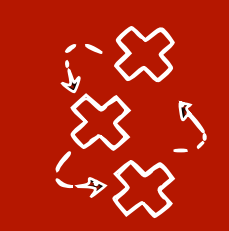


Causal Data Science

Lecture 11.2: Invariant causal prediction

Lecturer: Sara Magliacane

UvA - Spring 2023



Causal discovery overview

Constraint-based causal discovery

- Conditional independence tests
- Observational data
- Output: MEC
- SGS, PC

Score-based causal discovery

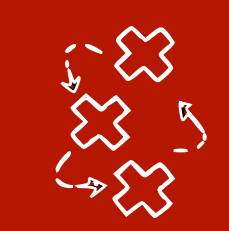
- Penalised likelihood
- Observational data
- Output: MEC
- GES

Restricted models

- Nonlinear additive noise, Linear Non-Gaussianity
- Observational data
- Output: DAG
- RESIT, LINGAM

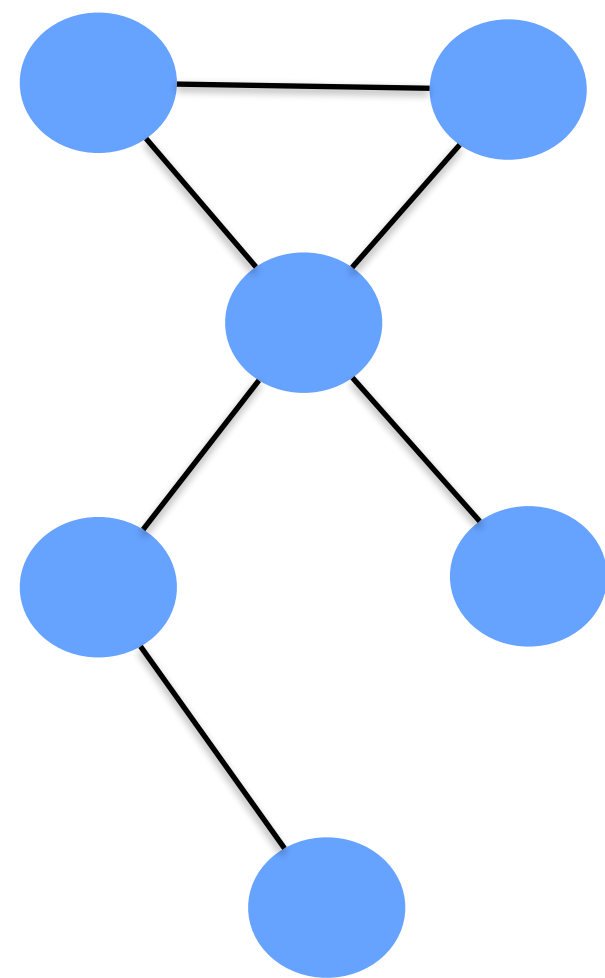
Interventional causal discovery / causal invariance

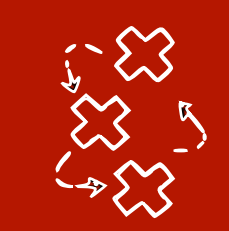
- Observational and Interventional data
- Output: parents of Y
- ICP



Intervention design/Experiment selection

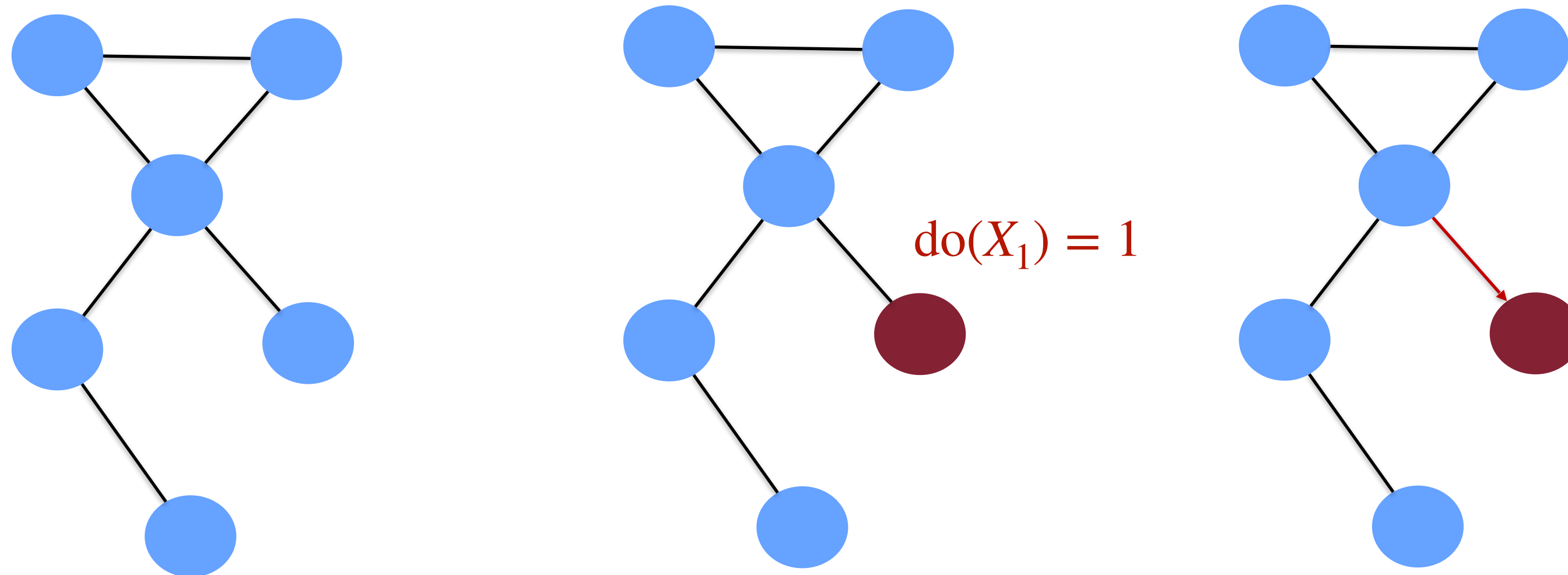
Design a set of interventions, so that we can **accurately** reconstruct **as much as possible** the causal graph **with the least samples**, also when **noisy**





