Causal discovery and Deep Learning

Faria et. al. 2022; Pearl et. al. 2018; Neal et. al. 2022; Schölkopf et. al. 2019; Bengio et. al. 2020; Peters et. al. 2017, Ke et. al. 2020, Brouillard et. al. 2020

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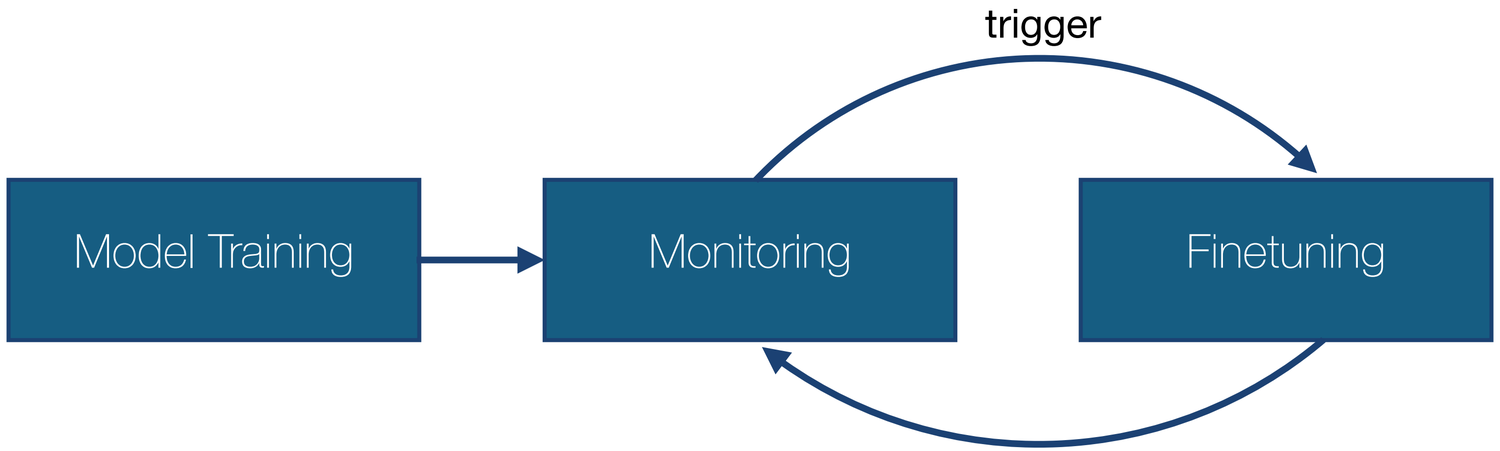
Deep Learning Sessions Portugal

Overview

- Limitations of current Deep Learning systems
- Causal Discovery
- Identifiability
- Interventions and Causal Discovery
- Latent interventions and Causal Discovery

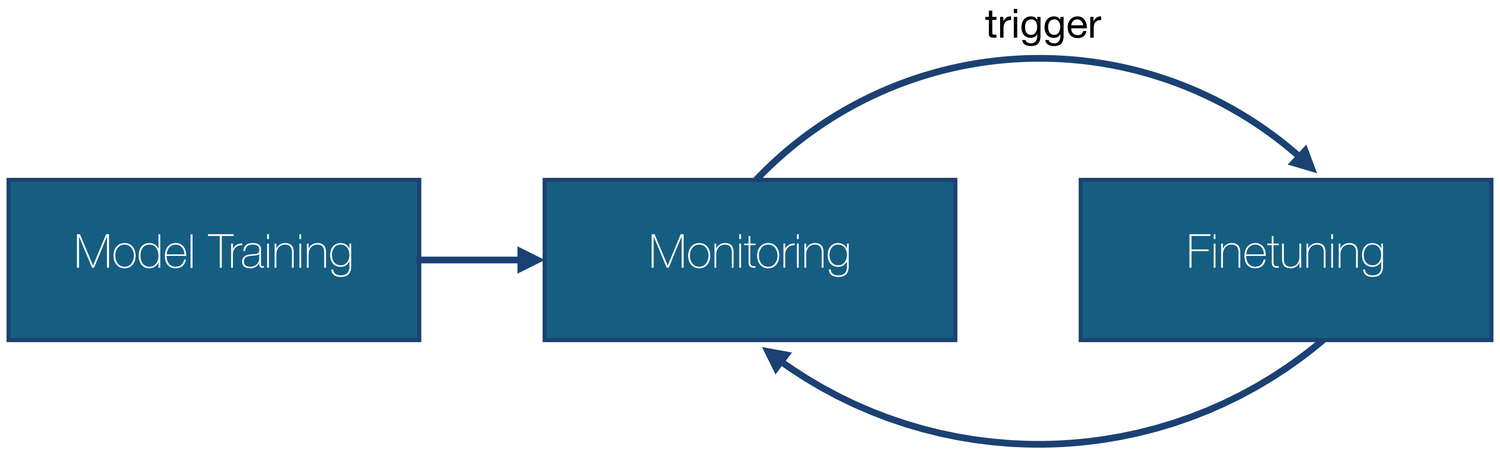
Limitations of current Deep Learning

- Distribution shifts.



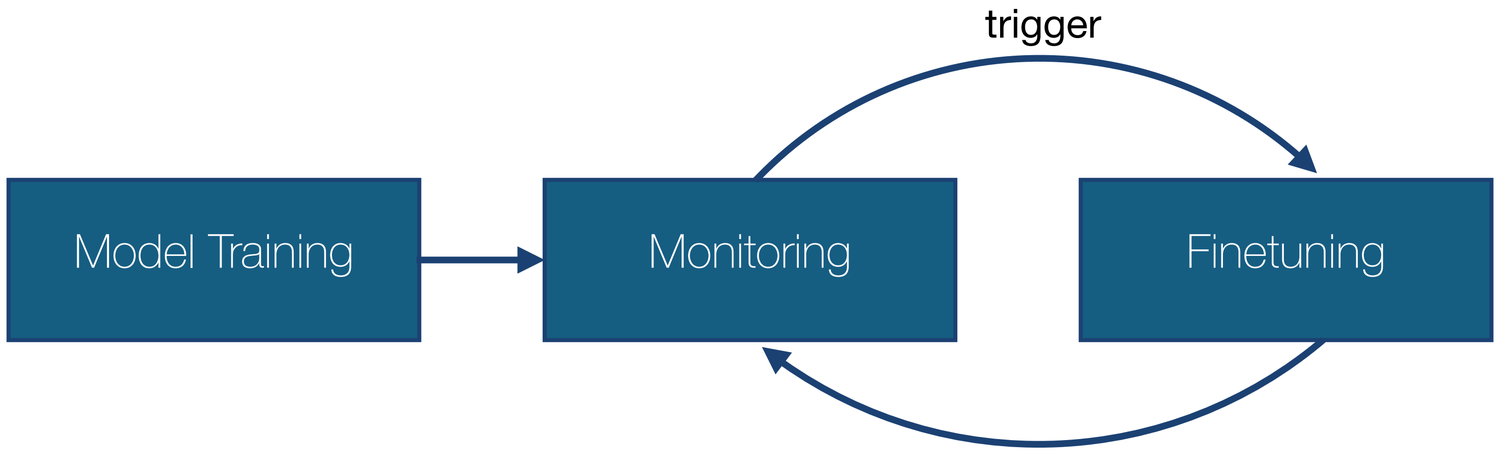
Limitations of current Deep Learning

- Distribution shifts.
- Model deployment drives distribution shifts.



Limitations of current Deep Learning

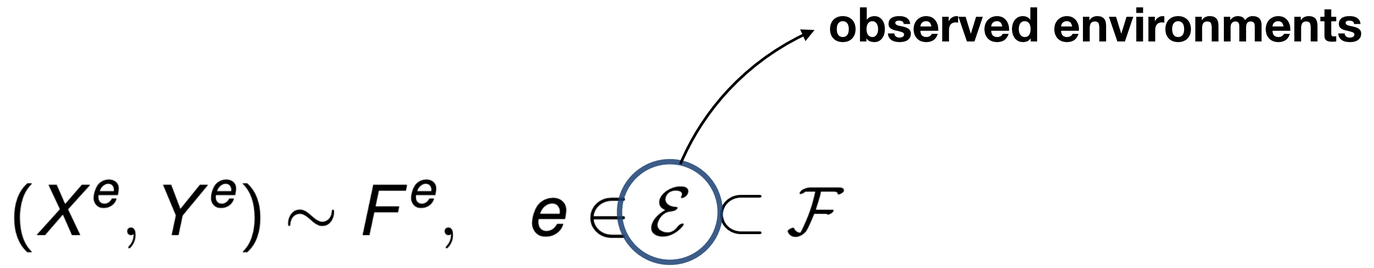
- Distribution shifts.
- Model deployment drives distribution shifts.
- Test-set performance vs generalization.
- Interpretability and scientific understanding



Benefits of causal predictors

- Causal predictors are optimally robust.

Consider the setting :



$$\hat{\beta} = \text{argmin}_\beta \max_{e \in \mathcal{F}} \mathbb{E}|Y^e - (X^e)^T \beta|^2$$

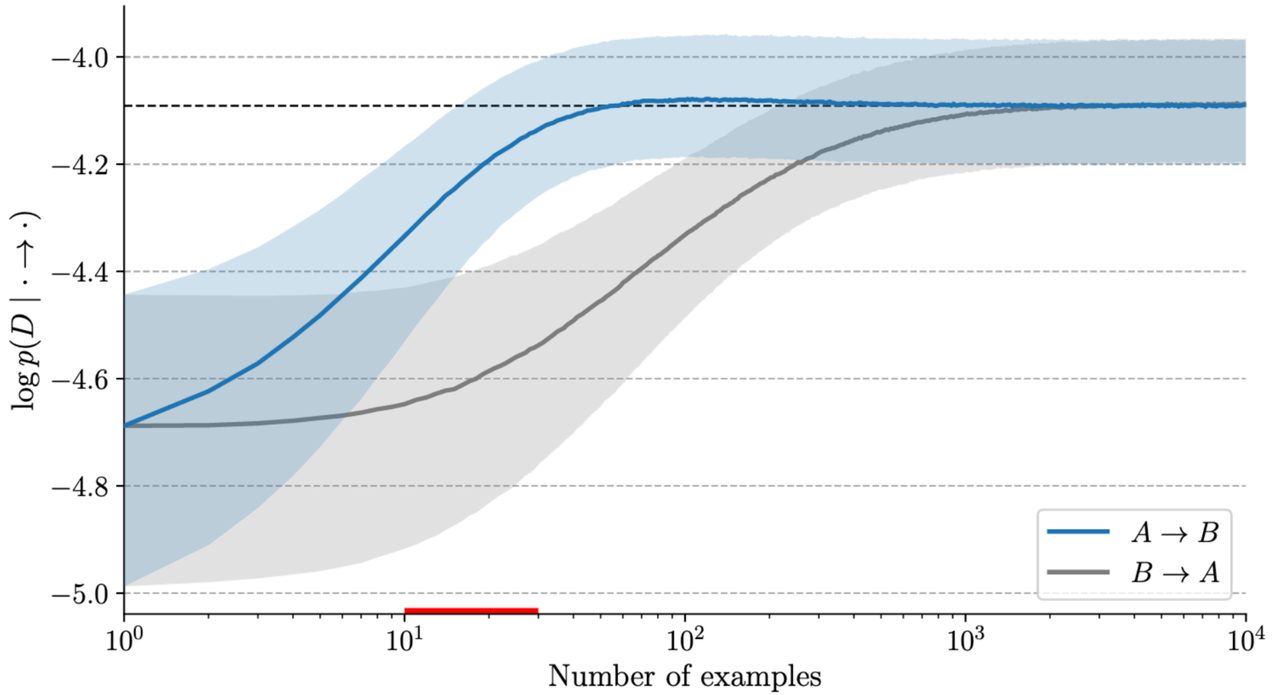
causal predictor

Causality $\Leftrightarrow$ **Prediction in heterogeneous scenarios/environments**

Causal inference using invariant prediction (Peters et. al. 2016)

Benefits of causal predictors

- Causal predictors are optimally robust.
- Fast and data efficient adaptation to transfer distribution.

