopf. Distinguishing cause from effect using observational data: methods and benchmarks. *The Journal of Machine Learning Research*, 17(1):1103–1204, 2016.
- [6] Jonas Peters, Peter Bühlmann, and Nicolai Meinshausen. Causal inference by using invariant prediction: identification and confidence intervals. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 78(5):947–1012, 2016.