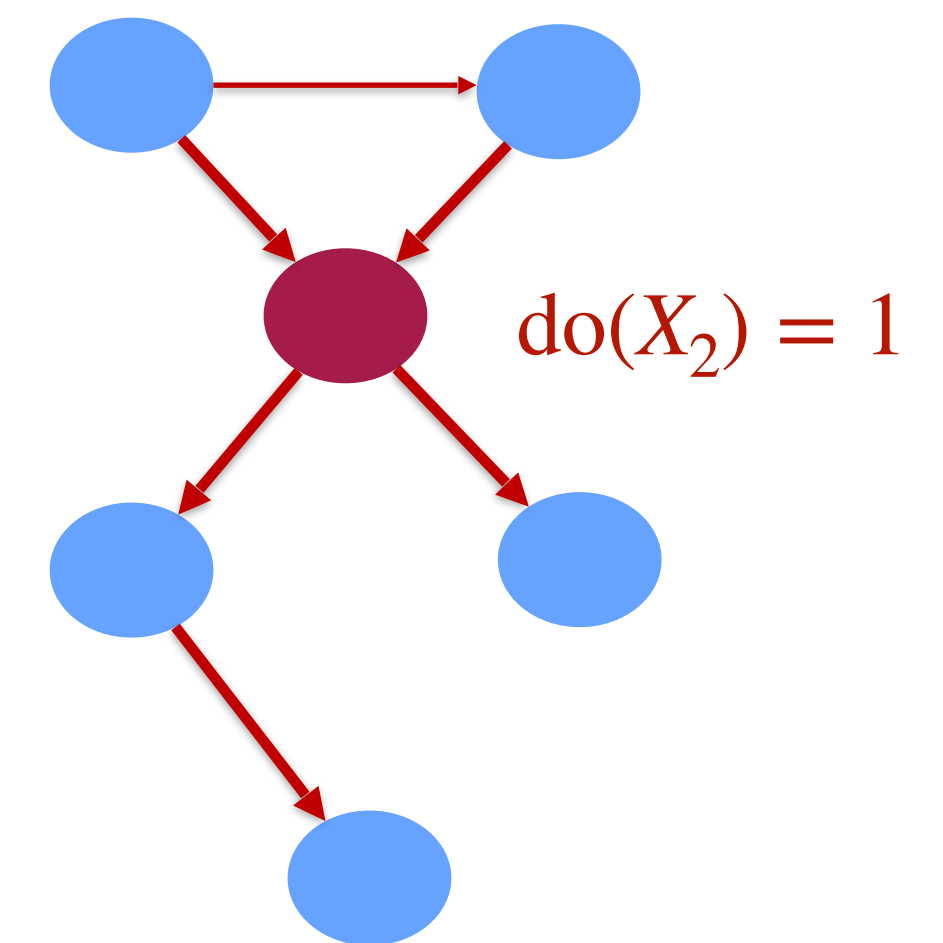
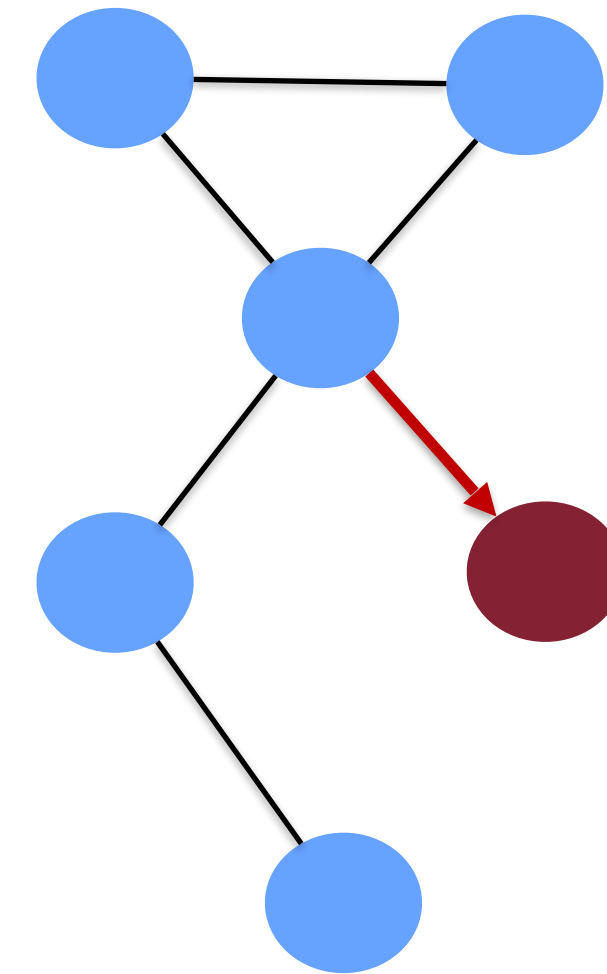
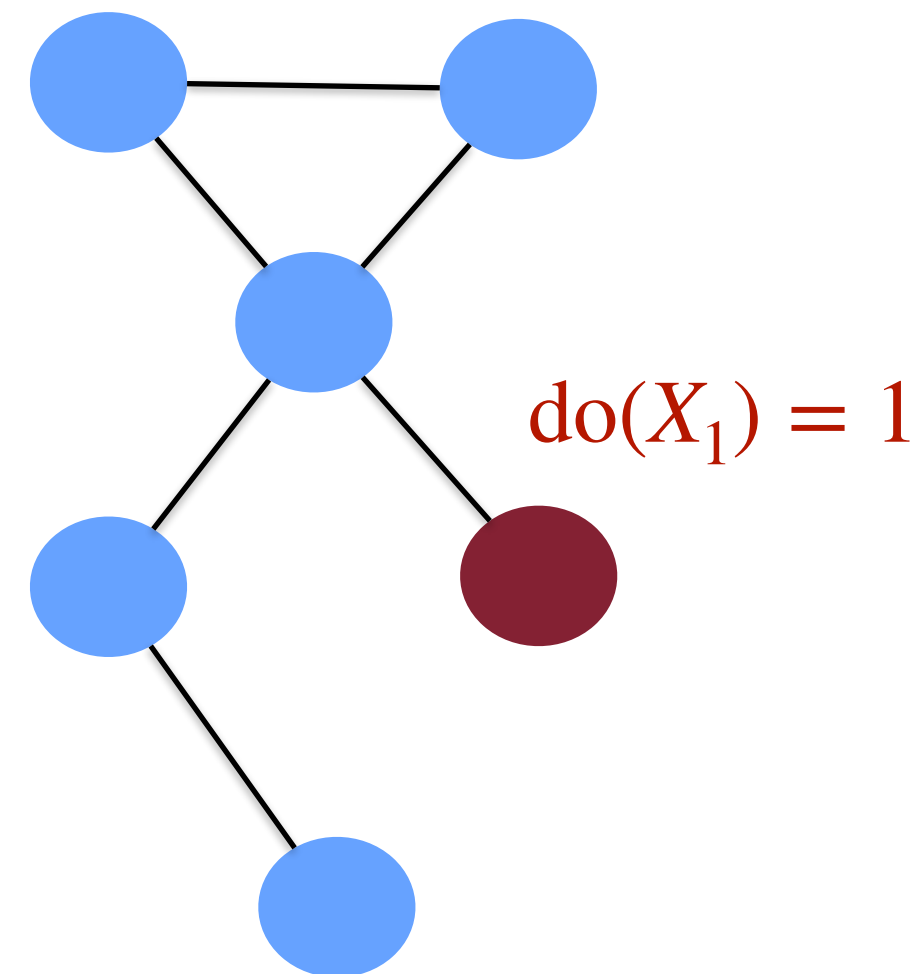
