Active Invariant Causal Prediction:
Experiment Selection Through Stability

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Joint work with Juan L. Gamella

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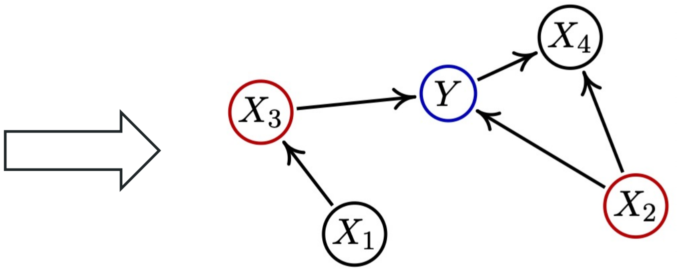
Causal structure learning

Setting

	Y	X_1	X_2	X_3	X_4
i=0	6.51	22.76	12.92	2.37	1.68
i=1	6.06	13.75	7.90	1.13	0.94
i=2	1.35	8.03	3.32	0.96	-0.15
i=3	1.53	-1.49	-0.14	-0.76	1.54
i=4	0.06	-3.64	-1.27	-0.22	0.04
i=5	-2.31	-11.15	-6.59	-1.76	-1.14
i=6	2.29	8.70	4.70	1.05	-1.24
i=7	0.98	1.23	0.87	0.37	0.76
i=8	5.22	19.16	10.54	2.20	-0.23
i=9	4.26	13.82	9.51	1.18	0.93
i=10	-0.60	-1.35	-1.40	-0.21	-0.05
i=11	-0.91	-3.50	-2.65	-0.45	-1.32
i=12	2.08	5.26	4.04	0.55	0.51
i=13	4.30	11.81	6.70	1.05	0.08
i=14	1.37	7.35	4.17	0.84	-1.56
i=...					

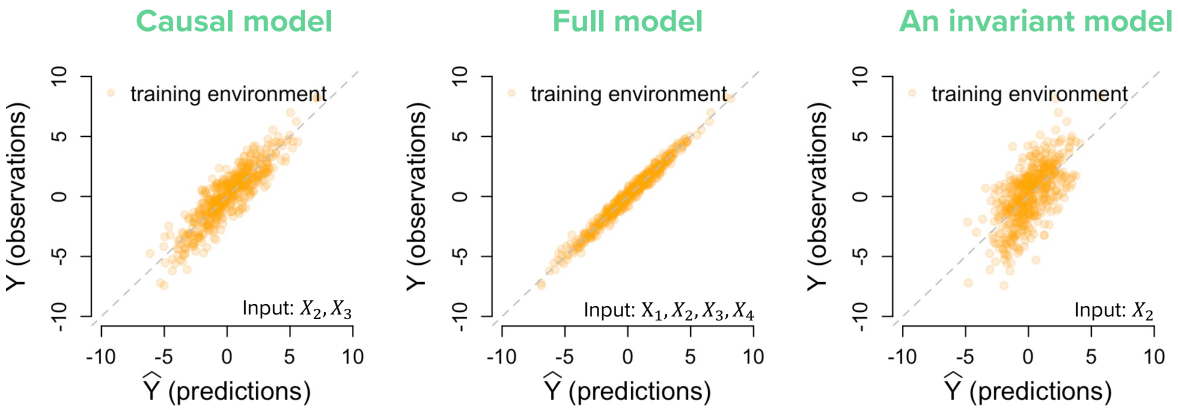


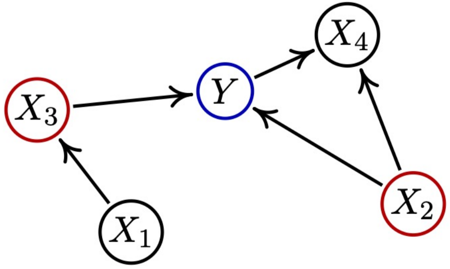
$$S^* = \text{parents}(Y) = \{X_2, X_3\}$$

