Causal Component Analysis

Liang Wendong^{1,2}, Armin Kekić¹, Julius von Kügelgen^{1,3}, Simon Buchholz¹, Michel Besserve¹, Luigi Gresele^{1,†}, Bernhard Schölkopf^{1,†}

¹ Max Planck Institute for Intelligent Systems, Tübingen

² ENS Paris-Saclay, Gif-sur-Yvette, France

³ University of Cambridge

[†] Joint supervision.







Causal Representation Learning (CRL) & Independent Component Analysis (ICA)

Causal Representation Learning (CRL) (Schölkopf et al., 2021) aims to identify *causally related* latent variables, together with a causal graph encoding their relationships.

CRL provides a principled definition of *disentanglement* (Bengio et al., 2013). Difficult problem; vast (and growing) literature, often based on strong assumptions. **Counterfactual data** (von Kügelgen* et al., 2021; Brehmer et al., 2022); **Temporal structure** (and **graph sparsity**) (Lachapelle and Lacoste-Julien, 2022; Lippe et al., 2022); **Parametric family of latent distributions** (Lachapelle, Rodriguez, et al., 2022; Squires et al., 2023; Buchholz et al., 2023); **Strong restrictions on the mixing function class**

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Independent Component Analysis (ICA) (Comon, 1994) aims to recover independent latent variables from observed mixtures thereof.

It is a special case of CRL, where the latent graph is known and empty.

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We introduce Causal Component Analysis (CauCA):

- Special case of CRL, presupposes knowledge of the causal graph;
- Generalization of ICA, causal components which support interventions.

Causal Bayesian networks (CBNs) and interventions (Pearl, 2009)

In a CBN with graph *G*, the conditional probabilities $\mathbb{P}_i(Z_i | \mathbf{Z}_{pa(i)})$ in the corresponding Markov factorization are called *causal mechanisms*. A CBNs consist of:

- a graph G & a collection of causal mechanisms $\{\mathbb{P}_i(Z_i \mid \mathbf{Z}_{pa(i)})\}_{i \in [d]}$.
- a collection of (stochastic) interventions $\{\{\widetilde{\mathbb{P}}_{j}^{k}(Z_{j} | \mathbb{Z}_{pa^{k}(j)})\}_{j \in \tau_{k}}\}_{k \in [K]}$ across K interventional regimes, with $\tau_{k} \subseteq V(G)$ intervention targets.

The joint probability for interventional regime k is given by:

$$\mathbb{P}^{k}(\mathsf{Z}) := \begin{cases} \prod_{i=1}^{d} \mathbb{P}_{i}(Z_{i} \mid \mathsf{Z}_{\mathsf{pa}(i)}) & k = 0\\ \prod_{j \in \tau_{k}} \widetilde{\mathbb{P}}_{j}^{k}\left(Z_{j} \mid \mathsf{Z}_{\mathsf{pa}^{k}(j)}\right) \prod_{i \notin \tau_{k}} \mathbb{P}_{i}\left(Z_{i} \mid \mathsf{Z}_{\mathsf{pa}(i)}\right) & \forall k \in [K] \end{cases}$$

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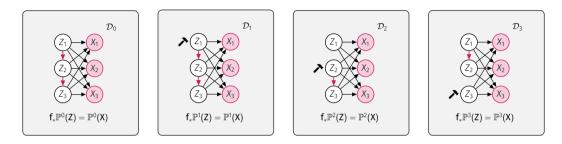
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Causal mechanisms are *modular*:

We can modify some without affecting the others (Pearl, 2009; Peters et al., 2017).

CauCA based on multiple interventions

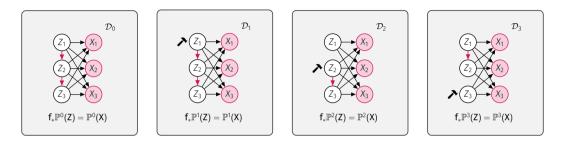


We are given multiple datasets \mathcal{D}_k generated by stochastic interventions on Z,

$$\mathcal{D}_k := \left(\tau_k, \left\{\mathbf{x}^{(n,k)}\right\}_{n=1}^{N_k}\right), \quad \text{with} \quad \mathbf{x}^{(n,k)} = \mathbf{f}\left(\mathbf{z}^{(n,k)}\right) \quad \text{and} \quad \mathbf{z}^{(n,k)} \stackrel{\text{i.i.d.}}{\sim} \mathbb{P}^k,$$

where \mathbb{P}^{k} are **nonparametric** distributions of **z**, and **f** is a **diffeomorphism**.

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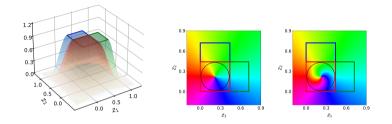
Our goal: Identify both the f and the $\{\mathbb{P}_i^k(z_i|\mathbf{z}_{pa(i)})\}_{i,k}$.