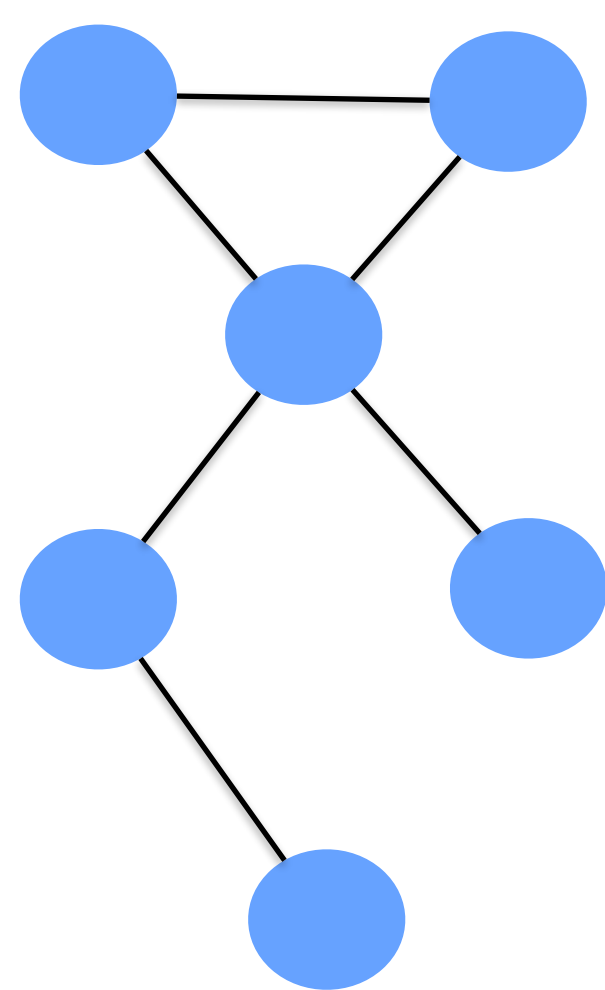
Intervention design/Experiment selection