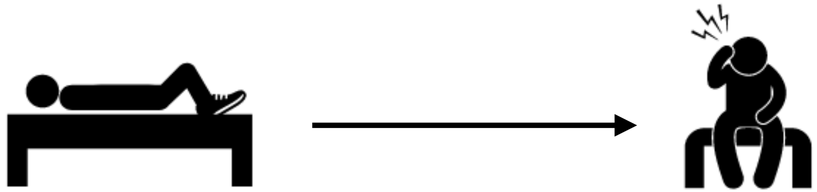


A Meta-Transfer Objective for Learning to Disentangle Causal Mechanisms (Bengio et. al. 2019)

What if we do not know the causal model ?

Causal Discovery

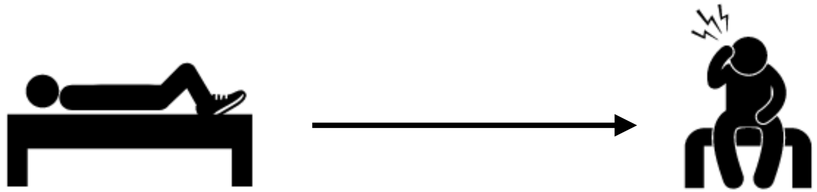
- Say we have a dataset.



Introduction to Causal Inference (Neal et. al. 2022)

Causal Discovery

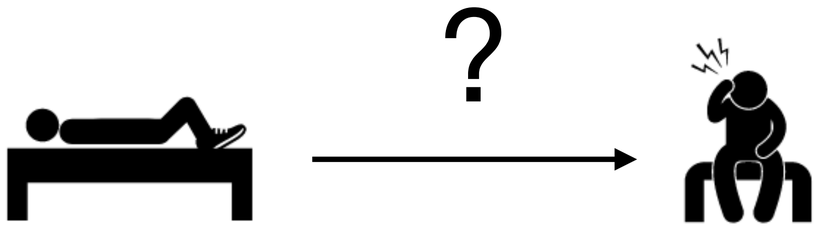
- Say we have a dataset.
- Cause-effect relation?



Introduction to Causal Inference (Neal et. al. 2022)

Causal Discovery

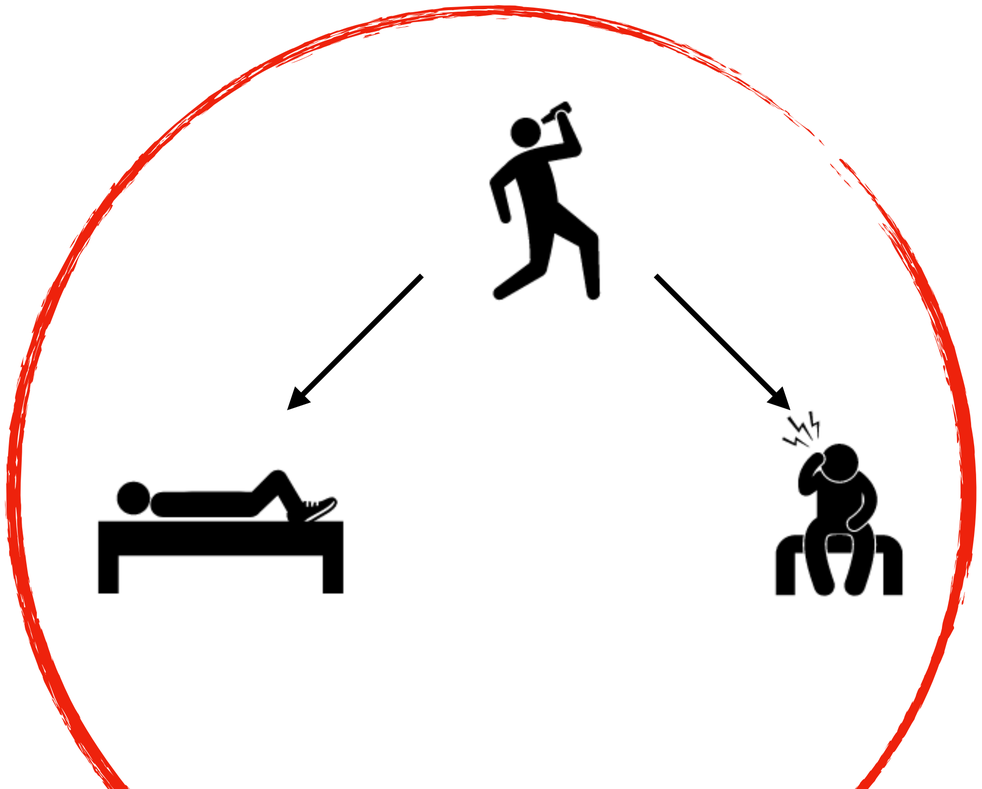
- Say we have a dataset.
- Cause-effect relation?
- **Correlation is not causation**



Introduction to Causal Inference (Neal et. al. 2022)

Causal Discovery

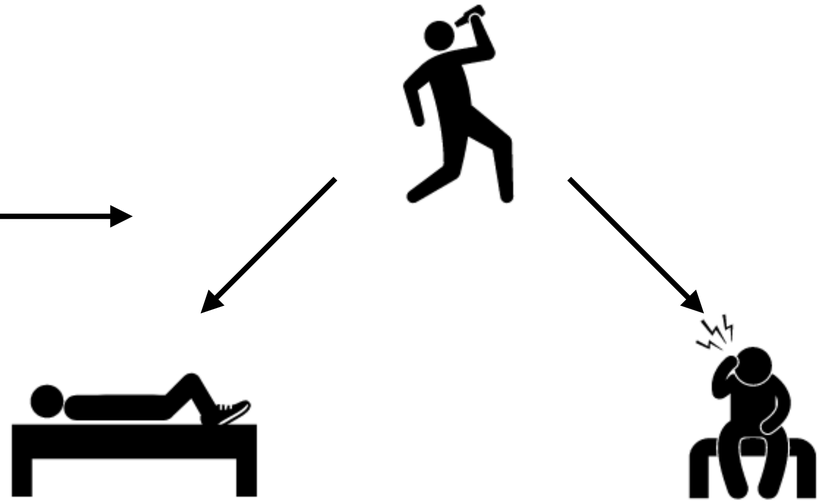
- Say we have a dataset.
- Cause-effect relation?
- **Correlation is not causation**
- Domain-expertise
- Hidden Confounding



Data-driven Causal Discovery

dataset (of observations)

