

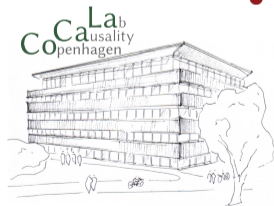
Invariant Policy Learning: A Causal Perspective

Sorawit Saengkyongam

Copenhagen Causality Lab (CoCaLa), University of Copenhagen

Joint work with Nikolaj Thams, Jonas Peters and Niklas Pfister.

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Contextual bandits: Covariates, Action, Reward

Goal: We consider the problem of learning policies that are robust with respect to shifts in the environments.

Setting: (Offline) Contextual Bandits

X: context (observed); **A:** action;

R: reward; **U:** context (unobserved)

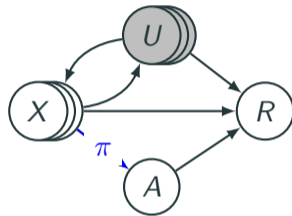


Figure 1: Graphical model of the setting

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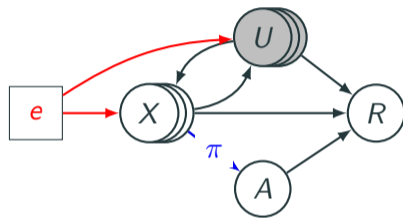


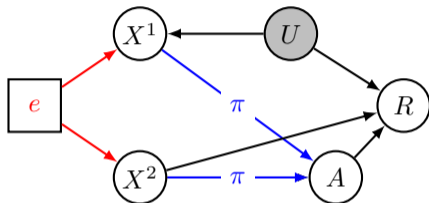
Figure 1: Graphical model of the setting

We assume additionally that data is collected from different environments, $e \in \mathcal{E}$, changing the covariate distributions. Future changes in distribution is represented as new environments.

- E.g. records from different hospitals, countries or experimental setups.

Example: Association flips between environments

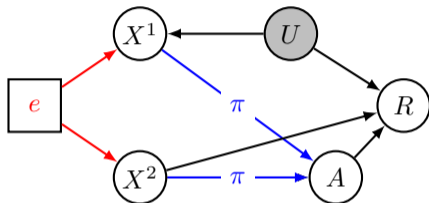
$$\mathcal{S}(\pi, \mathbf{e}) : \begin{cases} U := \epsilon_U \\ X^1 := \gamma_e U + \epsilon_{X^1} \\ X^2 := \alpha_e + \epsilon_{X^2} \\ A := g_\pi(X^1, X^2, \epsilon_A) \\ R := \begin{cases} \beta_1 X^2 + U + \epsilon_R, & \text{if } A = 0 \\ \beta_2 X^2 - U + \epsilon_R, & \text{if } A = 1 \end{cases} \end{cases}$$



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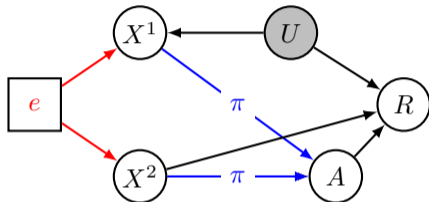


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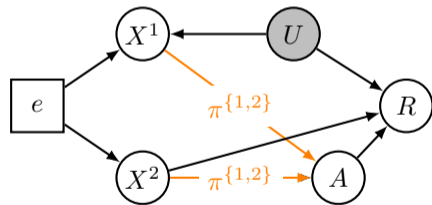
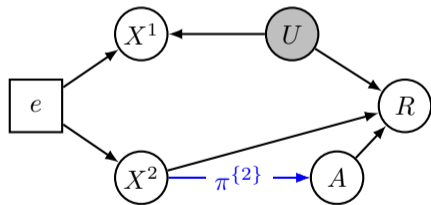
We do not assume that the graph is known! Instead, we seek for non-invariant features and exclude those from policy learning.

Invariance

A set of covariates X^S is **invariant** if it holds that

$$e \perp\!\!\!\perp_{\mathcal{G}^S} R \mid X^S.$$

A policy π is **invariant** w.r.t. a set S if π depends only on X^S .



$e \perp\!\!\!\perp_{\mathcal{G}^{\{2\}}} R \mid X^{\{2\}}$ but $e \not\perp\!\!\!\perp_{\mathcal{G}^{\{1,2\}}} R \mid X^{\{1,2\}}$.