Design a set of interventions, so that we can **accurately** reconstruct **as much as possible** the causal graph **with the least samples**, also when **noisy**



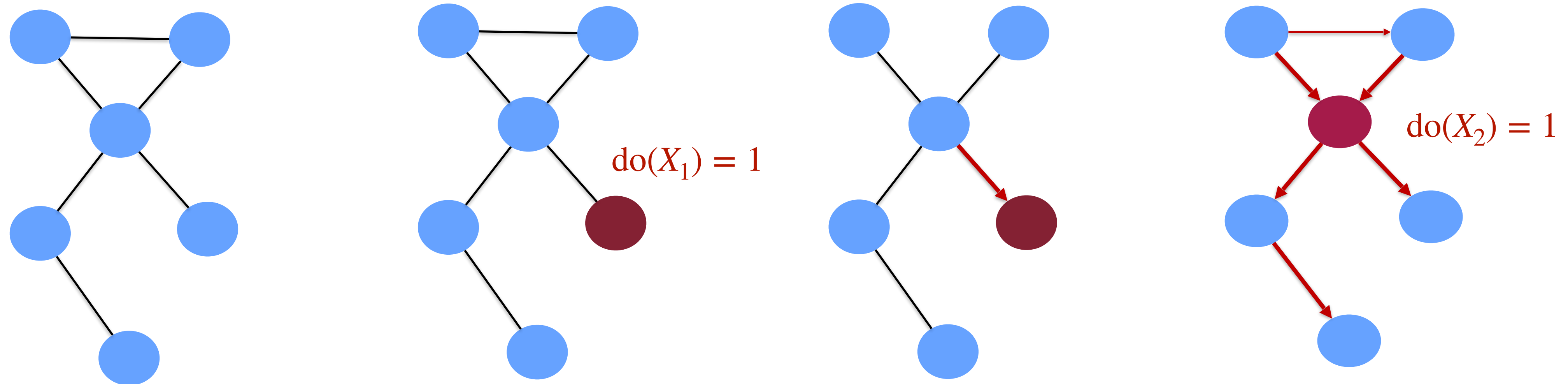
Intervention design/Experiment selection

Design a set of interventions, so that we can **accurately** reconstruct **as much as possible** the causal graph **with the least samples**, also when **noisy**

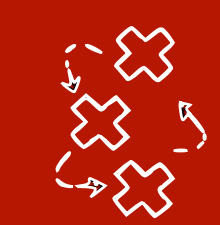


Intervention design/Experiment selection

Design a set of interventions, so that we can **accurately** reconstruct **as much as possible** the causal graph **with the least samples**, also when **noisy**

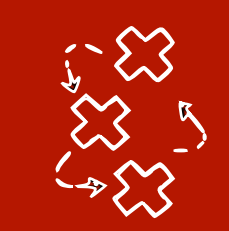


We formalised an algorithm/policy based on the concept of **central node** for forests with noisy interventions and for DAGs with noiseless interventions.



Learning from multiple contexts

- Now we cannot decide which intervention to perform (**intervention design**)
 - We then also have **known intervention targets**, e.g. $\text{do}(S = 1)$
- Instead, somebody gives us a **set of data from multiple contexts**
 - Possibly **unknown intervention targets**
 - Possibly **soft interventions** instead of **perfect interventions**



Invariant Causal Prediction example

$$\begin{cases} X_1 = \varepsilon_1 \\ Y = X_1 + \varepsilon_Y \\ X_2 = Y + \varepsilon_{X_2} \end{cases}$$

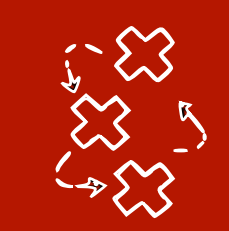
$$\varepsilon_1, \varepsilon_Y \sim N(0, 1), \quad \varepsilon_{X_2} \sim N(0, 0.01)$$

$$M1: Y \sim X_1$$

$$M2: Y \sim X_2$$

$$X_1 \rightarrow Y \rightarrow X_2$$

M2 has smaller error



Invariant Causal Prediction example

$$\begin{cases} X_1 = \varepsilon_1 \\ Y = X_1 + \varepsilon_Y \\ X_2 = Y + \varepsilon_{X_2} \end{cases}$$

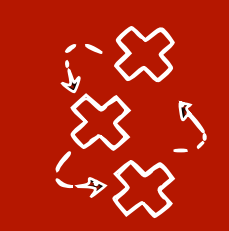
$\varepsilon_1, \varepsilon_Y \sim N(0, 1), \varepsilon_{X_2} \sim N(0, 0.01)$