Identifiability results for a nontrivial latent graph

Consider the example where the latent graph is given by $z_1 \rightarrow z_2 \rightarrow z_3$:

Requirement of interventions	Learned representation $\hat{z}=\hat{f}^{-1}(x)$	Reference
1 intervention per node	$[h_1(z_1), h_2(z_1, z_2), h_3(z_1, z_2, z_3)]$	Thm. 4.2 <i>(i)</i>
1 perfect intervention per node	$[h_1(z_1), h_2(z_2), h_3(z_3)]$	Thm. 4.2 <i>(ii)</i>
1 intervention per node for z_1 and z_2 , plus $ \overline{pa}(3) (\overline{pa}(3) +1) = 2 \times 3$ imperfect interventions on z_3 with "variability" assumption	$[h_1(z_1), h_2(z_2), h_3(z_2, z_3)]$	Prop. D.1
1 perfect intervention on z_1 and $2+1=3$ perfect fat-hand interventions on (z_2, z_3)	$[h_1(z_1), h_2(z_2, z_3), h_3(z_2, z_3)]$	Thm. 4.5

Negative results: non-identifiability when some assumptions are violated



Our paper also contributes 4 non-identifiability results when:

- The assumption of *interventional discrepancy* is violated;
- At least 1 of the variables is not intervened on (when the graph is not empty);
- At least 2 variables are not intervened on (when the graph is empty, i.e., ICA);
- When the targets of interventions are totally unknown.

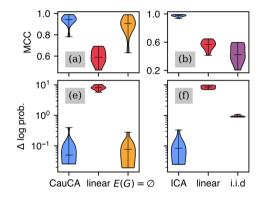
These results show that our assumptions are necessary, even for CRL.

Identifiability results for a trivial latent graph (ICA)

Consider the example when the latent graph is empty (i.e., no arrows):

Requirement of interventions	Learned representation $\hat{z} = \hat{f}^{-1}(x)$	Reference
1 intervention on any two nodes respectively	$[h_1(z_1), h_2(z_2), h_3(z_3)]$	Prop. 4.6
1 intervention on <i>z</i> ₁ and 2 fat-hand interven- tions on (<i>z</i> ₂ , <i>z</i> ₃)	$[h_1(z_1), h_2(z_2, z_3), h_3(z_2, z_3)]$	Corollary 4.8
1 intervention on z_1 and 4 fat-hand interven- tions on (z_2, z_3) with "variability" assumption	$[h_1(z_1), \pi[h_2(z_2), h_3(z_3)]]$	Prop. 4.9
1 intervention per node on any two nodes re- spectively with unknown order	$\pi [h_1(z_1), h_2(z_2), h_3(z_3)]$	Prop. E.6
6 fat-hand interventions on (z_1, z_2, z_3) with "variability" assumption	$\pi [h_1(z_1), h_2(z_2), h_3(z_3)]$	Hyvärinen et al., 2019, Thm. 1

Summary of our main contributions



We introduce a likelihood-based approach using normalizing flows to estimate both the unmixing function and the causal mechanisms.

Our method effectively recovers the latent causal components in synthetic experiments.

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- Impossibility results for CauCA also apply for CRL.
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By studying CauCA, we gain insights into the minimal assumptions required for CRL.

Thank you for your attention!

Poster Session: Wed 13 Dec 8:45 a.m. PST — 10:45 a.m. PST Location: Great Hall & Hall B1+B2 #827 Paper: https://arxiv.org/abs/2305.17225 Code: https://github.com/akekic/causal-component-analysis

References i

References

Ahuja, Kartik et al. (2022). "Interventional Causal Representation Lear	" ning". In: arXiv
preprint arXiv:2209.11924.	

Bengio, Yoshua et al. (2013). **"Representation learning: A review and new perspectives".** In: *IEEE transactions on pattern analysis and machine intelligence* 35.8, pp. 1798–1828.

- Brehmer, Johann et al. (2022). "Weakly supervised causal representation learning". In: arXiv preprint arXiv:2203.16437.
- Buchholz, Simon et al. (2023). "Learning Linear Causal Representations from Interventions under General Nonlinear Mixing". In: arXiv preprint arXiv:2306.02235.
- Comon, Pierre (1994). "Independent component analysis, a new concept?" In: Signal processing 36.3, pp. 287–314.

References ii

- Hyvärinen, Aapo et al. (2019). **"Nonlinear ICA using auxiliary variables and generalized contrastive learning".** In: *The 22nd International Conference on Artificial Intelligence and Statistics*. PMLR, pp. 859–868.
- Lachapelle, Sébastien and Simon Lacoste-Julien (2022). **"Partial Disentanglement via Mechanism Sparsity".** In: *arXiv preprint arXiv:2207.07732*.
- Lachapelle, Sébastien, Pau Rodriguez, et al. (2022). "Disentanglement via mechanism sparsity regularization: A new principle for nonlinear ICA". In: Conference on Causal Learning and Reasoning. PMLR, pp. 428–484.
- Lippe, Phillip et al. (2022). "Citris: Causal identifiability from temporal intervened sequences". In: International Conference on Machine Learning. PMLR, pp. 13557–13603.
- Pearl, Judea (2009). *Causality.* Cambridge university press.
- Peters, Jonas et al. (2017). Elements of causal inference: foundations and learning algorithms. The MIT Press.
- Schölkopf, Bernhard et al. (2021). **"Toward causal representation learning".** In: *Proceedings of the IEEE* 109.5, pp. 612–634.

References iii

- - Squires, Chandler et al. (2023). *Linear Causal Disentanglement via Interventions.*
 - Varici, Burak et al. (2023). **"Score-based Causal Representation Learning with Interventions".** In: arXiv preprint arXiv:2301.08230.
- von Kügelgen*, Julius et al. (2021). "Self-Supervised Learning with Data Augmentations Provably Isolates Content from Style". In: Advances in Neural Information Processing Systems (NeurIPS). Vol. 34.