Goal: Infer causal parents of target variable Y

Causal models generalize

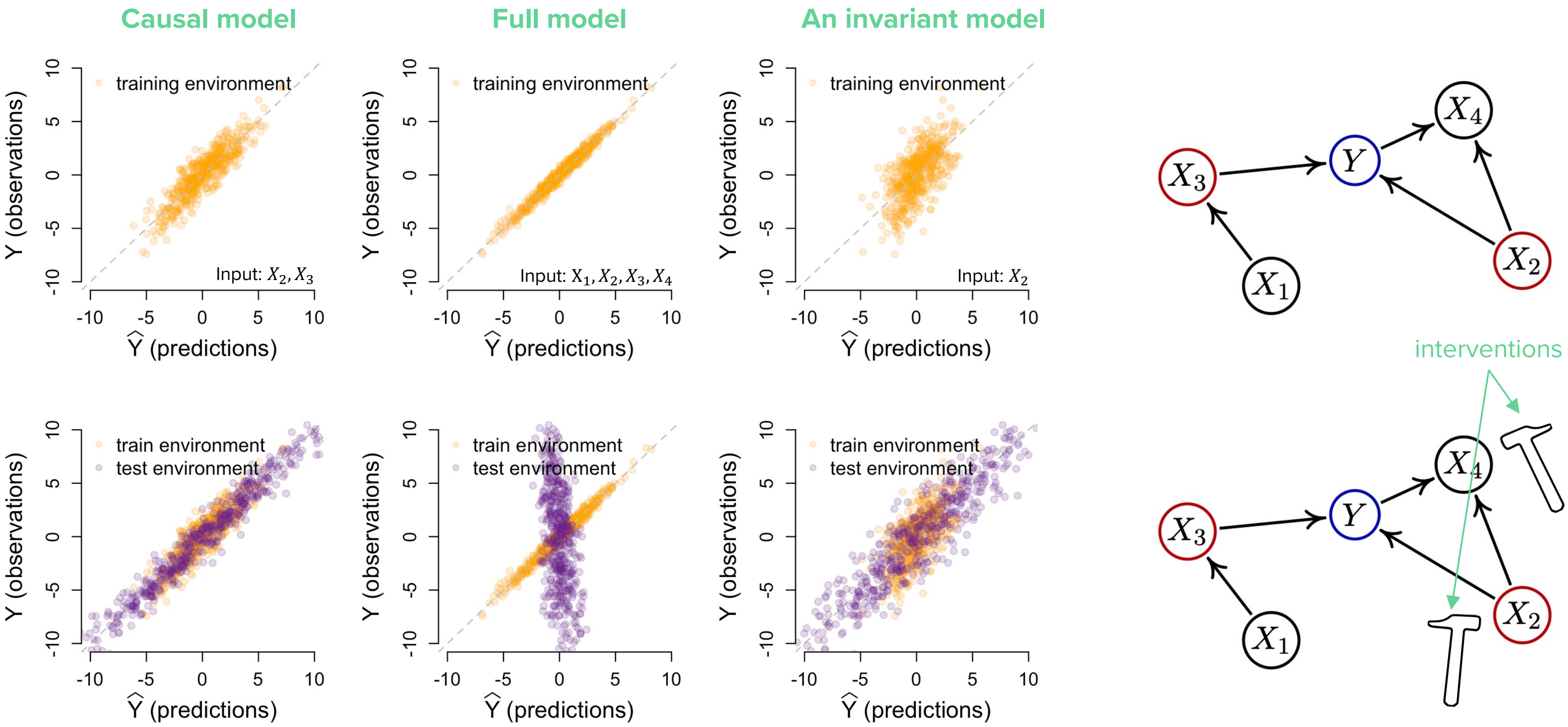
Invariant models are potentially causal





Causal models generalize

Invariant models are potentially causal



Invariant Causal Prediction (ICP)

Peters et al. (2016)

Key observation As long as we avoid interventions on the response Y itself, for all environments $e, f \in \mathcal{E}$ and for all x

$$Y^e \big| X^e_{S^*} = x \quad \overset{d}{=} \quad Y^f \big| X^f_{S^*} = x$$

S^* are the causal parents of Y

Idea: *Find* invariant conditional distributions to estimate $S^* \coloneqq \mathrm{parents}(Y)$

Other sets of predictor variables may also satisfy this invariance!

Peters et al. (2016). *Causal inference using invariant prediction: identification and confidence intervals*

Invariant Causal Prediction (ICP)

Invariant models are potentially causal

Definition We call a set of variables S invariant under a set of environments $\mathcal{E}$ if for all $e, f \in \mathcal{E}$ and for all x

$$Y^e \middle| X_S^e = x \quad \overset{d}{=} \quad Y^f \middle| X_S^f = x$$

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Invariant Causal Prediction (ICP)
Method

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$$Y^e \,\big|\, X_S^e = x \quad \overset{d}{=} \quad Y^f \,\big|\, X_S^f = x$$

Invariant Causal Prediction:

1. Given data from different environment, find **all** invariant sets

2. Return **intersection** of these: $\hat{S} := \cap_{S:\text{invariant}} S$

Disclaimer: Some simplifications in this talk…

Peters et al. (2016). *Causal inference using invariant prediction: identification and confidence intervals*

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Assumptions

- Acyclicity
- No hidden confounders
- No interventions on Y

Peters et al. (2016). *Causal inference using invariant prediction: identification and confidence intervals*

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Peters et al. (2016); Heinze-Deml et al. (2018); Pfister et al. (2019)

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Invariant Causal Prediction:

1. Given data from different environment, find **all** invariant sets

   Based on testing null hypothesis of "invariance across environments" $H_{0,S}$ for all S

2. Return **intersection** of these: $\hat{S} := \cap_{S:\, H_{0,S} \text{ not rejected}} S$

Invariant Causal Prediction (ICP)

Method

Definition We call a set of variables S invariant under a set of environments $\mathcal{E}$ if for all $e, f \in \mathcal{E}$ and for all x

$$Y^e \middle| X_S^e = x \quad \overset{d}{=} \quad Y^f \middle| X_S^f = x$$

Invariant Causal Prediction:

Guarantee:

$$P(\hat{S} \subseteq S^*) \geq P(H_{0,S^*} \text{ not rejected}) \geq 1 - \alpha$$

Null hypothesis for testing invariance of the true causal parents S^*

Peters et al. (2016). *Causal inference using invariant prediction: identification and confidence intervals*

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Invariant Causal Prediction:

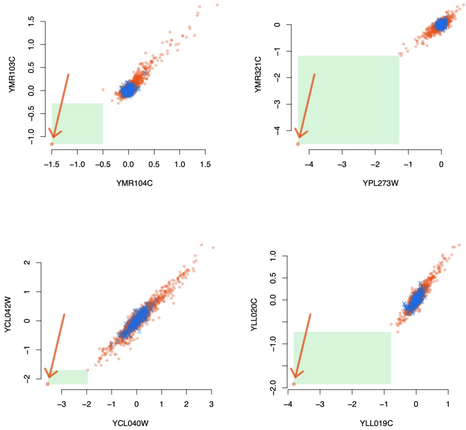
1. Given data from different environment, find **all** invariant sets

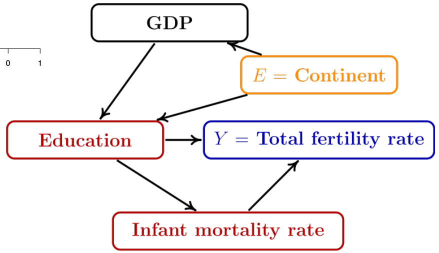
Focus of this talk!