M1: $Y \sim X_1$ M2: $Y \sim X_2$

$$X_1 \rightarrow Y \rightarrow X_2$$

$$X_1 \rightarrow Y \quad X_2 \text{ do}(X_2)$$

M2 has smaller error
but it fails in $\text{do}(X_2)$



Invariant Causal Prediction example

$$\begin{cases} X_1 = \varepsilon_1 \\ Y = X_1 + \varepsilon_Y \\ X_2 = Y + \varepsilon_{X_2} \end{cases}$$

$$\varepsilon_1, \varepsilon_Y \sim N(0, 1), \quad \varepsilon_{X_2} \sim N(0, 0.01)$$

$$M1: Y \sim X_1$$

$$M2: Y \sim X_2$$

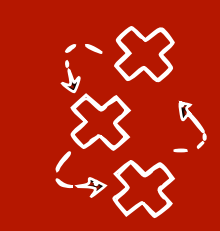
$$X_1 \rightarrow Y \rightarrow X_2$$

Using causal parents of Y helps
with DISTRIBUTION SHIFTS



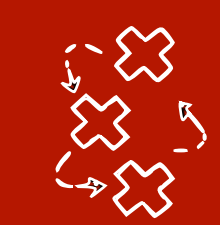
Invariant Causal Prediction (ICP) [Peters et al 2016]

- Given a target variable Y and features (X_1, \dots, X_p) , we want to **find the causal parents of Y , i.e. $\text{Pa}(Y)$**



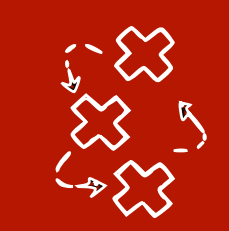
Invariant Causal Prediction (ICP) [Peters et al 2016]

- Given a target variable Y and features (X_1, \dots, X_p) , we want to **find the causal parents of Y , i.e. $\text{Pa}(Y)$**
- We assume we have access to **a set of different environments E** (e.g. interventional or observational data), s.t. for $e \in E$, $(X_1^e, \dots, X_p^e, Y^e) \sim P^e$



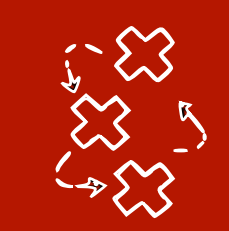
Invariant Causal Prediction (ICP) [Peters et al 2016]

- Given a target variable Y and features (X_1, \dots, X_p) , we want to **find the causal parents of Y , i.e. $\text{Pa}(Y)$**
- We assume we have access to **a set of different environments E** (e.g. interventional or observational data), s.t. for $e \in E$, $(X_1^e, \dots, X_p^e, Y^e) \sim P^e$
- We further assume that in **none of the environments Y is intervened upon**
- We can then show that $e, f \in E : P^e(Y^e | \text{Pa}(Y^e)) = P^f(Y^f | \text{Pa}(Y^f))$



Invariant Causal Prediction example

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = -2Y + \epsilon_2 \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases}$$

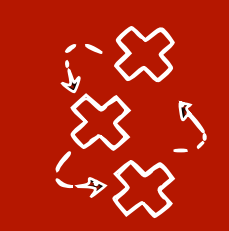


Invariant Causal Prediction example

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = -2Y + \epsilon_2 \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases}$$

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = 1 \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases}$$

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = 10Y + \epsilon_Y \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases}$$

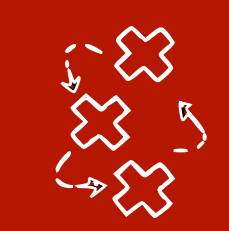


Invariant Causal Prediction example

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = -2Y + \epsilon_2 \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases} \quad E = 0$$

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = 1 \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases} \quad E = 1$$

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = 10Y + \epsilon_Y \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases} \quad E = 2$$



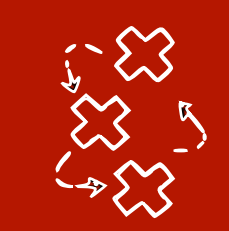
Invariant Causal Prediction example

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = -2Y + \epsilon_2 \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases} \quad E = 0$$

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = 1 \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases} \quad E = 1$$

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = 10Y + \epsilon_Y \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases} \quad E = 2$$

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = \begin{cases} -2Y + \epsilon_2 & \text{if } E = 0 \\ 1 & \text{if } E = 1 \\ 10Y + \epsilon_Y & \text{if } E = 2 \end{cases} \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases}$$