causal discovery method



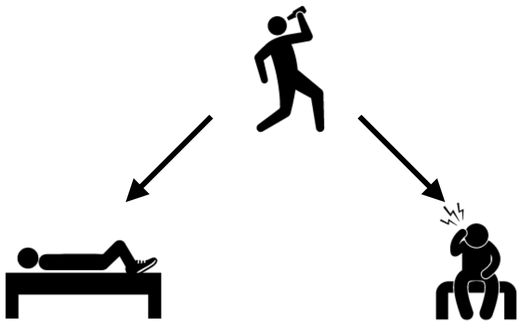
Identifiability

 independent from  given 

Identifiability

independent from

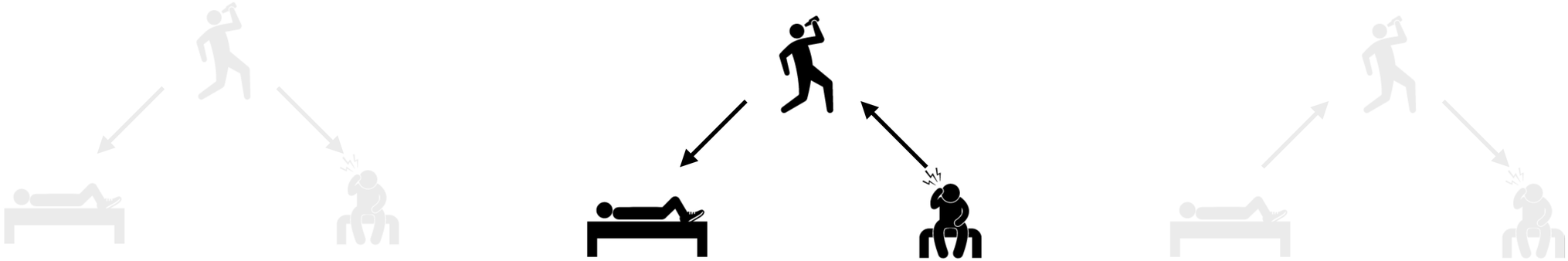
given



Identifiability

independent from

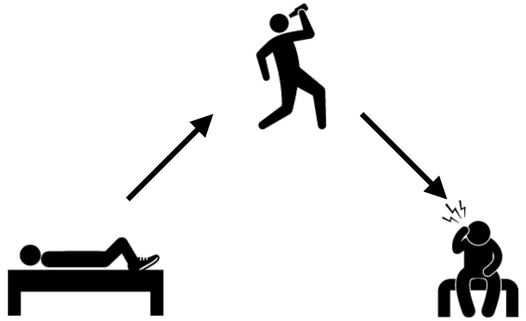
given



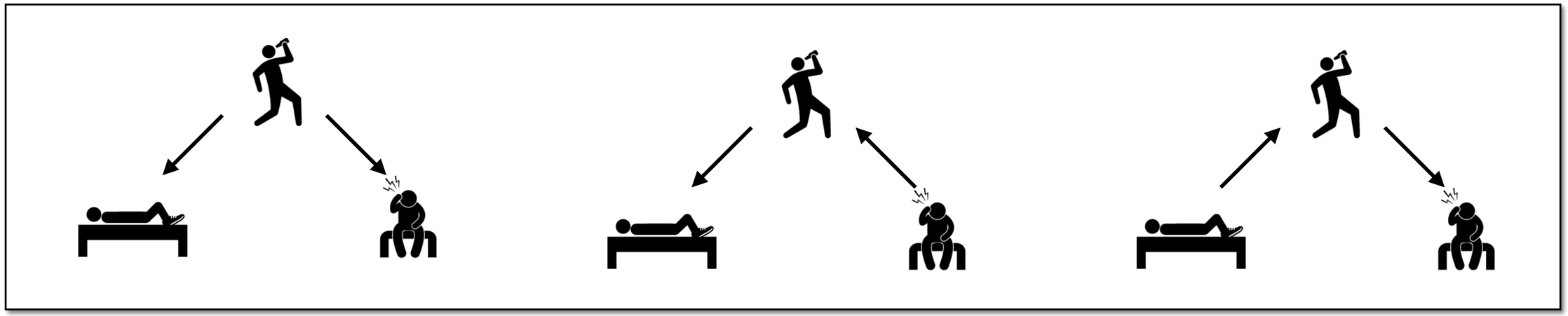
Identifiability

independent from

given



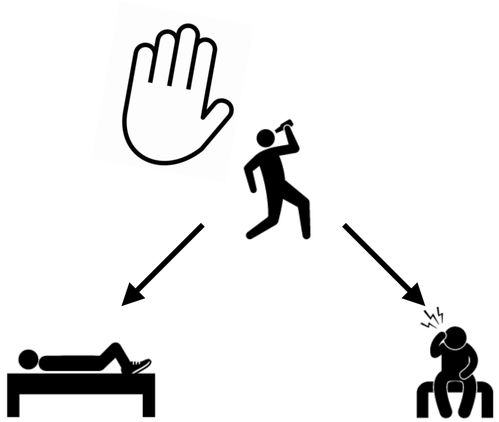
Identifiability



Markov Equivalence class

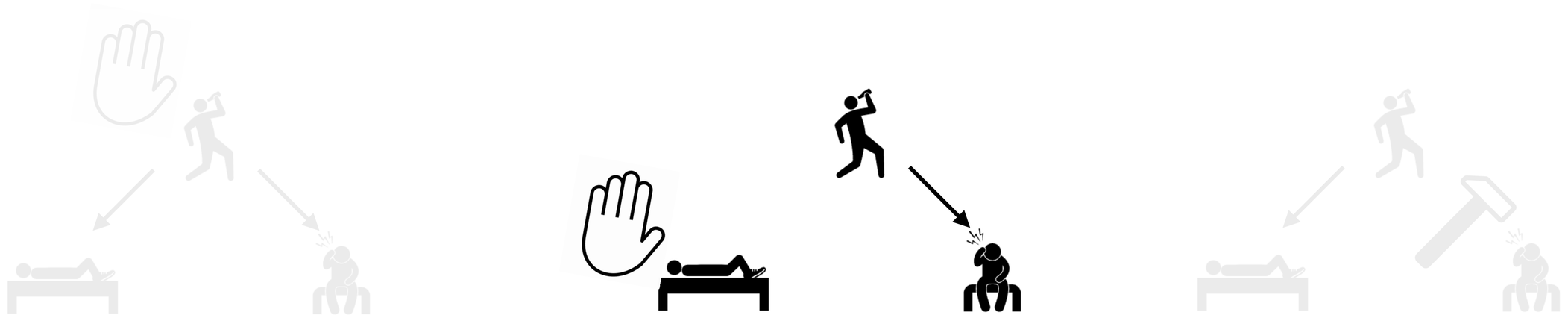
Interventions

- Science; hypotheses; experiments (interventions)



Interventions

- Science; hypotheses; experiments (interventions)

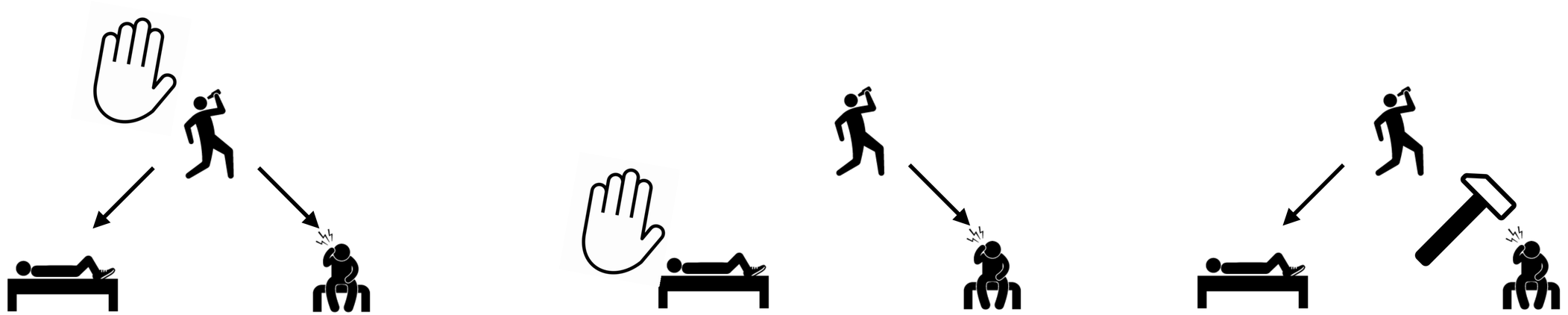


Interventions

- Science; hypotheses; experiments (interventions)

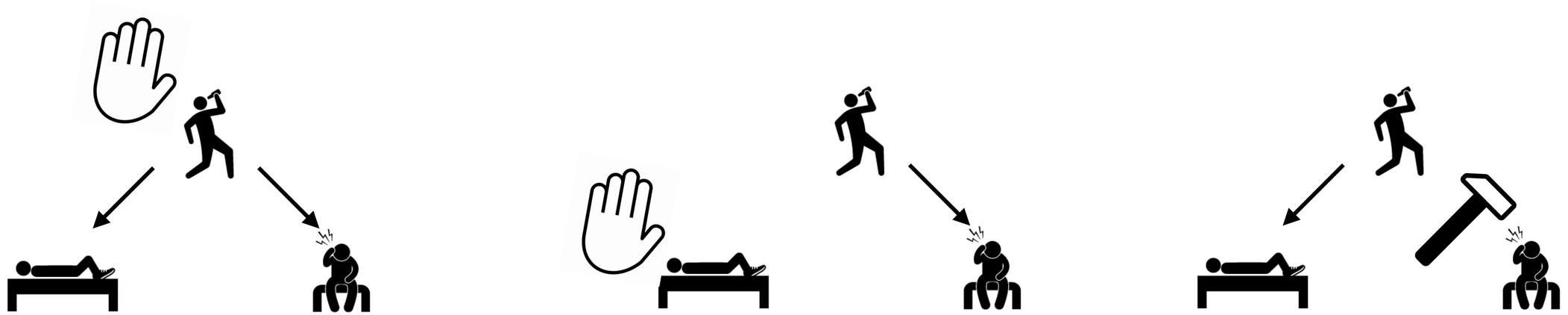
Interventions

- Science; hypotheses; experiments (interventions)
- Causal discovery with intervention data



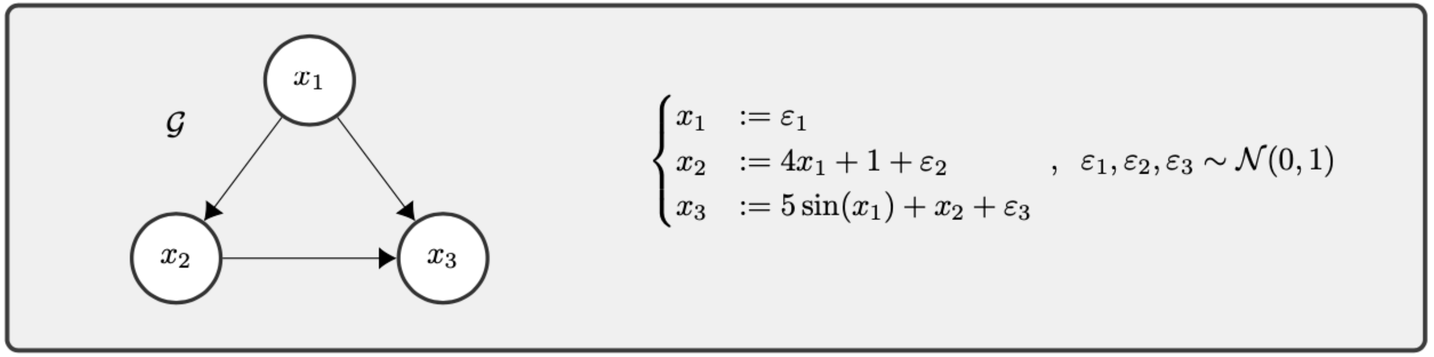
Interventions

- Science; hypotheses; experiments (interventions)
- Causal discovery with intervention data
- **Complex**; **expensive**; **unethical**.

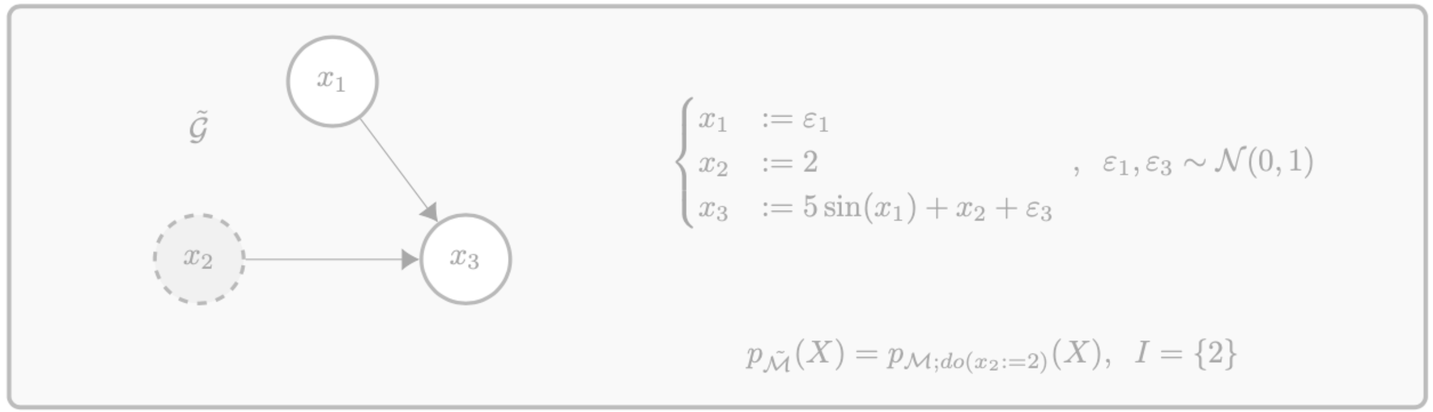


Structural Causal Models

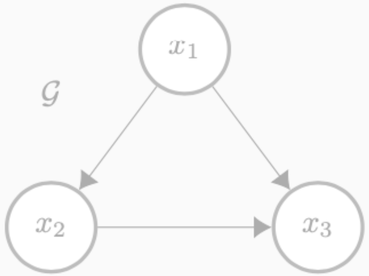
Structural causal models



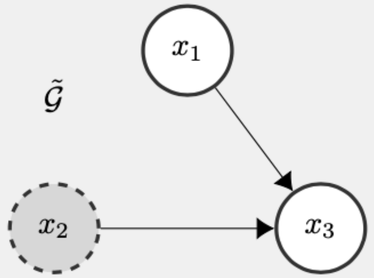
$$p_{\mathcal{M}}(X) = p_{\mathcal{M}}(x_3|x_2, x_1)p_{\mathcal{M}}(x_2|x_1)p_{\mathcal{M}}(x_1)$$