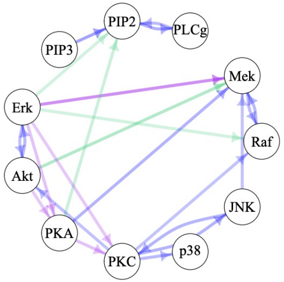
2. Return **intersection** of these: $\hat{S} := \cap_{S:\, H_{0,S} \text{ not rejected}} S$

Invariant Causal Prediction (ICP)
Applications

- Gene perturbation experiments for yeast
  - Data: Kemmeren et al. (2014)
  - Application of ICP: Meinshausen et al. (2016)
  - Environments: wild-type vs. gene deletions
- Fertility rate modeling
  - Data: UN World population prospects (2013)
  - Application of nonlinear ICP: Heinze-Deml et al. (2018)
  - Environments: Different continents
- Protein-signaling network estimation
  - Flow cytometry data: Sachs et al. (2005)
  - Application of ICP: Meinshausen et al. (2016)
  - Environments: Different experimental conditions







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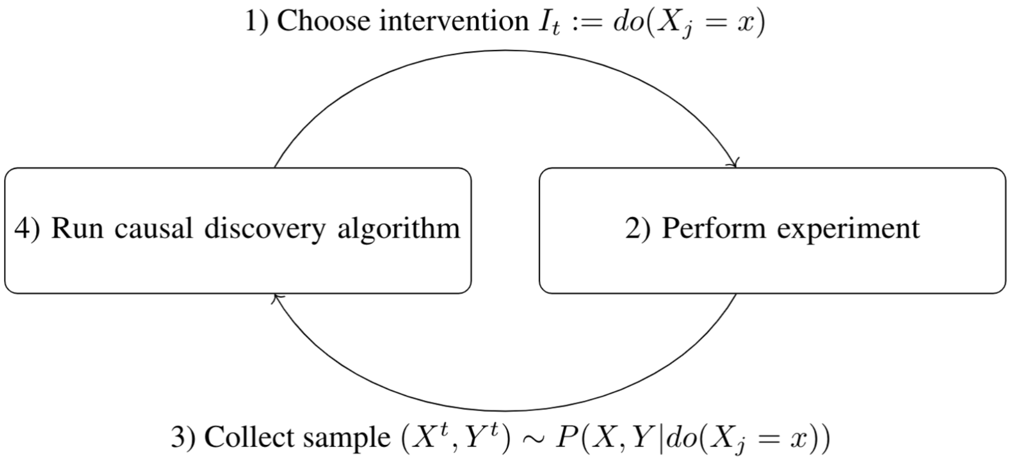
Active causal learning
Setting

Definition Learning a causal model while being able to actively perform interventions

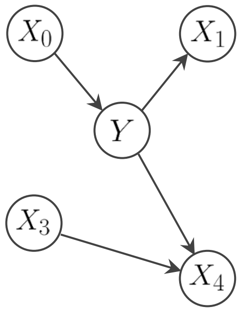
experiments



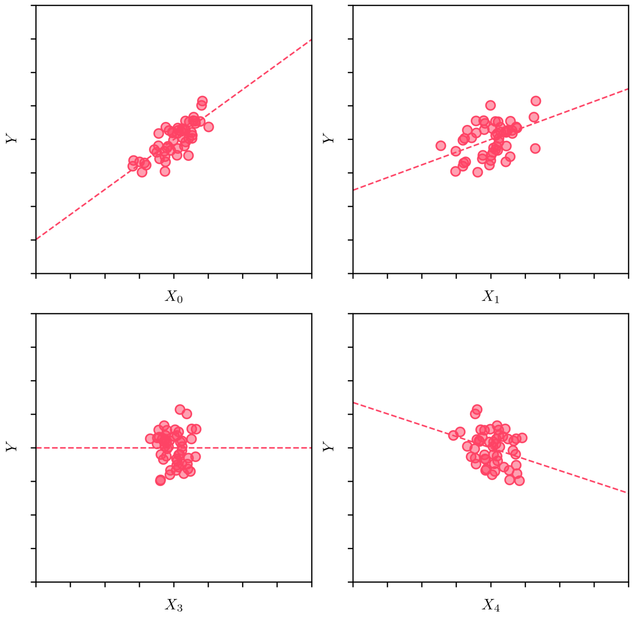
Invariant Causal Prediction (ICP)

Example

ICP: 1. Find **all** invariant sets; 2. Return **intersection** of these



Environment 1



Invariant sets*

$S \subseteq \{X_0, X_1, X_3, X_4\}$

ICP Estimate

$\hat{S} = \emptyset$

estimate for causal parents

*Invariant sets: $\emptyset$, $\{X_0\}$, $\{X_1\}$, $\{X_3\}$, $\{X_4\}$, $\{X_0, X_1\}$, $\{X_0, X_3\}$, $\{X_0, X_4\}$, $\{X_1, X_3\}$, $\{X_1, X_4\}$, $\{X_3, X_4\}$, $\{X_0, X_1, X_3\}$, $\{X_0, X_1, X_4\}$, $\{X_1, X_3, X_4\}$, $\{X_0, X_3, X_4\}$, $\{X_0, X_1, X_3, X_4\}$

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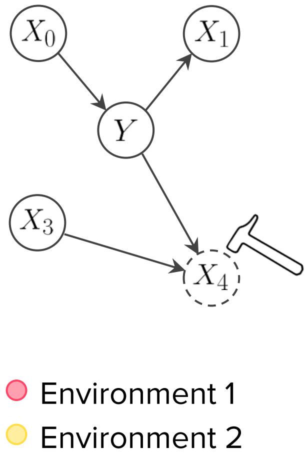