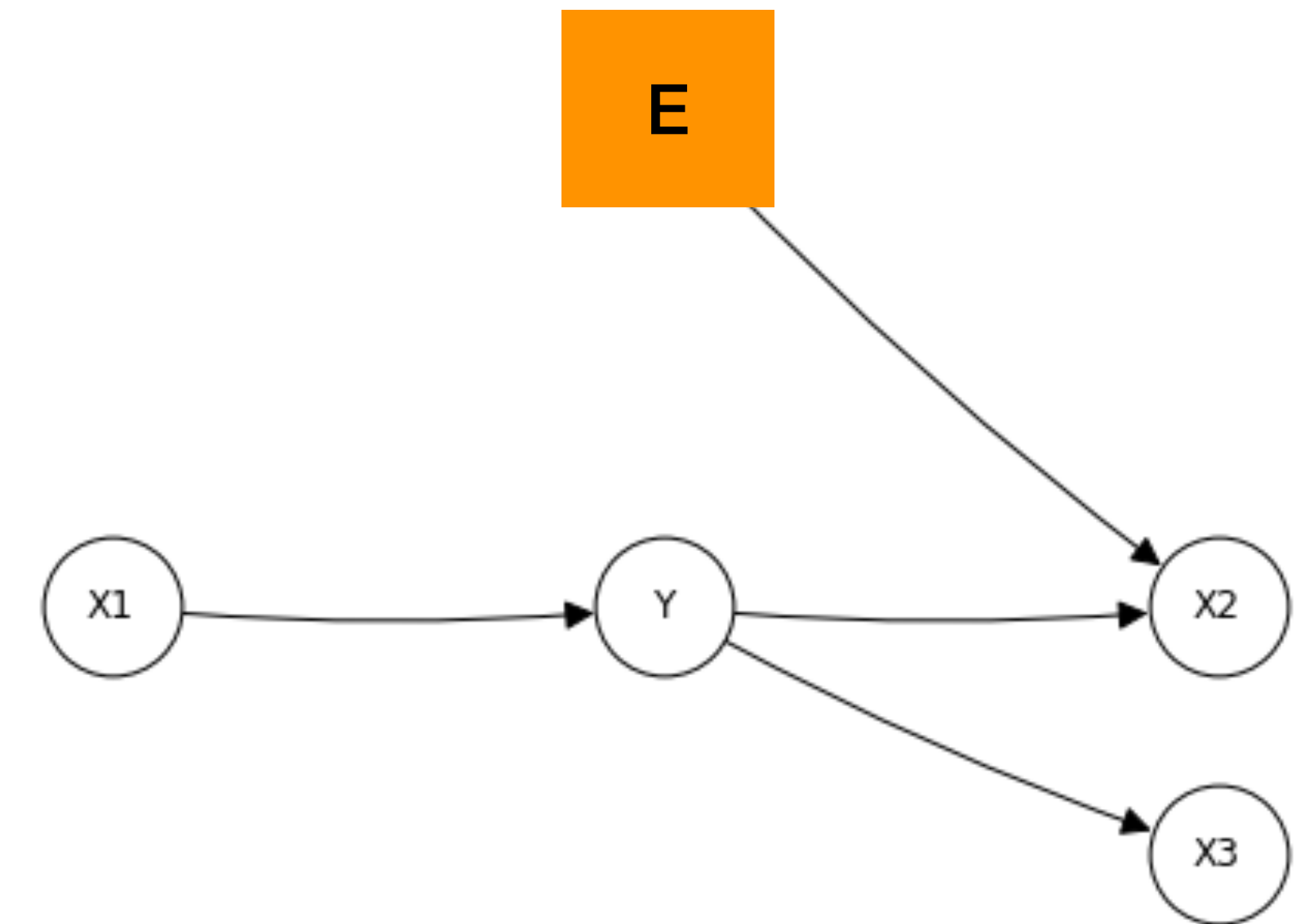
Invariant Causal Prediction example

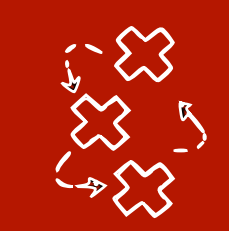
$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = -2Y + \epsilon_2 \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases} \quad E = 0$$

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = 1 \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases} \quad E = 1$$

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = 10Y + \epsilon_Y \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases} \quad E = 2$$

$$\begin{cases} \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_Y \sim \mathcal{N}(0,1) \\ X_1 = 10 + \epsilon_1 \\ Y = 3X_1 + \epsilon_Y \\ X_2 = \begin{cases} -2Y + \epsilon_2 & \text{if } E = 0 \\ 1 & \text{if } E = 1 \\ 10Y + \epsilon_Y & \text{if } E = 2 \end{cases} \\ X_3 = 2Y + 0.1\epsilon_3 \end{cases}$$



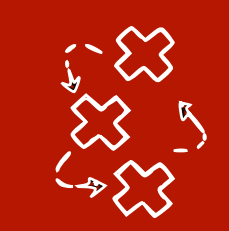


Invariant Causal Prediction example 2

$$\begin{cases} X_1 = \varepsilon_1 \\ Y = X_1 + \varepsilon_Y \\ X_2 = Y + \varepsilon_{X_2} \end{cases} \begin{array}{l} \longrightarrow \text{do}(X_1=1) \\ \longrightarrow \text{unchanged} \\ \longrightarrow \text{do}(X_2=1) \end{array}$$

$\varepsilon_1, \varepsilon_Y \sim N(0, 1), \varepsilon_{X_2} \sim N(0, 0.01)$

$$P^e(Y^e | \text{Pa}(Y^e)) = P^f(Y^f | \text{Pa}(Y^f))$$



Invariant Causal Prediction example 2

env e_1

$$\begin{cases} X_1 = \varepsilon_1 \end{cases}$$

$$\begin{cases} Y = X_1 + \varepsilon_Y \end{cases}$$

$$\begin{cases} X_2 = Y + \varepsilon_{X_2} \end{cases}$$

$$\varepsilon_1, \varepsilon_Y \sim N(0, 1), \varepsilon_{X_2} \sim N(0, 0.01)$$

env e_2

$$\longrightarrow \text{do}(X_1 = 1)$$

\longrightarrow unchanged

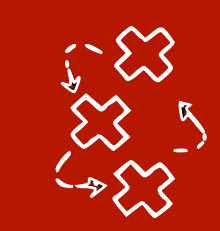
$$\longrightarrow \text{do}(X_2 = 1)$$

$$X_1 \rightarrow Y \rightarrow X_2 \quad \text{env } e_1$$

$$X_1 \rightarrow Y \quad X_2 \quad \text{env } e_2$$

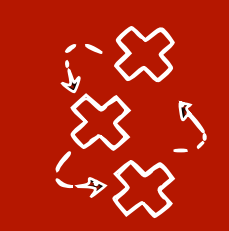


$$Y \perp\!\!\!\perp E \mid X_1 \Rightarrow X_1 \in \text{Pa}(Y)$$



Invariant Causal Prediction (ICP)

