# Exogenous Isomorphism for Counterfactual Identifiability

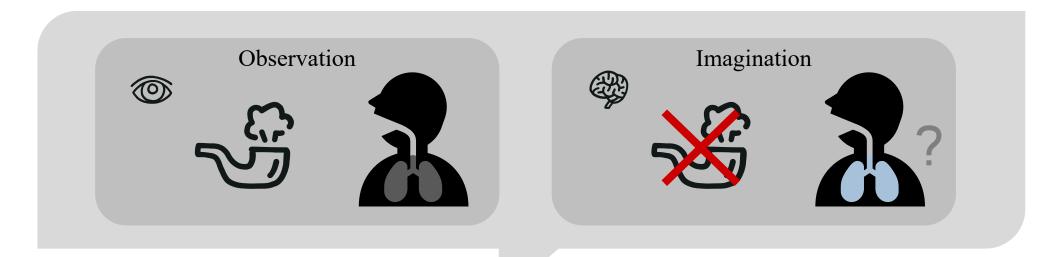
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## Counterfactual Identifiability

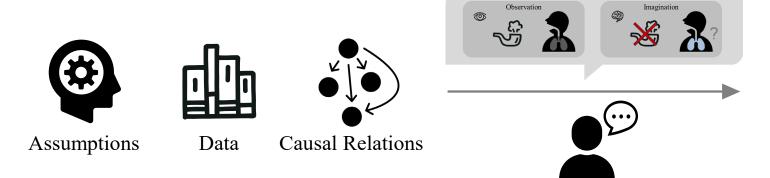
• Counterfactual is about answering "what-if" questions



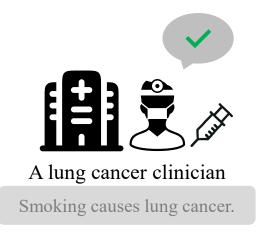


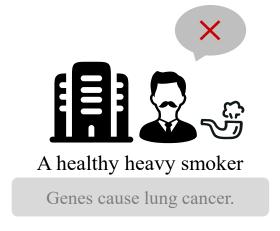
#### Counterfactual Identifiability

• Inconsistent answers may be produced.



Option A. Yes
Option B. No
Option C. Not Sure?

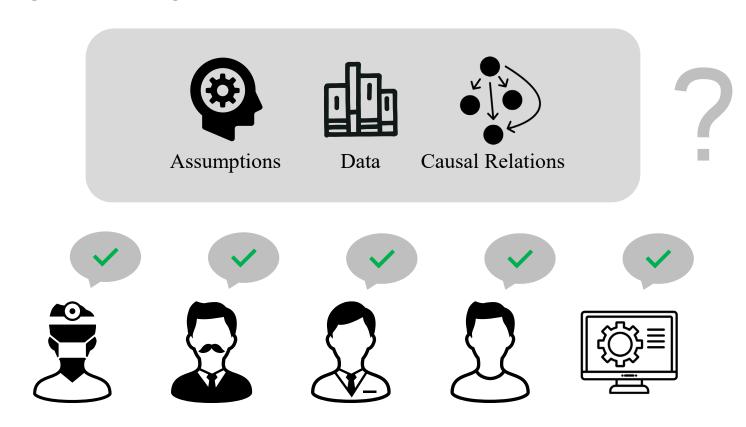






#### Counterfactual Identifiability

- Counterfactual Identifiability
  - How strong must the guarantees be for consistent answers?



The coloring house



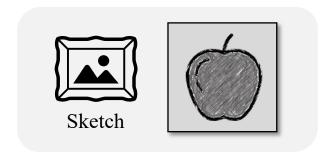


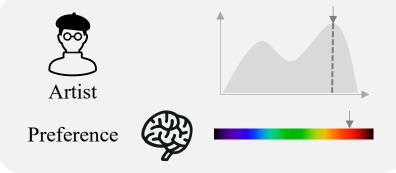












Unaware of the sketch, the artist randomly selects a color.

i.e.