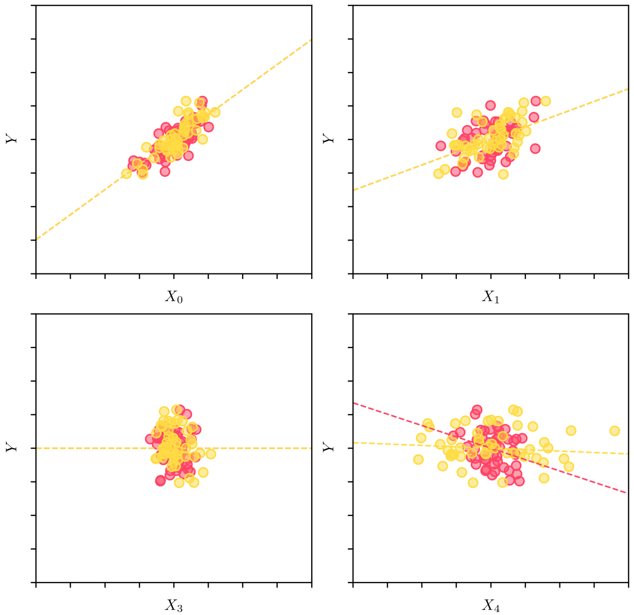

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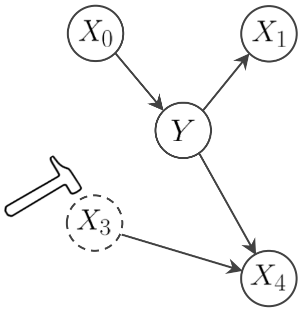
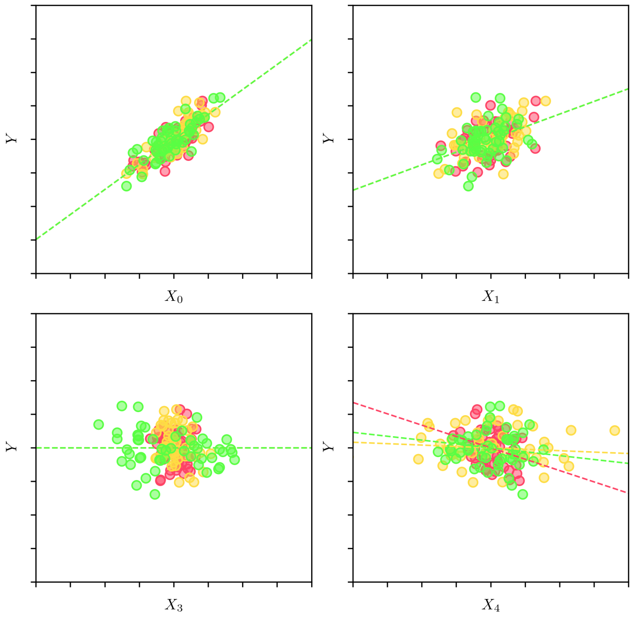


- Environment 1
- Environment 2
- Environment 3



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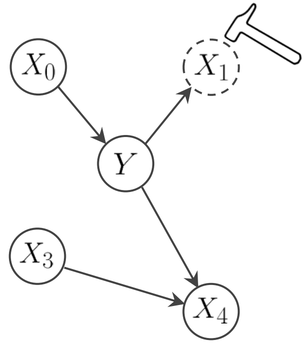
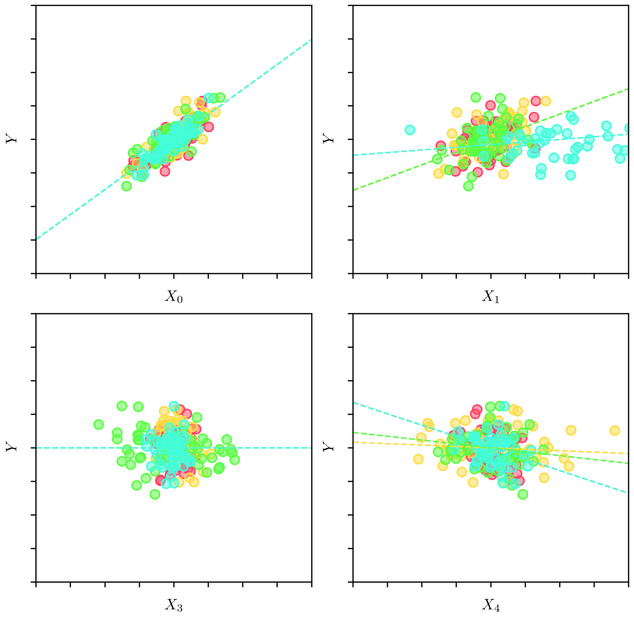


- Environment 1
- Environment 2
- Environment 3
- Environment 4



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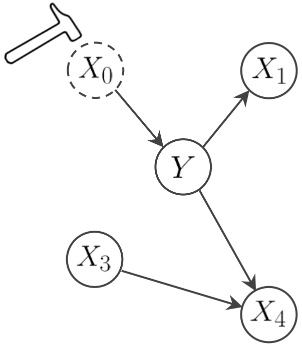
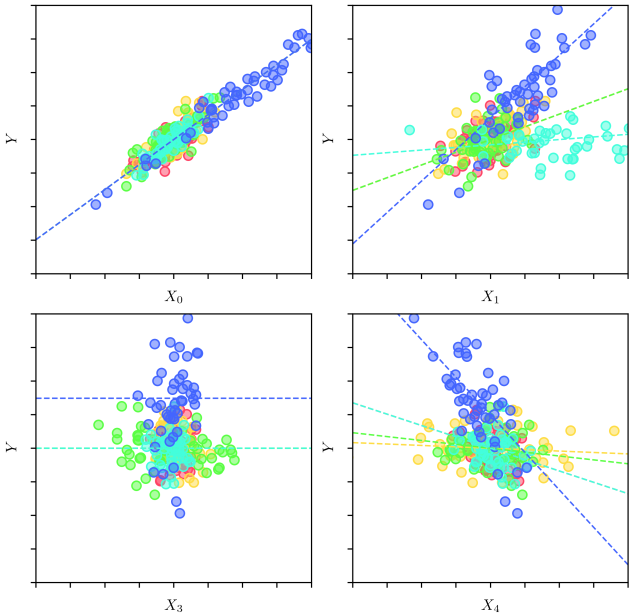