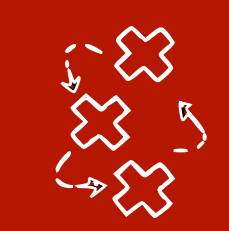
- We assume we have access to **a set of different environments E** (e.g. interventional or observational data), s.t. for $e \in E$, $(X_1^e, \dots, X_p^e, Y^e) \sim P^e$
- We further assume that in **none of the environments Y is intervened upon**



Invariant Causal Prediction (ICP)

- We assume we have access to **a set of different environments E** (e.g. interventional or observational data), s.t. for $e \in E$, $(X_1^e, \dots, X_p^e, Y^e) \sim P^e$
- We further assume that in **none of the environments Y is intervened upon**
- We represent the environment index with E
- If there are no latent confounders, one can prove that:

$$\bigcap_{S \subseteq \{1, \dots, p\} \text{ s.t. } Y \perp\!\!\!\perp E | S} S \subseteq \text{Pa}(Y)$$



Invariant Causal Prediction example 3

env e_1

$$\begin{cases} X_1 = \varepsilon_1 \\ Y = X_1 + \varepsilon_Y \\ X_2 = Y + \varepsilon_{X_2} \end{cases}$$

$$\varepsilon_1, \varepsilon_Y \sim N(0, 1), \varepsilon_{X_2} \sim N(0, 0.01)$$

env e_2

$$\rightarrow \text{do}(X_1 = 1)$$

$$X_1 \rightarrow Y \rightarrow X_2 \quad \text{env } e_1$$

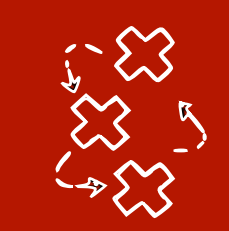
$$X_1 \rightarrow Y \rightarrow X_2 \quad \text{env } e_2$$

$$\begin{array}{c} \varepsilon \\ \swarrow \\ X_1 \rightarrow Y \rightarrow X_2 \end{array}$$

$$Y \perp\!\!\!\perp \varepsilon \mid X_1$$

$$Y \not\perp\!\!\!\perp \varepsilon \mid X_1, X_2$$

$$\begin{aligned} \{X_1\} \cap \{X_1, X_2\} &= \{X_1\} \\ \Rightarrow X_1 &\in \text{Pa}(Y) \end{aligned}$$



Invariant Causal Prediction example 4

env e_1

$$\begin{cases} X_1 = \varepsilon_1 \\ Y = X_1 + \varepsilon_Y \\ X_2 = Y + \varepsilon_{X_2} \end{cases}$$

$$\varepsilon_1, \varepsilon_Y \sim N(0, 1), \varepsilon_{X_2} \sim N(0, 0.01)$$

$$\text{pa}(X_2) = ?$$

$$\begin{aligned} X_2 &\perp\!\!\!\perp \varepsilon | X_1 \\ X_2 &\perp\!\!\!\perp \varepsilon | X_1, Y \\ X_2 &\perp\!\!\!\perp \varepsilon | Y \end{aligned}$$

env e_2

$$\rightarrow \text{do}(X_1 = 1)$$

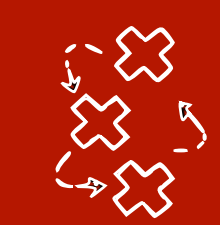
$$X_1 \rightarrow Y \rightarrow X_2 \quad \text{env } e_1$$

$$X_1 \rightarrow Y \rightarrow X_2 \quad \text{env } e_2$$

$$\begin{array}{c} \varepsilon \\ \swarrow \\ X_1 \rightarrow Y \rightarrow X_2 \end{array}$$

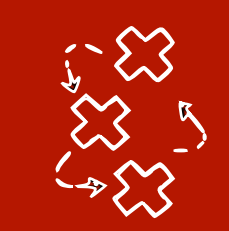
$$\{X_1\} \cap \{X_1, Y\} \cap \{Y\} = \emptyset$$

$$\emptyset \in \text{pa}(X_2)$$



Invariant Causal Prediction (ICP)

- We assume we have access to **a set of different environments E** (e.g. interventional or observational data), s.t. for $e \in E$, $(X_1^e, \dots, X_p^e, Y^e) \sim P^e$
- We further assume that in **none of the environments Y is intervened upon**
- Approximate test on residuals for each $S \subseteq \{1, \dots, p\}$
 - Fit linear regression with S and let $R = Y - \hat{f}(X_S)$
 - Test null hypothesis that mean and variance of R are the same across E
 - Combine the two p-values and reject S if the combined p-value $\leq \alpha$