Structural causal models



$$\begin{cases} x_1 & := \varepsilon_1 \\ x_2 & := 4x_1 + 1 + \varepsilon_2 \\ x_3 & := 5\sin(x_1) + x_2 + \varepsilon_3 \end{cases}, \quad \varepsilon_1, \varepsilon_2, \varepsilon_3 \sim \mathcal{N}(0,1)$$



$$\begin{cases} x_1 & := \varepsilon_1 \\ x_2 & := 2 \\ x_3 & := 5\sin(x_1) + x_2 + \varepsilon_3 \end{cases}, \quad \varepsilon_1, \varepsilon_3 \sim \mathcal{N}(0,1)$$

$$p_{\tilde{\mathcal{M}}}(X) = p_{\mathcal{M};do(x_2:=2)}(X), \quad I = \{2\}$$

$$p_{\tilde{\mathcal{M}}}(X) = p_{\mathcal{M}}(x_3|x_2,x_1)p_{\mathcal{M};\mathrm{do}(x_2:=2)}(x_2)p_{\mathcal{M}}(x_1)$$

Structural causal models

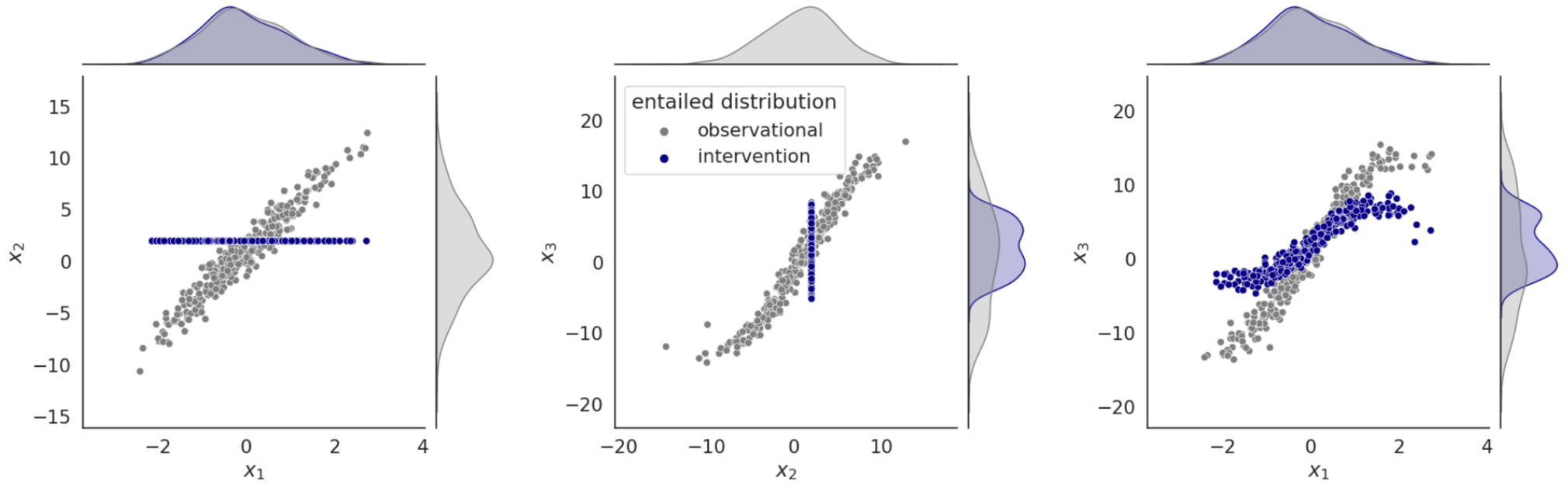
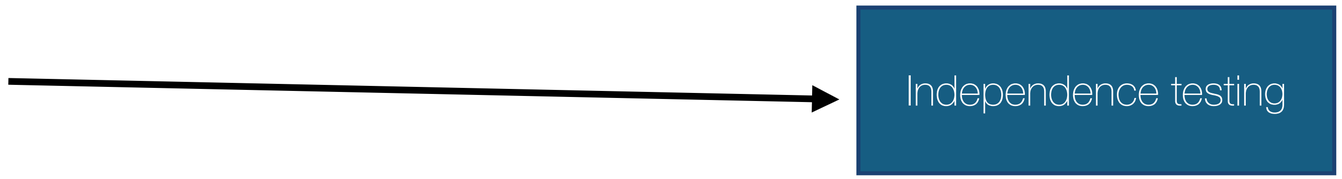


Figure 2.5: Samples from the observational SCM in Figure 2.2, and intervention SCM in Figure 2.4.

Causal Discovery Methods

- Constrained-Based
- Score based
- Hybrid
- Others



Causal Discovery Methods

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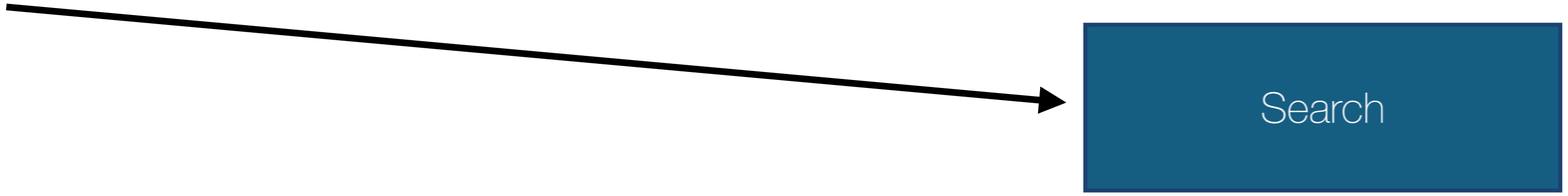

Causal Discovery Methods

- Constrained-Based
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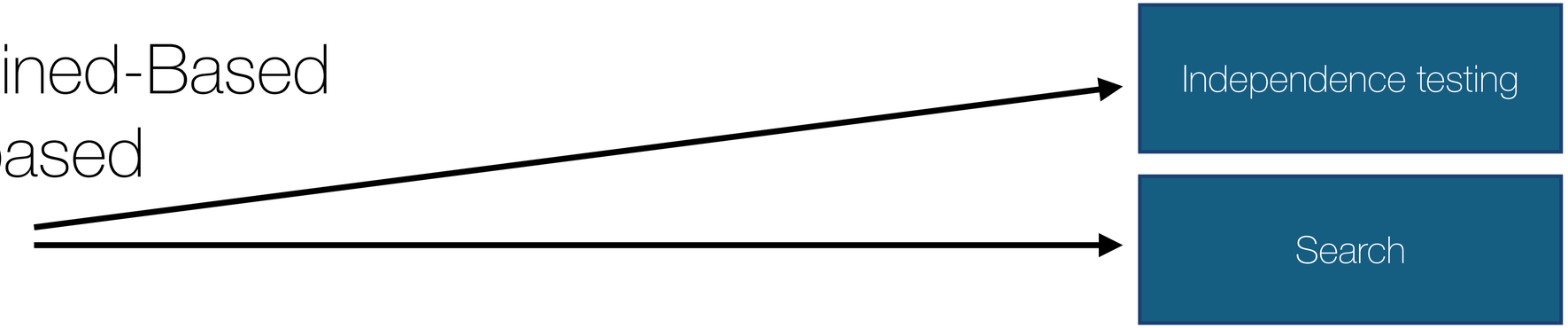


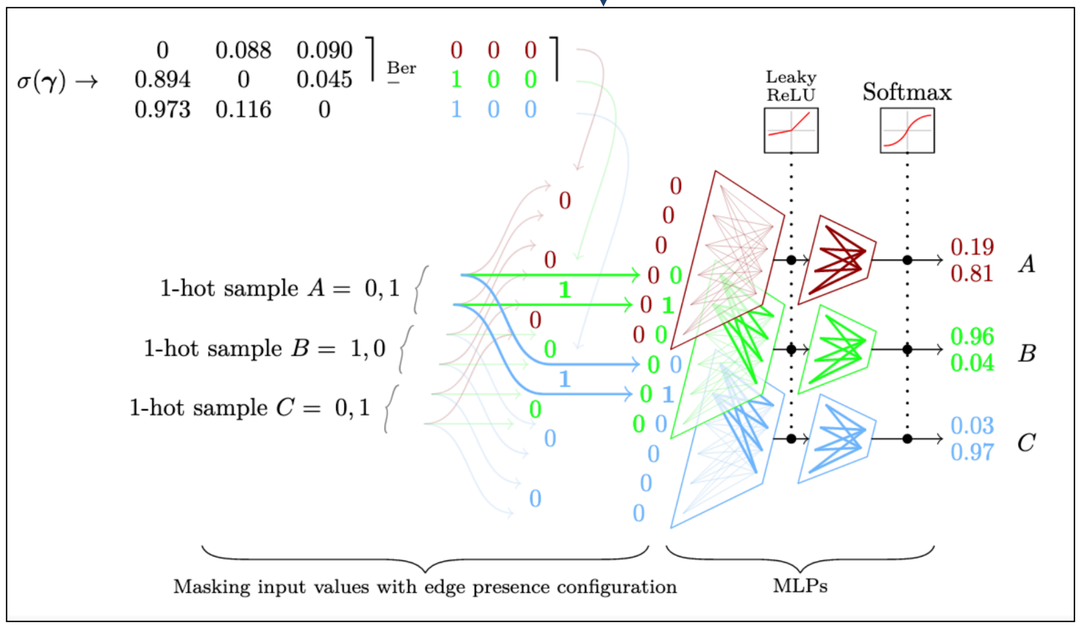
Score based methods with deep learning

$$\Lambda^* = \arg\max_{\Lambda} S(\Lambda)$$

$$S(\Lambda) = \max_{\theta} \mathbb{E}_{\mathcal{G}\sim \mathrm{DAG}(\mathcal{G};\Lambda)} \left[\log p(\mathcal{D}|\mathcal{G},\theta) + \log p(\mathcal{G}) \right]$$