Endogenous



Exogenous













Observational Query:







Counterfactual Query:





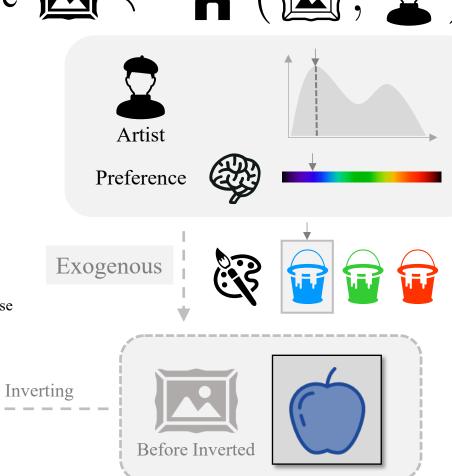
The inverse coloring house

• The inverse coloring house

Sketch

Endogenous

Colored



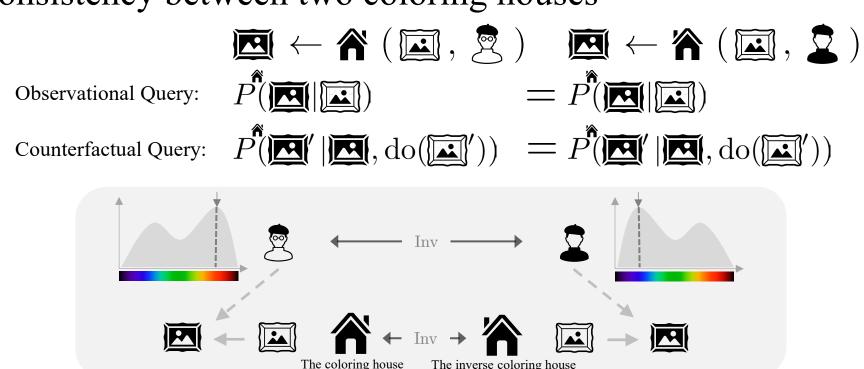
Unaware of the sketch, the artist randomly selects a color.

i.e. 🔟 🗓

and have exactly opposite preferences.

i.e.  $P(\mathbb{R}^n) = P(\operatorname{Inv}(\mathbb{R}^n))$ 

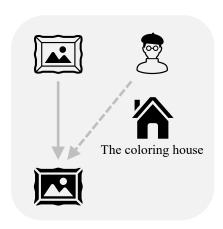
• The consistency between two coloring houses



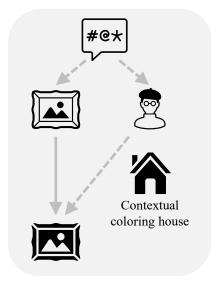
$$(\mathbf{A}, \mathbf{B}) = (\mathbf{A}, \operatorname{Inv}(\mathbf{B}))$$