- Environment 1
- Environment 2
- Environment 3
- Environment 4
- Environment 5



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$\{X_0\}, \{X_0, X_3\}$

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$$\hat{S} = \{X_0\}$$

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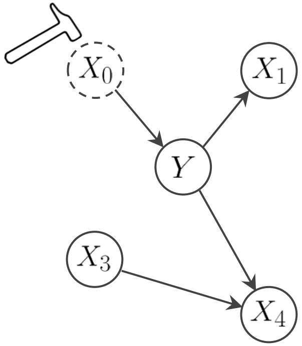

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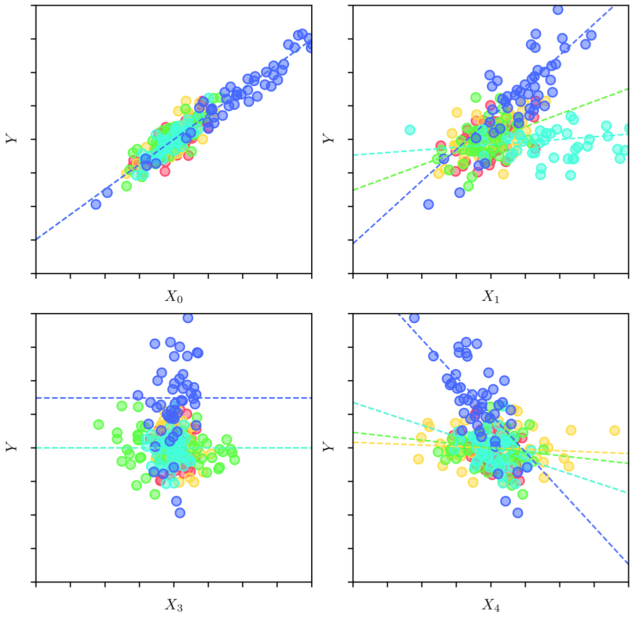

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$\{X_0\}, \{X_0, X_3\}$

ICP Estimate

$$\hat{S} = \{X_0\}$$

Did we need all these environments?

Invariant Causal Prediction (ICP)

Example

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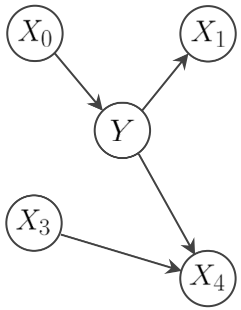

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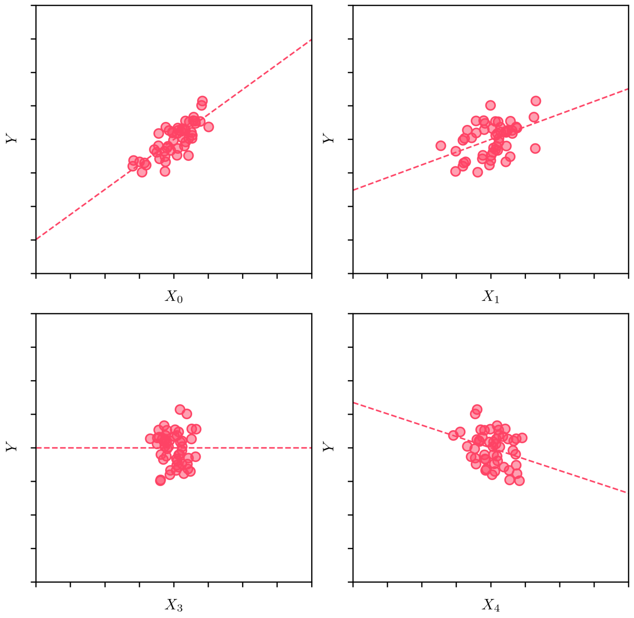

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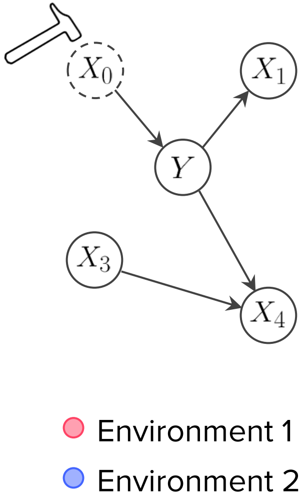
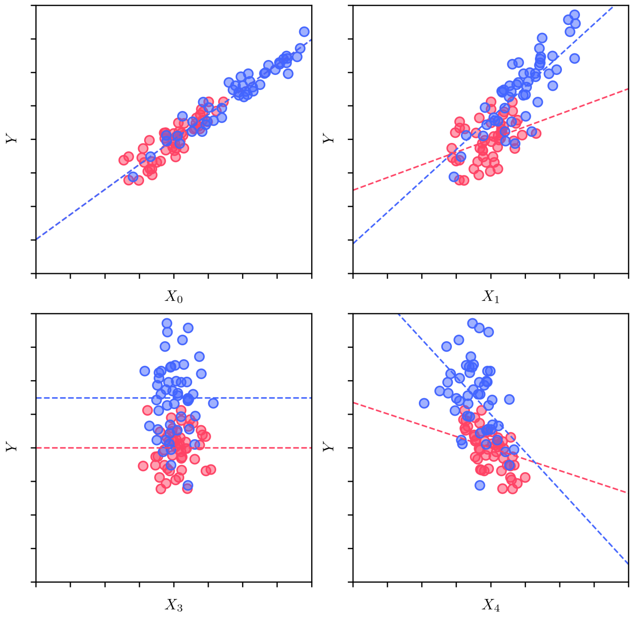
Invariant Causal Prediction (ICP)