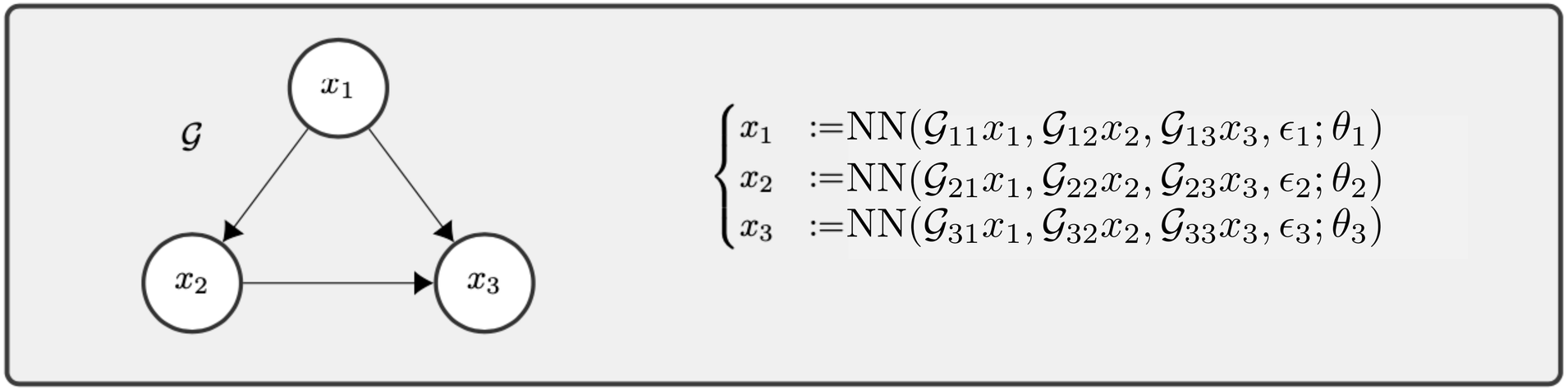
(most of the time) approximated w/ fully factorized Bernoulli

Penalize dense graphs/enforce acyclicity



Ke et. al. 2020

Score based methods with deep learning



Similar to doing LASSO for all of the variables at once w/ acyclicity constraints.

Ke et. al. 2020

Interventions and Causal Discovery

Causal discovery with intervention data

$$\Lambda^*, \tilde{\mathcal{M}}^* = \arg\max_{\Lambda, \tilde{\mathcal{M}}} S(\Lambda, \tilde{\mathcal{M}})$$

$$S(\Lambda, \tilde{\mathcal{M}}) = \max_{\theta, \phi} \mathbb{E}_{\mathcal{G} \sim \mathrm{DAG}(\mathcal{G}; \Lambda)} \Big[\mathbb{E}_{k \sim p(k)} \big[\log p(\mathcal{D}^k | \mathcal{G}, \theta^k, \tilde{\mathcal{M}}^{(k)}) + \log p(\mathcal{G}) \big] \Big]$$

Intervention specific parameters

Intervention variables

Brouillard et. al. 2020

Differentiable Causal Discovery Under Latent Interventions



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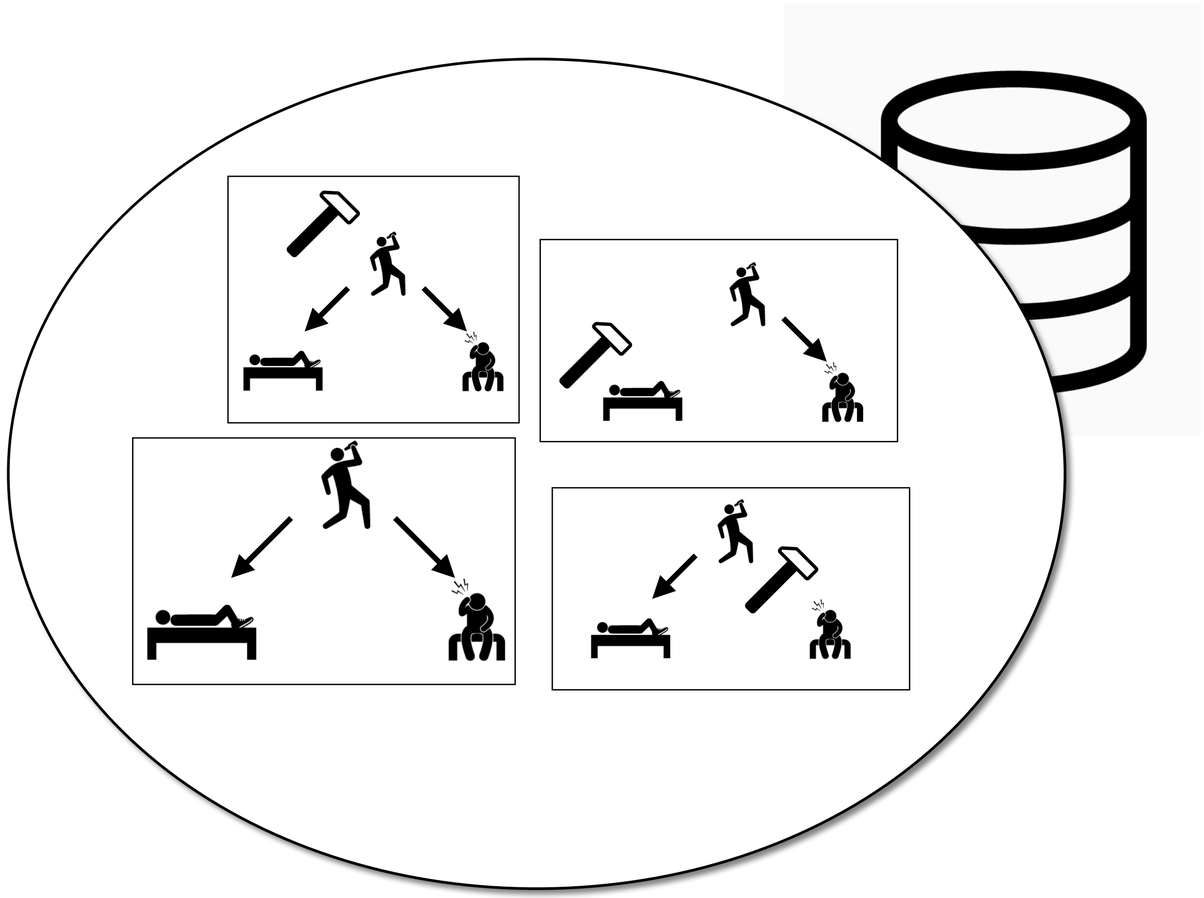
Unbabel

TÉCNICO LISBOA

ellis

Latent interventions

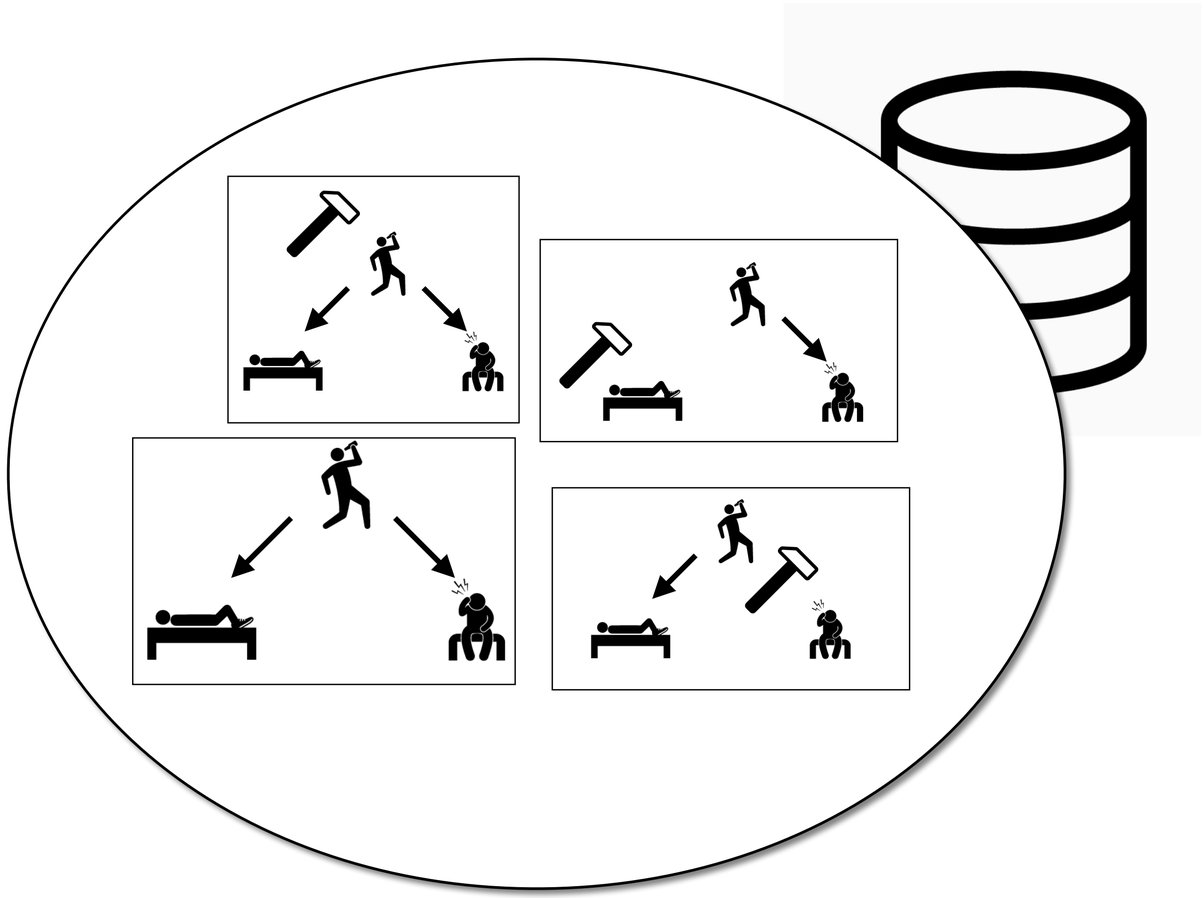


Mixture of experimental regimes.

For each sample:

- do not know correspondence to intervention regime;

Latent interventions



Mixture of experimental regimes.

For each sample:

- do not know correspondence to intervention regime;

For each intervention:

- do not know experimental conditions

Can we recover latent interventions?