Maximizing the worst-case reward

Objective: Distributional Robustness

$$\operatorname{argmax}_{\pi \in \Pi} V^{\mathcal{E}}(\pi), \quad \text{where } V^{\mathcal{E}}(\pi) := \inf_{e \in \mathcal{E}} \mathbb{E}^{\pi, e} [R].$$

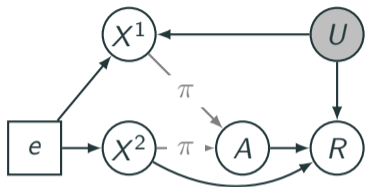
Under certain assumptions solving the distributionally robust objective amounts to finding an optimal invariant policy.

Theorem

Consider an invariant policy $\pi^* \in \operatorname{argmax}_{\pi \in \Pi_{\text{inv}}} \sum_{e \in \mathcal{E}^{\text{obs}}} \mathbb{E}^{\pi, e} [R]$. Under “strong environments” assumption, it holds that

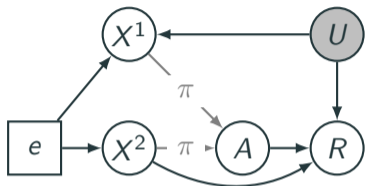
$$\forall \pi \in \Pi : \quad V^{\mathcal{E}}(\pi) \leq V^{\mathcal{E}}(\pi^*).$$

“Strong environments” Assumption

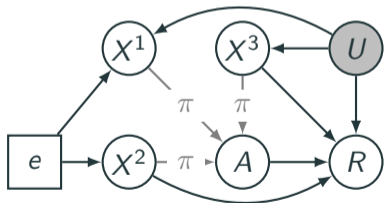


Strong environments: There exists $e \in \mathcal{E}$ such that $X^1 \perp\!\!\!\perp U$ in e .

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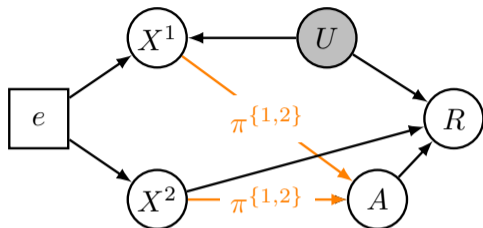


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Testing invariance



We have,

$e \not\perp_{\pi^{\{1,2\}}} R \mid X^{\{1,2\}}$
and $e \not\perp_{\pi^{\{1,2\}}} R \mid X^{\{2\}}$
(but $e \perp_{\pi^{\{2\}}} R \mid X^{\{2\}}$).

Given $S \subseteq \{1, \dots, d\}$, we resample the data to mimick¹ the policy π^S .

To test invariance: 1) bundle all environments, 2) fit regression, 3) test whether prediction residuals are equally distributed across environments².

¹Nikolaj Thams et al. (2021). "Statistical Testing under Distributional Shifts". In: *arXiv preprint arXiv:2105.10821*

²Christina Heinze-Deml et al. (2018). "Invariant Causal Prediction for Nonlinear Models". In: *Journal of Causal Inference* 6.2

Limitations of Subset Search

- (i) Computational efficiency
 - Variable screening
 - Greedy search

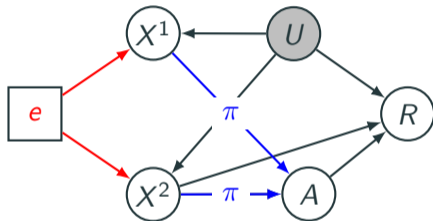
Limitations of Subset Search

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- (ii) No invariant sets when U acts on the parents

Limitations of Subset Search

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There is no invariant set!!

HSIC-X: Exploiting Independent Instruments Identification and Distribution Generalization

Sorawit Saengkyongam

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Instrumental Variable (IV) Setting

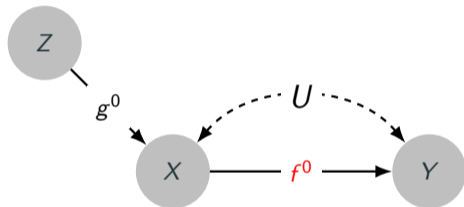
We consider the following structural causal model M^0

$$Z := \epsilon_Z$$

$$U := \epsilon_U$$

$$X := g^0(Z, U, \epsilon_X)$$

$$Y := f^0(X) + h^0(U, \epsilon_Y)$$



where $Z \in \mathbb{R}^r$ are **instruments**, $U \in \mathbb{R}^q$ are unobserved variables, $X \in \mathbb{R}^d$ are **predictors**, $Y \in \mathbb{R}$ is a **response**, and $(\epsilon_Z, \epsilon_U, \epsilon_X, \epsilon_Y)$ are jointly independent noise variables. The **causal function** f^0 satisfies **independence restriction** $Y - f^0(X) \perp\!\!\!\perp Z$.