Heterogeneity plays a key role

ICP: 1. Find **all** invariant sets; 2. Return **intersection** of these





Invariant sets*

$S = \{X_0\} \cup W$

$\forall\, W \subseteq \{X_1, X_3, X_4\}$

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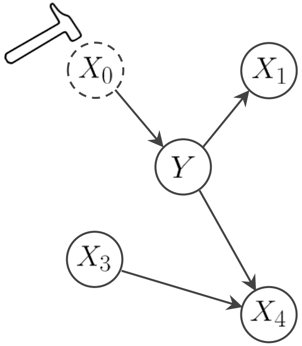
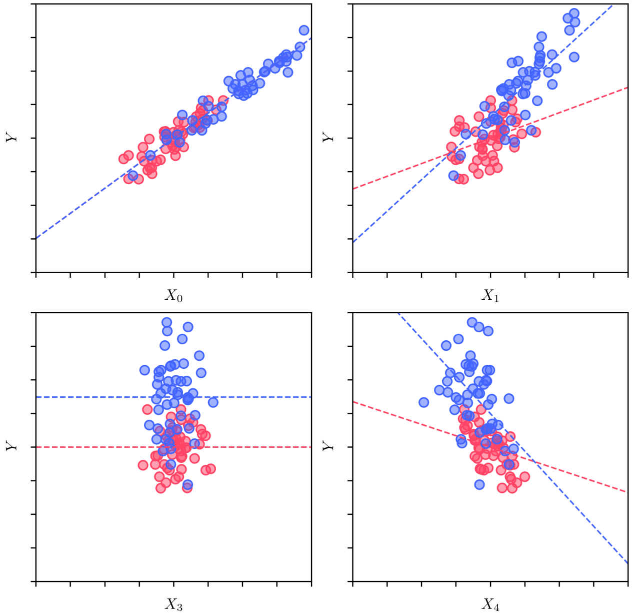


Environment 1

Environment 2



Invariant sets*

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ICP Estimate

$$\hat{S} = \{X_0\}$$

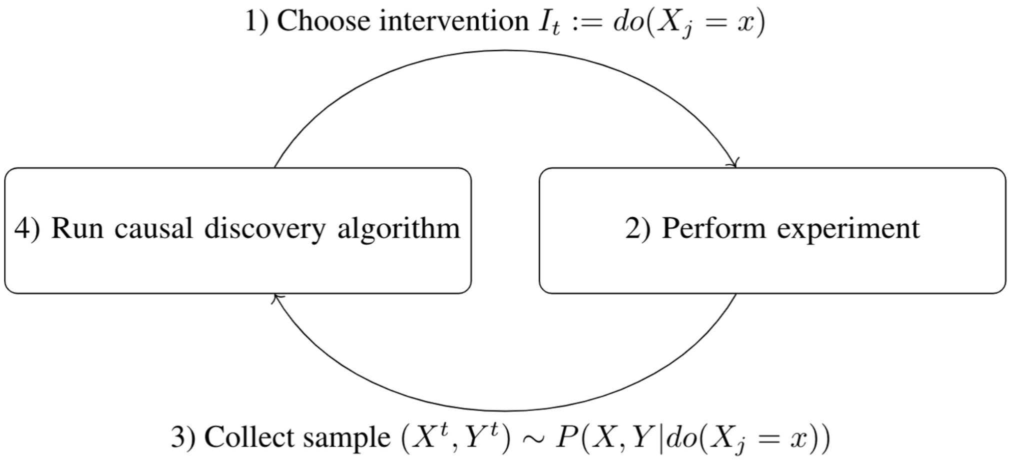
Some environments are more informative than others!

Active causal learning

Setting

Definition Learning a causal model while being able to actively perform interventions

experiments



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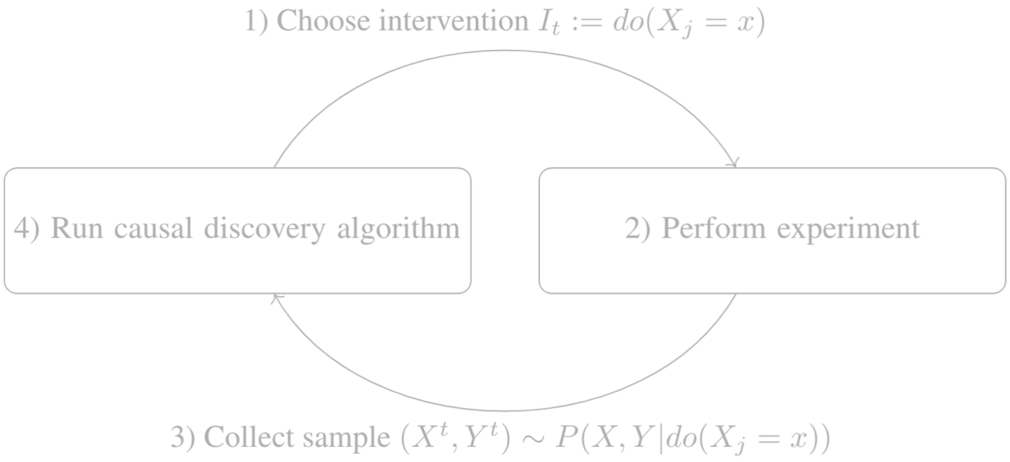