Intervention recovery

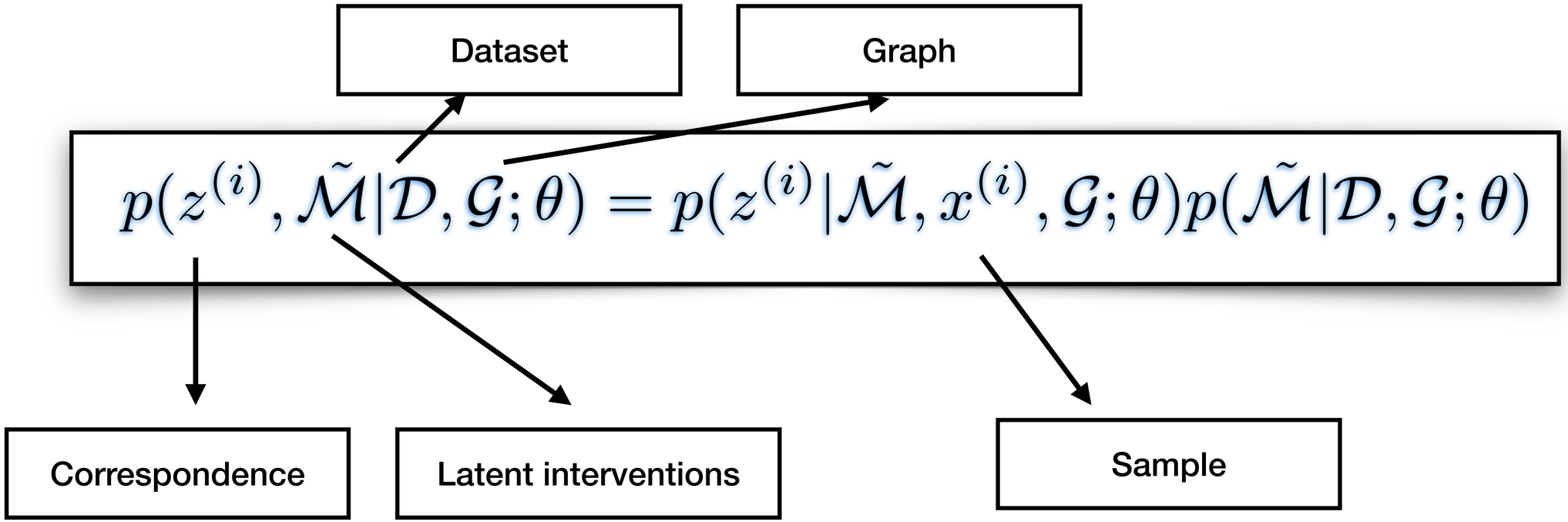
- Given the causal graph.
- Recover interventions and correspondences.
- Propose joint distribution

Infinite mixture of intervention SCMs

+

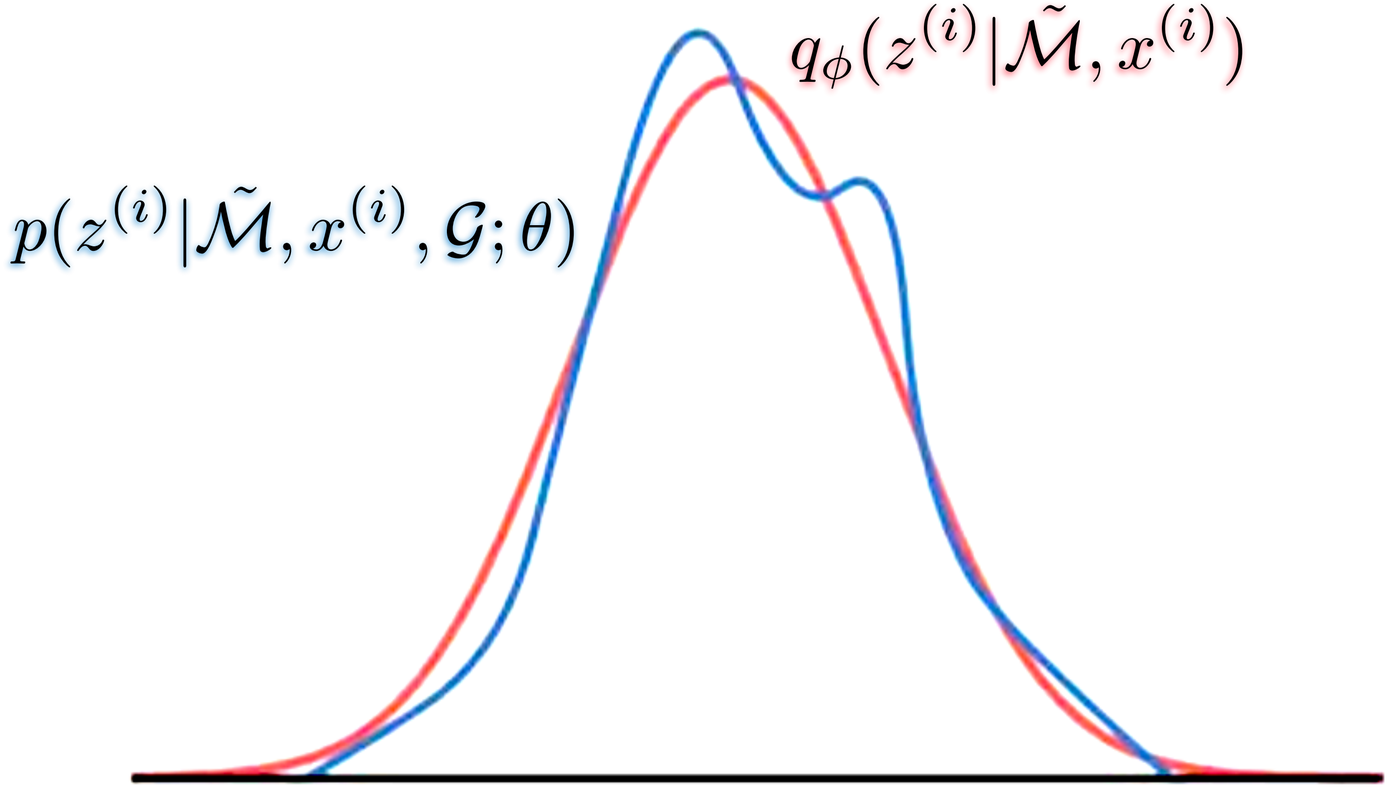
Prior distribution for the interventions
(Dirichlet process)

Approximate posterior inference



Approximate posterior inference

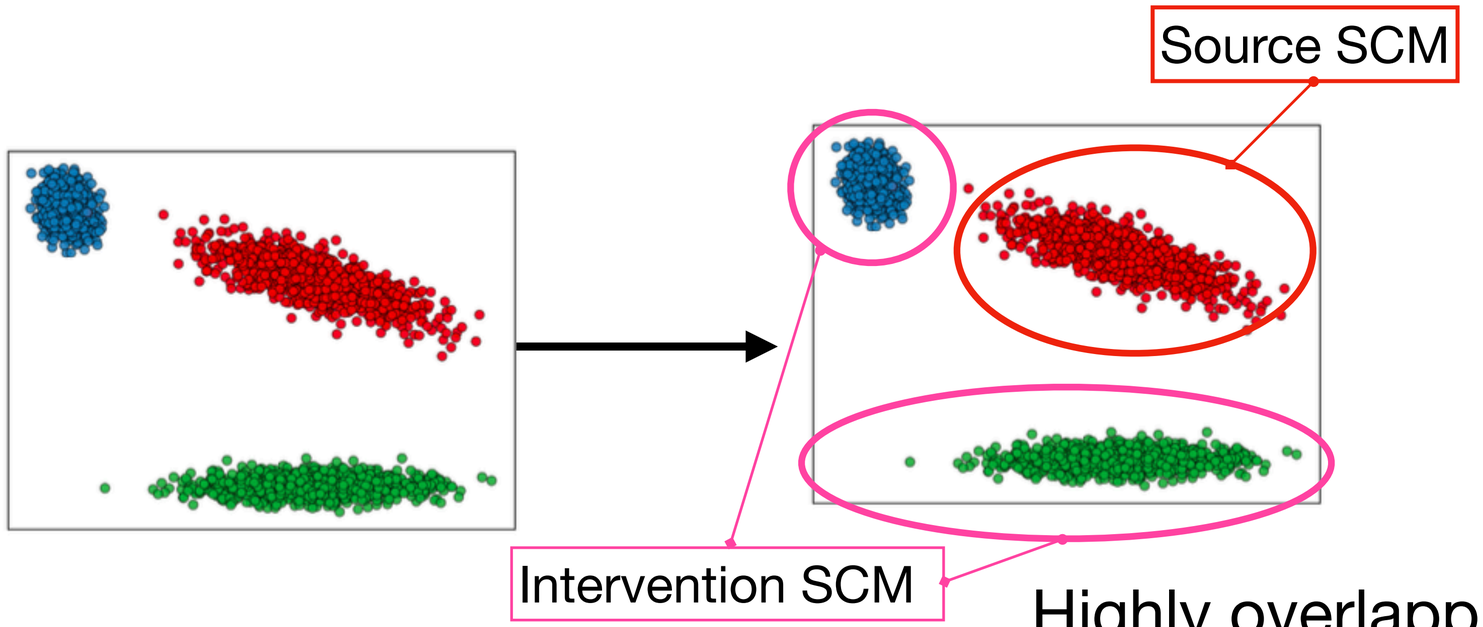
- Variational inference



Approximate posterior inference

- Variational inference

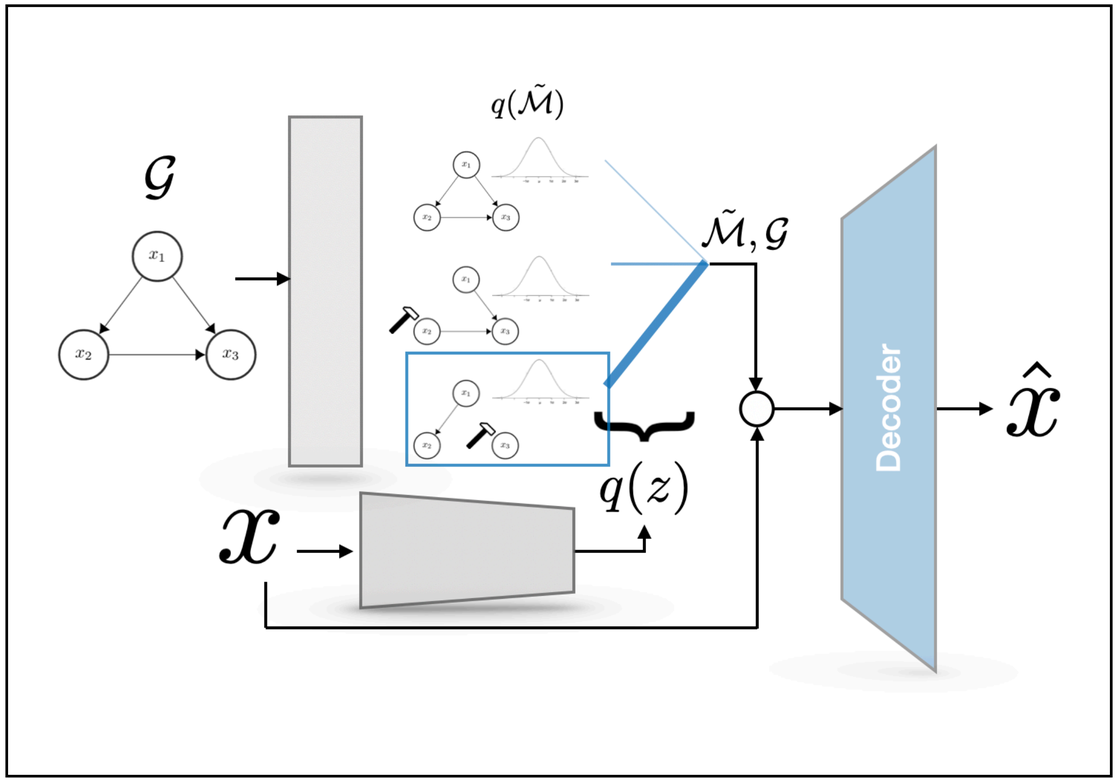
Similar to a clustering problem
(each cluster as few degrees of freedom)