Identification of f^0 : Moment restriction vs Independence restriction

E.g., consider a linear causal function $f^0(x) = x^\top \theta^0$ for some $\theta^0 \in \mathbb{R}^d$.

Classical IV approach

Identification of f^0 is based on the (conditional) **moment restriction**:

$$\mathbb{E}[Y - X^\top \theta \mid Z] = 0. \quad (1)$$

f^0 is not identifiable when $\mathbb{E}[X \mid Z] = 0$.

Independence-based IV

Identification of f^0 is based on the **independence restriction**:

$$Y - X^\top \theta \perp\!\!\!\perp Z. \quad (2)$$

We can identify f^0 even if $\mathbb{E}[X \mid Z] = 0$.

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The independence restriction (2) yields

- (i) Strictly stronger identifiability results.
- (ii) (in some settings) More efficient estimators (e.g., under weak instruments).

Example: Non-additive Instruments

Consider the following SCM

$$\begin{aligned}Z &:= \epsilon_Z \\U &:= \epsilon_U \\X &:= ZU + \epsilon_X \\Y &:= X + U + \epsilon_Y,\end{aligned}\tag{3}$$

with $\mathcal{F} = \{f \mid f(x) = \theta x\}$, where $(\epsilon_Z, \epsilon_U, \epsilon_X, \epsilon_Y)$ are jointly independent standard Gaussian variables.

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Here, we have $\mathbb{E}[X|Z] = Z \mathbb{E}[U] + \mathbb{E}[\epsilon_X] = 0$ and therefore one cannot identify the causal function based only on the [moment restriction](#). Nonetheless, the causal function can be identified with the [independence restriction](#).

Independence-based IV with HSIC

Given $(\mathbf{X}, \mathbf{Y}, \mathbf{Z})$, our method aims to find a function \hat{f} that minimizes the dependency between the residuals $\mathbf{Y} - \hat{f}(\mathbf{X})$ and the instruments \mathbf{Z} .

We propose the HSIC-X ('X' for 'exogenous') estimator:

$$\hat{f} := \arg \min_{f \in \mathcal{F}} \widehat{\text{HSIC}}(\mathbf{Y} - f(\mathbf{X}), \mathbf{Z}), \quad (4)$$

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Two heuristics to alleviate the non-convexity issue:

- (i) Initialize the parameters in the first trial at the OLS/2SLS solutions.
- (ii) Restarting heuristic: Test for the independence restriction at the solution. If the test is rejected, randomly re-initialize the parameters and restart the optimization.

Under-identified IV and Distribution Generalization

In the under-identified case when Z is not rich enough to identify f^0 , we can still get a meaningful estimator where we find the most predictive invariant function.

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Theorem [Generalization to interventions on Z]

Let $\ell : \mathbb{R} \rightarrow \mathbb{R}$ be a convex loss function and \mathcal{I} be a set of interventions on Z . If the interventions \mathcal{I} is 'strong enough', then

$$\inf_{f \in \mathcal{F}_{\text{inv}}} \mathbb{E}_{M^0}[\ell(Y - f(X))] = \inf_{f \in \mathcal{F}} \sup_{i \in \mathcal{I}} \mathbb{E}_{M^0(i)}[\ell(Y - f(X))], \quad (5)$$

where $\mathcal{F}_{\text{inv}} := \{f_{\diamond} \in \mathcal{F} \mid Z \perp\!\!\!\perp Y - f_{\diamond}(X) \text{ under } \mathbb{P}_{M^0}\}$ is the space of invariant functions.

Under-identified IV and Distribution Generalization

Motivated by (5), we propose the HSIC-X-pen ('pen' for 'penalization') estimator:

$$\hat{f}^\lambda = \arg \min_{f \in \mathcal{F}} \widehat{\text{HSIC}}(\mathbf{Y} - f(\mathbf{X}), \mathbf{Z}) + \lambda \sum_{i=1}^n \ell(Y_i - f(X_i)), \quad (6)$$

where the tuning parameter $\lambda \in [0, \infty)$ is selected as the largest possible value for which an HSIC-based independence test between the residuals and the instruments is not rejected.

Contributions

Three contributions:

- (i) We discuss the use of the **independence restriction** $Y - f(X) \perp\!\!\!\perp Z$ in IV estimation and its implication on the identifiability of f^0 .
- (ii) We propose **HSIC-X**, a gradient-based learning method that exploits the independence restriction to estimate f^0 and prove its consistency.
- (iii) We propose to use the independence restriction for **distribution generalization** and prove theoretical guarantees.

- (i) How to estimate the prediction intervals?
- (ii) How to handle non-additive confounding effect?