$$P_{\Xi} = \text{Inv}_{\sharp} P_{\Xi}$$

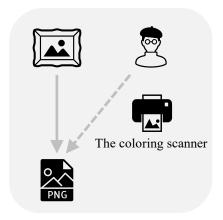
Other cases



Markovian

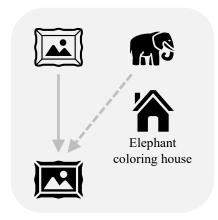


Not Markovian



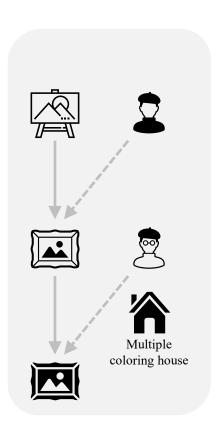
Different Endogenous

Domain



Different Exogenous

Domain



Multiple Variables

#### Identifiability from Isomorphisms

$$P_{\Xi} = \operatorname{Iso}_{\sharp} P_{\Xi}$$

Isomorphism	Mechanism Isomorphism	Distributional Isomorphism	Mechanistic Requirement	Structural Requirement
Counterfactual Equivalence (Peters et al., 2017)	$f^{(1)}(\mathbf{v}_{pa^{(1)}}, u^{(1)}) = f^{(2)}(\mathbf{v}_{pa^{(2)}}, u^{(1)})$	$P_{\mathbf{U}}^{(2)} = P_{\mathbf{U}}^{(1)}$	-	order
BGM Equivalence (Nasr-Esfahany et al. 2023)	$f^{(1)}(\mathbf{v}_{pa^{(1)}}, u^{(1)}) = f^{(2)}(\mathbf{v}_{pa^{(2)}}, g(u^{(1)}))$	-	bijection	graph
LCM Isomorphism (Brehmer et al. 2022)	$f^{(1)}(\mathbf{v}_{\mathrm{pa}^{(1)}}, u^{(1)}) = f^{(2)}(\mathbf{v}_{\mathrm{pa}^{(2)}}, \varphi(u^{(1)}))$	$P_{\mathbf{U}}^{(2)} = oldsymbol{arphi}_\sharp P_{\mathbf{U}}^{(1)}$	diffeomorphism	graph isomorphism
Domain Counterfactual Equivalence (Zhou et al. 2024)	$f^{(1)}(\mathbf{v}_{pa^{(1)}}, h_1(u^{(1)})) = f^{(2)}(\mathbf{v}_{pa^{(2)}}, h_2(u^{(2)}))$	$P_{\mathbf{U}}^{(k)} \sim \mathcal{N}(0, \mathbf{I})$	bijection	domain label
Exogenous Isomorphism (Ours)	$f^{(1)}(\mathbf{v}_{pa^{(1)}}, u^{(1)}) = f^{(2)}(\mathbf{v}_{pa^{(2)}}, h(u^{(1)}))$	$P_{\mathbf{U}}^{(2)} = \boldsymbol{h}_{\sharp} P_{\mathbf{U}}^{(1)}$	-	order

<sup>[1]</sup> Peters, J., Janzing, D., & Scholkopf, B. (2017). Elements of causal inference: Foundations and Learning Algorithms. MIT Press.

<sup>[2]</sup> Nasr-Esfahany, A., Alizadeh, M., & Shah, D. (2023). Counterfactual Identifiability of Bijective Causal Models. In Proceedings of the 40th International Conference on Machine Learning (pp. 25733–25754). PMLR.

<sup>[3]</sup> Brehmer, J., Haan, P., Lippe, P., & Cohen, T. (2022). Weakly supervised causal representation learning. In Advances in Neural Information Processing Systems (pp. 38319–38331). Curran Associates, Inc..

<sup>[4]</sup> Zhou, Z., Bai, R., Kulinski, S., Kocaoglu, M., & Inouye, D. (2024). Towards Characterizing Domain Counterfactuals for Invertible Latent Causal Models. In The Twelfth International Conference on Learning Representations.

## Identifiability from Isomorphisms

#### • Exogenous isomorphism



 $P_{\Xi} = \operatorname{Iso}_{\sharp} P_{\Xi}$ 

Recursive SCMs  $\mathcal{M}^{(1)}$  and  $\mathcal{M}^{(2)}$  are said to be **exogenously isomorphic**, denoted  $\mathcal{M}^{(1)} \sim_{\text{EI}} \mathcal{M}^{(2)}$ , if there exists a shared causal ordering  $\leq$  and function  $\mathbf{h}: \Omega_{\mathbf{U}}^{(1)} \to \Omega_{\mathbf{U}}^{(2)}$  satisfying:

- Component-wise bijection  $\mathbf{h} = (h_i)_{i \in \mathcal{I}}$ , where each  $h_i : \Omega_{U_i}^{(1)} \to \Omega_{U_i}^{(2)}$  is a bijection
- Exogenous distribution isomorphism  $P_{\mathbf{U}}^{(2)} = \mathbf{h}_{\sharp} P_{\mathbf{U}}^{(1)}$
- Causal mechanism isomorphism  $f^{(1)}(\mathbf{v}_{\mathrm{pa}^{(1)}},u^{(1)})=f^{(2)}(\mathbf{v}_{\mathrm{pa}^{(2)}},h(u^{(1)}))$

#### • Exogenous isomorphism implies counterfactual consistency

$$\mathcal{M}^{(1)} \sim_{\mathrm{EI}} \mathcal{M}^{(2)} \implies \mathcal{M}^{(1)} \sim_{\mathcal{L}_3} \mathcal{M}^{(2)}.$$

 $\sim_{L_3}$  is an equivalence relation over Structural Causal Models (SCMs), indicating that the models yield the same answers to any counterfactual statement.

- This includes counterfactual outcomes, counterfactual effects, joint counterfactuals, and nested counterfactuals.
- From the perspective of the Pearl Causal Hierarchy (PCH),  $\sim_{\mathcal{L}_3}$  implies that the complete counterfactual layer is identical, meaning the models are indistinguishable across the entire hierarchy.