Highly overlapping clusters
(not that noticeable in this 2D example)

Approximate posterior inference

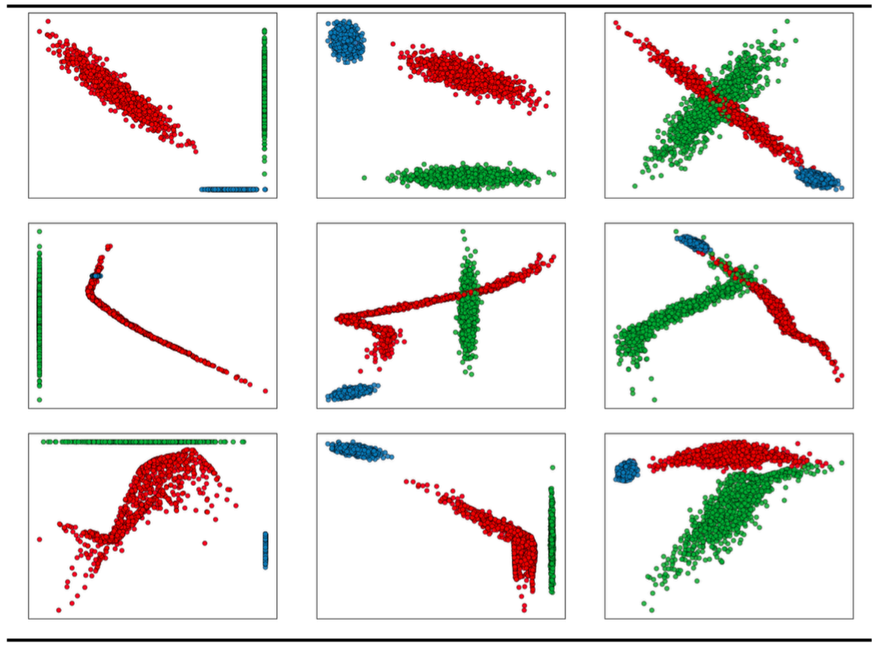
$$\max_{\theta,\phi} \sum_{i=1}^{N} \text{ELBO}_{q(z^{(i)},\tilde{\mathcal{M}};\phi)}\left(x^{(i)}, \mathcal{G}; \theta\right)$$



Experiments with single node interventions

Model Type	d = 10		d = 20	
	ER1	ER4	ER1	ER4
Stochastic Interventions:				
Linear Gaussian	0.9816 ± 0.019	0.9492 ± 0.007	0.9815 ± 0.005	0.9785 ± 0.006
Non-Linear Gaussian	0.9643 ± 0.015	0.9242 ± 0.006	0.9655 ± 0.005	0.9431 ± 0.003
Non-Linear Non-Gaussian	0.8314 ± 0.062	0.7812 ± 0.1074	0.8929 ± 0.027	0.8412 ± 0.087
Imperfect Interventions:				
Linear Gaussian	0.9262 ± 0.030	0.8802 ± 0.040	0.8072 ± 0.098	0.7819 ± 0.054
Non-Linear Gaussian	0.9541 ± 0.012	0.9205 ± 0.005	0.9670 ± 0.007	0.9434 ± 0.004
Non-Linear Non-Gaussian	0.9103 ± 0.004	0.9090 ± 0.004	0.9345 ± 0.005	0.9196 ± 0.005
Atomic Interventions:				
Linear Gaussian	0.9141 ± 0.0018	0.9148 ± 0.0021	0.9507 ± 0.0059	0.9461 ± 0.0030
Non-Linear Gaussian	0.9138 ± 0.0053	0.9195 ± 0.0041	0.9506 ± 0.0056	0.9435 ± 0.0032
Non-Linear Non-Gaussian	0.9100 ± 0.0056	0.9034 ± 0.0115	0.9314 ± 0.0104	0.9306 ± 0.0041

Table 3.2: Results for the single-node intervention experiment. The metric used is the average rand index.

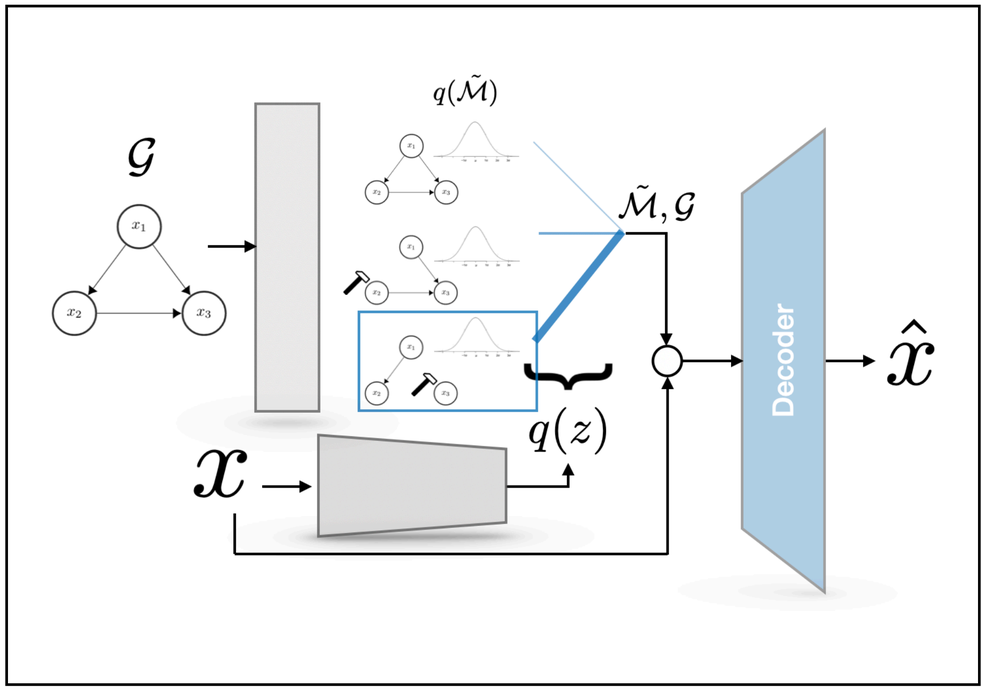


Can we recover the causal graph?

Score based method

$$\Lambda^* = \arg\max_{\Lambda} S(\Lambda)$$

$$S(\Lambda) = \max_{\theta,\phi} \mathbb{E}_{\mathcal{G}\sim \mathrm{DAG}(\mathcal{G};\Lambda)} \Big[\sum_{i=1}^{N} \mathrm{ELBO}_{q(z^{(i)},\tilde{\mathcal{M}};\phi)} \left(x^{(i)}, \mathcal{G}; \theta\right) + \log p(\mathcal{G}) \Big]$$



Model variants

- **“latent”** (new)

For each sample:

- do not know correspondence to intervention regime;

For each intervention:

- do not know experimental conditions

Model variants

- “latent” (new)
- **“unknown”**

For each sample:

- ~~do not~~ know correspondence to intervention regime;

For each intervention:

- do not know experimental conditions

Model variants

- “latent” (new)
- “unknown”
- **“known”**

For each sample:

- ~~do not~~ know correspondence to intervention regime;

For each intervention:

- ~~do not~~ know experimental conditions

Model variants

- “latent” (new)
- “unknown”
- “known”
- **“observational”**

assume there is no intervention data.

Model variants

- “latent” (new)
- “unknown”
- “known”
- “observational”
- **“semi-supervised”** (new)

Model variants

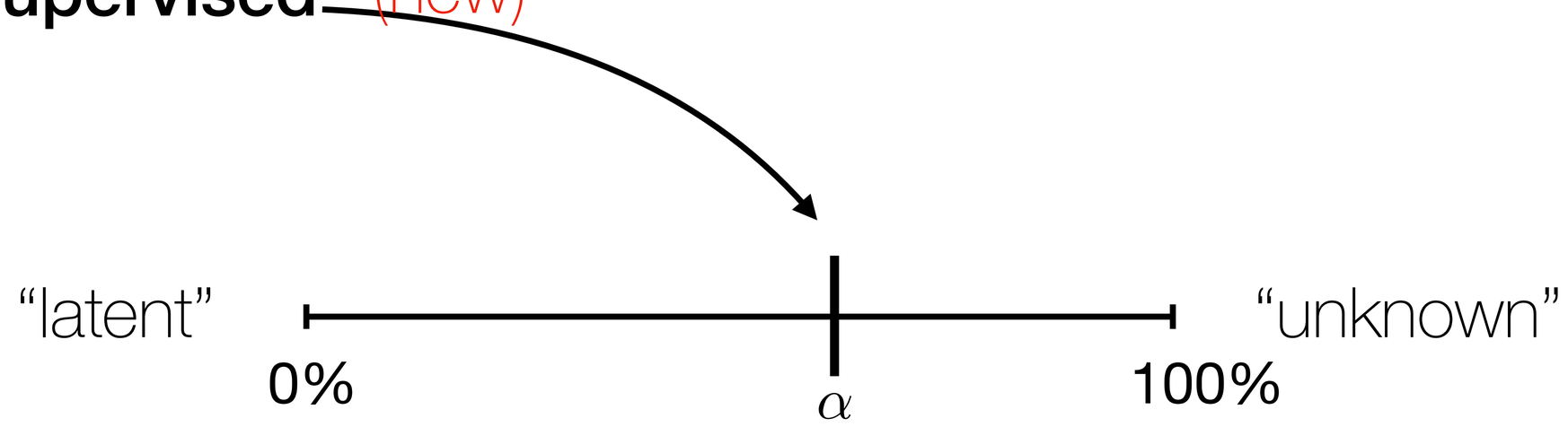
- “latent” (new)
- “unknown”
- “known”
- “observational”
- **“semi-supervised”** (new)