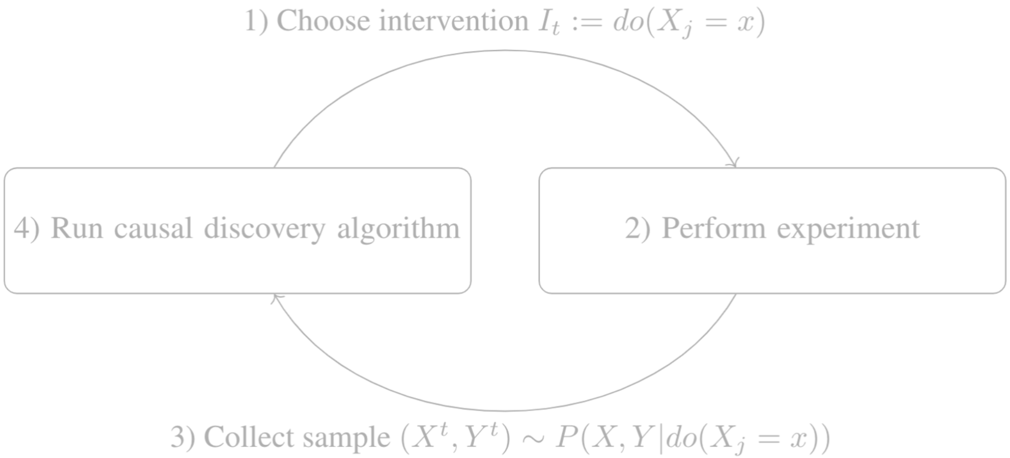
How do you select informative experiments?

Active causal learning

Informative intervention

Definition Learning a causal model while being able to actively perform interventions

experiments



Informative intervention: The one after which the largest number of parents appear in the estimate

Active causal learning

Informative intervention

Lemma *If a parent is directly intervened on, then it appears on all invariant sets*

Treat **direct interventions on parents** as maximally informative

Intervention selection strategies

Some proposals

- **Key idea:** After each experiment observe how the invariant sets change
- Collection of invariant sets has properties one can exploit for experiment selection:

Proposition *Parents appear on at least half of all invariant sets*

⇒ ***Ratio strategy:*** Do not intervene on variables that appear less often

Lemma *If the marginal distribution of Y is invariant under a set of environments, then none of the interventions were performed upstream of the response*

⇒ ***Empty-set strategy:*** If after an intervention the marginal distribution of Y is invariant, discard the intervention target from future interventions

Intervention selection strategies

Some proposals

Ratio strategy Do not intervene on variables that appear on less than half of the invariant sets

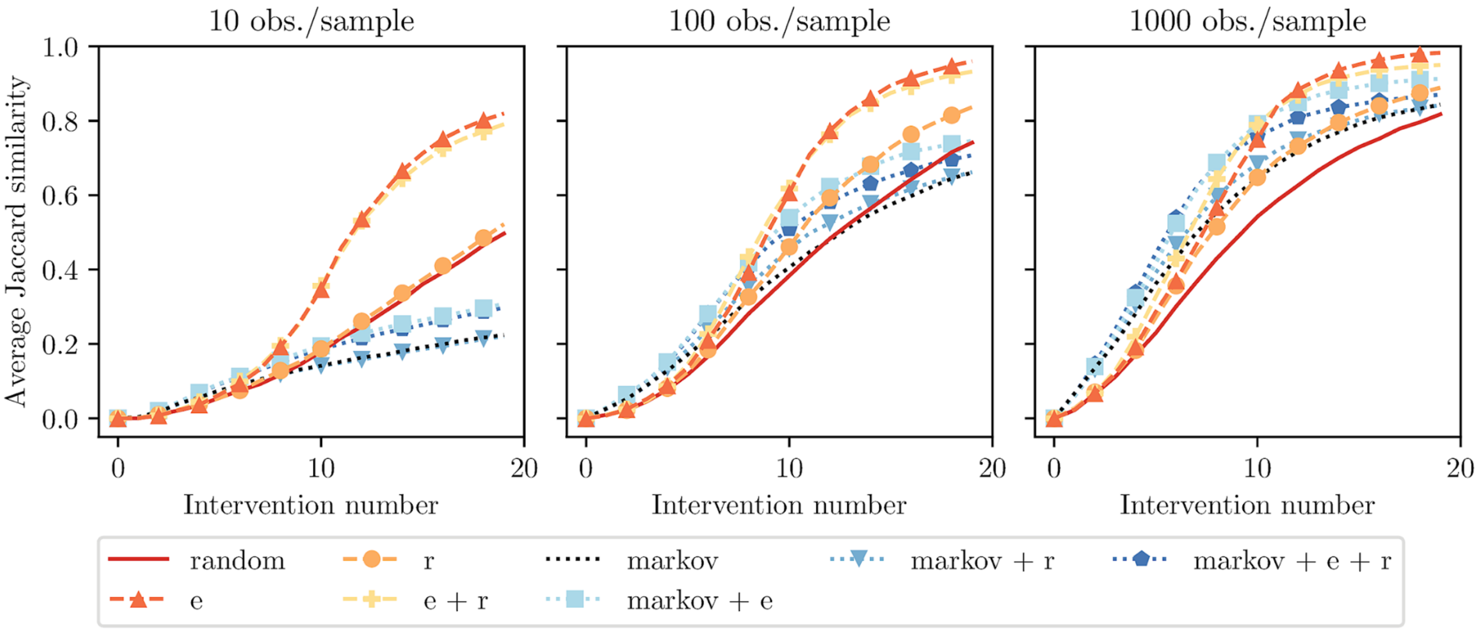
Empty-set strategy If after an intervention the marginal distribution of Y is invariant, discard the intervention target from future interventions