ICP improves with more interventions

$$E \rightarrow X_1 \rightarrow X_2 \rightarrow Y$$

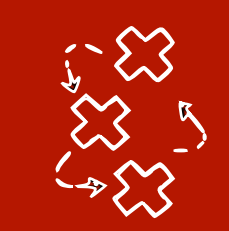
$$\left. \begin{array}{l} E \perp\!\!\!\perp Y | X_1 \\ E \perp\!\!\!\perp Y | X_2 \\ E \perp\!\!\!\perp Y | X_1, X_2 \end{array} \right\} \cap \emptyset$$

+ new environment e^3

$$X_2 = f^{\text{new}}(X_1, \varepsilon_2)$$

$$E \rightarrow X_1 \rightarrow \vec{X}_2 \rightarrow Y$$

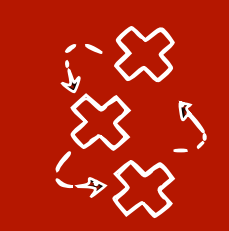
$$\begin{array}{l} E \perp\!\!\!\perp Y | X_2 \quad \cap \quad X_2 \in \text{Pa}(Y) \\ E \perp\!\!\!\perp Y | X_2, X_1 \end{array}$$



ICP improves with more interventions

- We assume we have access to **a set of different environments E** (e.g. interventional or observational data), s.t. for $e \in E$, $(X_1^e, \dots, X_p^e, Y^e) \sim P^e$
- We further assume that in **none of the environments Y is intervened upon**
- We represent the environment index with E , no latent confounders
- If the **environment variable causes all (X_1, \dots, X_p)**

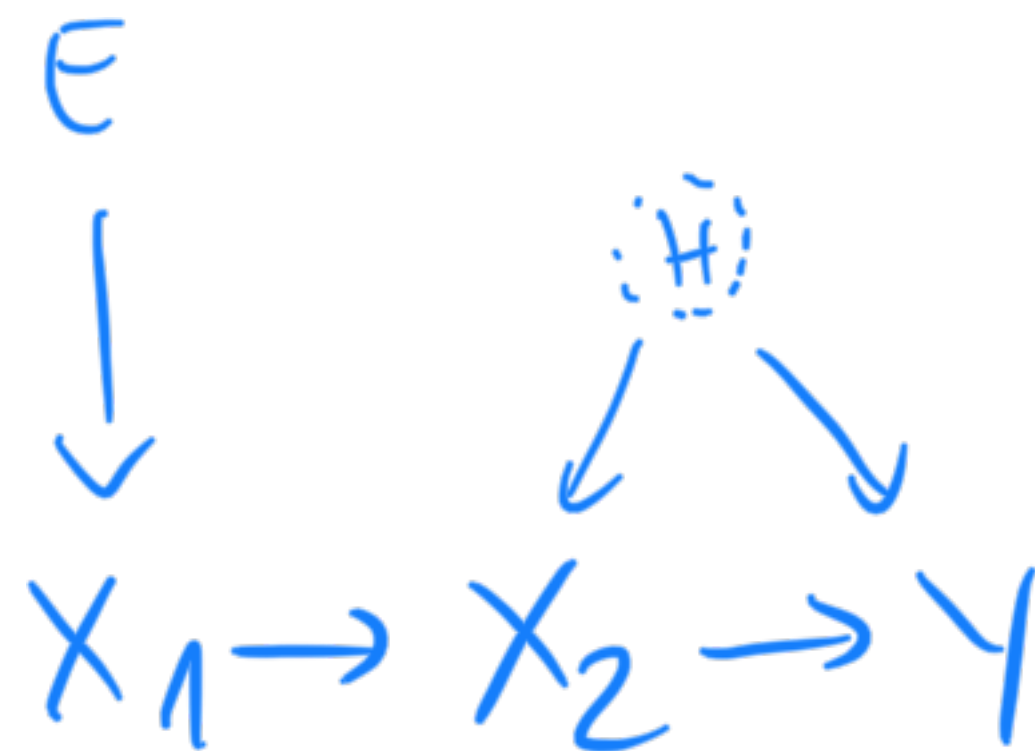
$$\text{Pa}(Y) = \bigcap_{S \subseteq \{1, \dots, p\} \text{ s.t. } Y \perp\!\!\!\perp E | S} S$$



Invariant Causal Prediction - latent confounders

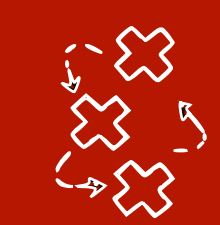
- If there are latent confounders, one can prove that:

$$\bigcap_{S \subseteq \{1, \dots, p\} \text{ s.t. } Y \perp\!\!\!\perp E | S} S \subseteq \text{Anc}(Y)$$



$$Y \not\perp\!\!\!\perp E | X_2$$

$$Y \perp\!\!\!\perp E | X_1 \Rightarrow X_1 \in \text{Anc}(Y)$$
$$Y \perp\!\!\!\perp E | X_1, X_2$$



Learning from multiple contexts

- Now we cannot decide which intervention to perform (**intervention design**)
 - We then also have **known intervention targets**, e.g. $\text{do}(S = 1)$
- Instead, somebody gives us a **set of data from multiple contexts**
 - Possibly **unknown intervention targets**
 - Possibly **soft interventions** instead of **perfect interventions**

**ICP finds subsets of parents,
what about finding (an
equivalence class of) the
causal graph?**