## To Achieve Exogenous Isomorphism

• EI-identifiability problem

$$egin{aligned} \mathcal{A} &\models & \mathcal{M}^{(1)} \sim_{\square} \mathcal{M}^{(2)} \ &\Longrightarrow & \mathcal{M}^{(1)} \sim_{\operatorname{EI}} \mathcal{M}^{(2)} \ &\Longrightarrow & \mathcal{M}^{(1)} \sim_{\mathcal{L}_3} \mathcal{M}^{(2)} \end{aligned}$$

Under what assumptions  $\mathcal{A}$  does the model equivalence class  $\sim_{\square}$  imply  $\sim_{\text{EI}}$ ?

#### Bijective SCMs

Assumption (a). The causal mechanisms are **bijective** with respect to the exogenous variables.

Assumption (b). The structural causal model is **Markovian**.

Assumption (c). The **causal order** is given.

Assumption (d). The **observational distribution** is available.

Assumption (e). The model induces identical **counterfactual transport** (e.g., Knothe–Rosenblatt transport).

#### Triangular Monotonic SCMs

Assumption (a). The causal mechanisms are **monotonic** with respect to the exogenous variables.

Assumption (b). The structural causal model is Markovian.

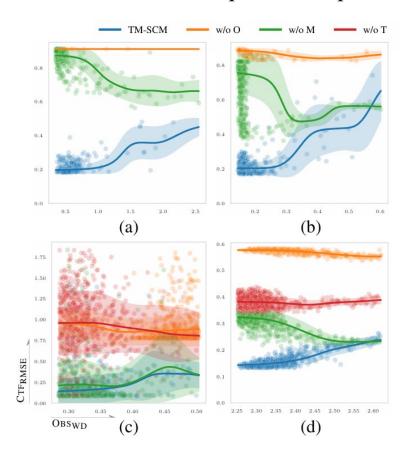
Assumption (c). The **causal order** is given.

Assumption (d). The **observational distribution** is available.

- The model equivalence classes that satisfy the above assumptions entails EI-identifiability.
- As a result, counterfactual identifiability are ensured within these classes.

#### **Ablation Study**

• Ablation experiments on synthetic datasets with neural network-based Triangular Monotonic SCMs provide empirical support for the theoretical results.



Метнор		ER-DIAG-50	ER-Tril-50
DNME	- w/o O w/o M	$0.53_{\pm 0.05} \ 0.78_{\pm 0.05} \ 0.62_{\pm 0.04}$	$\begin{array}{c} \textbf{0.51}_{\pm \textbf{0.12}} \\ 0.89_{\pm 0.10} \\ 0.58_{\pm 0.10} \end{array}$
TNME	- w/o O w/o M	$0.47_{\pm 0.05}$ $11.24_{\pm 20.98}$ $0.62_{\pm 0.04}$	$egin{array}{c} 0.55_{\pm 0.12} \ 6.41_{\pm 9.84} \ 0.73_{\pm 0.21} \end{array}$
CMSM	- w/o O w/o M w/o T	$\begin{array}{c} \textbf{0.37}_{\pm \textbf{0.05}} \\ 2.64_{\pm 3.72} \\ 1.69_{\pm 2.60} \\ 0.64_{\pm 0.05} \end{array}$	$egin{array}{c} \mathbf{0.42_{\pm 0.12}} \\ 2.12_{\pm 2.49} \\ 0.75_{\pm 0.49} \\ 1.25_{\pm 1.29} \\ \end{array}$
TVSM	- w/o O w/o M w/o T	$0.46_{\pm 0.05} \\ 0.79_{\pm 0.04} \\ 0.53_{\pm 0.05} \\ 0.67_{\pm 0.05}$	$\begin{array}{c} \textbf{0.50}_{\pm \textbf{0.12}} \\ 0.88_{\pm 0.10} \\ 0.53_{\pm 0.11} \\ 0.78_{\pm 0.12} \end{array}$

#### Summary

- We introduced exogenous isomorphism ensuring consistency across all counterfactual queries.
- We identified and proved that two specific classes of models satisfy EI-identifiability.
- Empirical results on neural SCMs and synthetic datasets support our theoretical claims.
- This work provides a principled foundation for learning counterfactually reliable models.

#### **THANKS**

Full paper is available at: https://arxiv.org/abs/2505.02212



Code is available at: https://github.com/cyisk/tmscm