Markov strategy Picking intervention targets from within the Markov blanket

Policy A combination of the above strategies

Experiments

Simulations

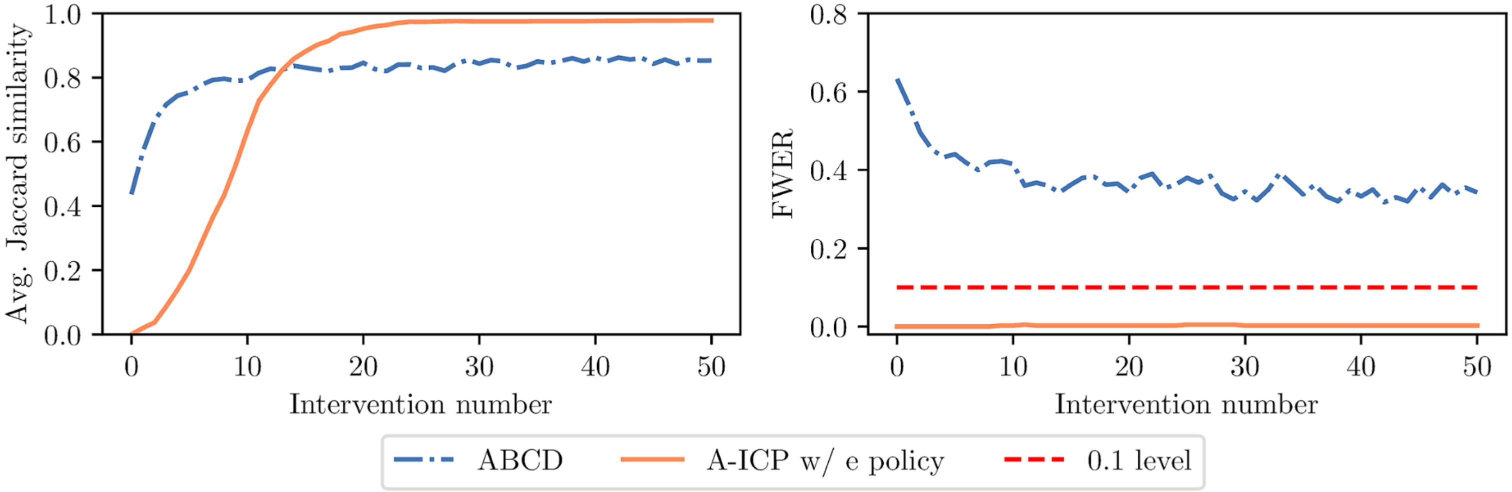


Strategies e - empty set r – ratio markov - markov blanket

Jaccard similarity $\frac{|\hat{S} \cap S^*|}{|\hat{S} \cup S^*|}$

Experiments

Comparison with Bayesian approach ABCD



Jaccard similarity $\frac{|\hat{S} \cap S^*|}{|\hat{S} \cup S^*|}$

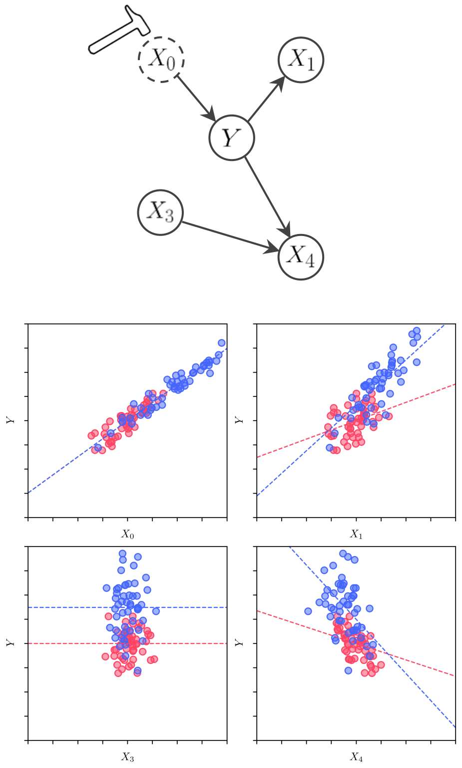
FWER $\hat{P}(\hat{S} \not\subseteq S^*)$

Agrawal et al. (2019). *ABCD-Strategy: Budgeted Experimental Design for Targeted Causal Structure Discovery*

Active Invariant Causal Prediction

Summary

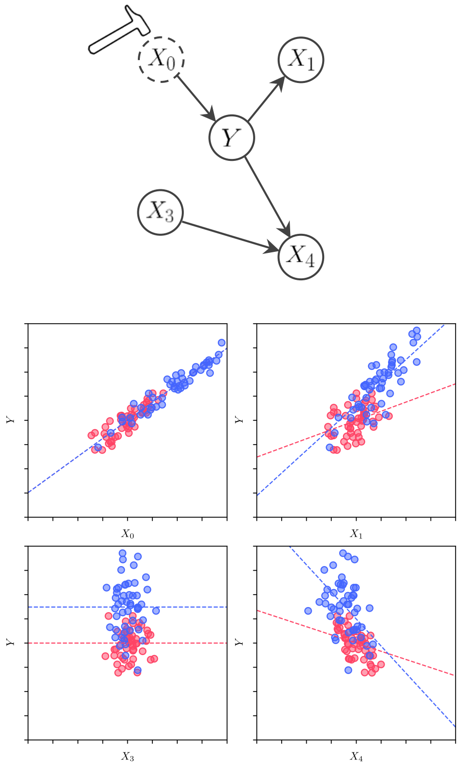
- Causal models are invariant and generalize
- Invariant models (wrt. some observed environments) are potentially causal
- Heterogeneity plays a key role in Invariant Causal Prediction
- Some environments are more informative than others
- In A-ICP, we collect informative new environments by observing which models are invariant given current environments
- This may help to find the causal model more quickly



Active Invariant Causal Prediction

Discussion

- ICP does not require knowledge of intervention locations
  - Robust to off-target effects (not acting on Y)
  - Can combine existing environments with unknown intervention targets with actively collected environments
  - But we also discard information we have for the actively collected environments – potential to improve A-ICP



Thank you!

Some references

J. L. Gamella and C. Heinze-Deml. *Active Invariant Causal Prediction: Experiment Selection through Stability. NeurIPS 2020*

C. Heinze-Deml, J. Peters and N. Meinshausen. *Invariant Causal Prediction for Nonlinear Models. Journal of Causal Inference 6 (2), 2018*

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