For each sample:

- (fraction) know correspondence to intervention regime;

For each intervention:

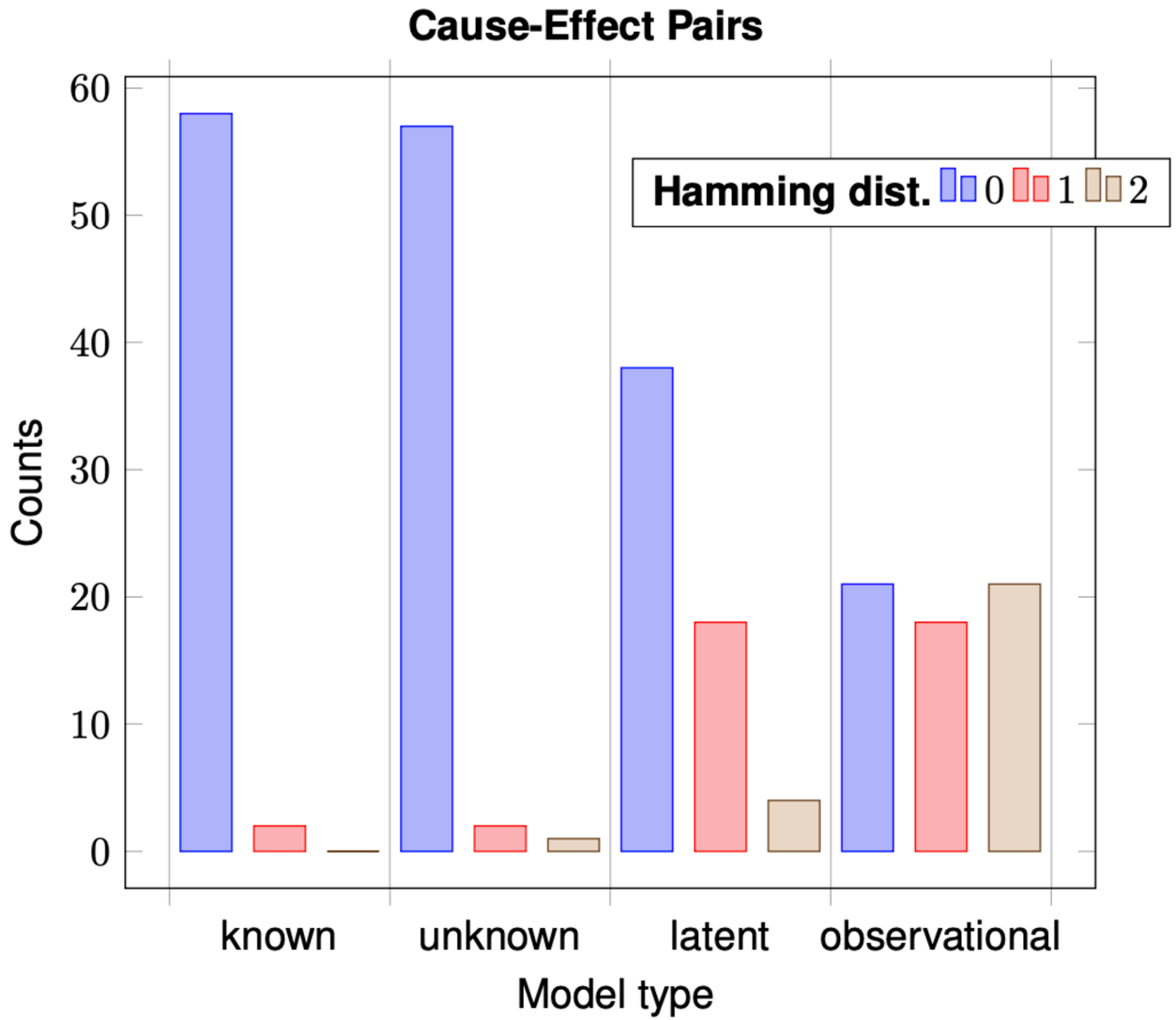
- do not know experimental conditions

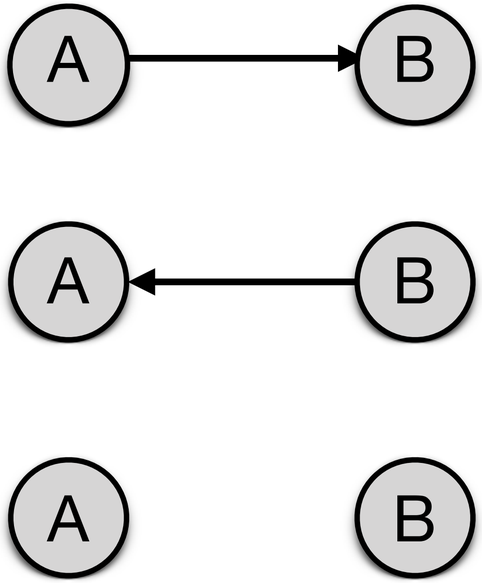


Fraction of samples with correspondences.

Experiments

Experiments with cause effect pairs





Experiments on synthetic data

Model Type	e	latent	unknown	known	observational
		Stochastic Interventions:			
Linear Gaussian		5.9 ± 6.2	3.4 ± 3.2	0.5 ± 1.3	10.3 ± 7.8
Non-Linear Gaussian	1	12.2 ± 3.9	10.3 ± 2.5	7.0 ± 3.6	13.7 ± 3.8
Non-Linear Non-Gaussian		8.7 ± 6.6	8.0 ± 2.7	6.6 ± 2.2	11.3 ± 5.0
Linear Gaussian		27.2 ± 6.2	24.1 ± 5.8	15.6 ± 6.0	39.6 ± 5.0
Non-Linear Gaussian	4	35.8 ± 3.8	30.3 ± 5.3	27.7 ± 4.3	37.5 ± 5.2
Non-Linear Non-Gaussian		36.1 ± 4.4	35.5 ± 8.1	31.5 ± 5.6	40.2 ± 6.9
		Imperfect Interventions:			
Linear Gaussian		5.8 ± 4.2	6.2 ± 3.06	4.7 ± 3.6	10.4 ± 2.9
Non-Linear Gaussian	1	9.3 ± 2.4	8.9 ± 2.5	7.8 ± 3.9	10.5 ± 2.8
Non-Linear Non-Gaussian		8.8 ± 3.0	9.1 ± 3.5	7.9 ± 1.4	11.5 ± 5.4
Linear Gaussian		35.9 ± 8.3	29.7 ± 5.6	17.7 ± 7.9	39.1 ± 9.1
Non-Linear Gaussian	4	32.1 ± 6.0	32.6 ± 5.8	32.8 ± 5.4	39.8 ± 9.3
Non-Linear Non-Gaussian		30.4 ± 12.2	30.2 ± 11.2	25.8 ± 3.9	36.7 ± 9.8

Table 4.1: Hamming distances on synthetic 10 variable SCMs.

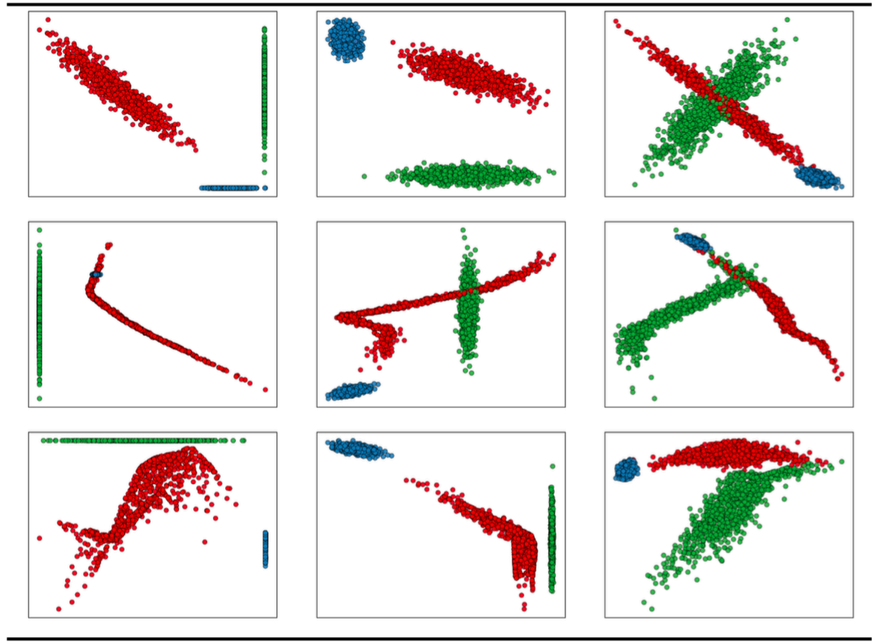


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Table 4.1: Hamming distances on synthetic 10 variable SCMs.

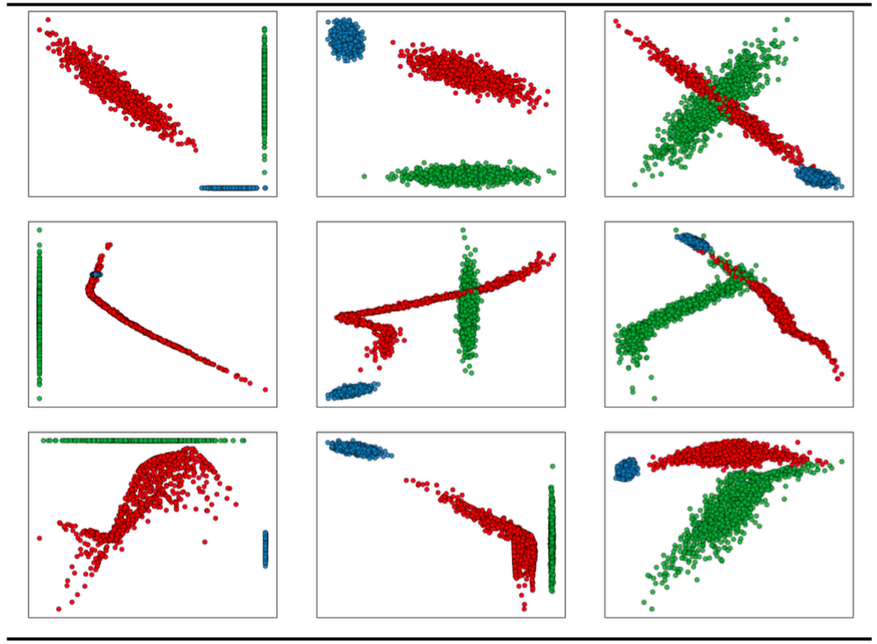

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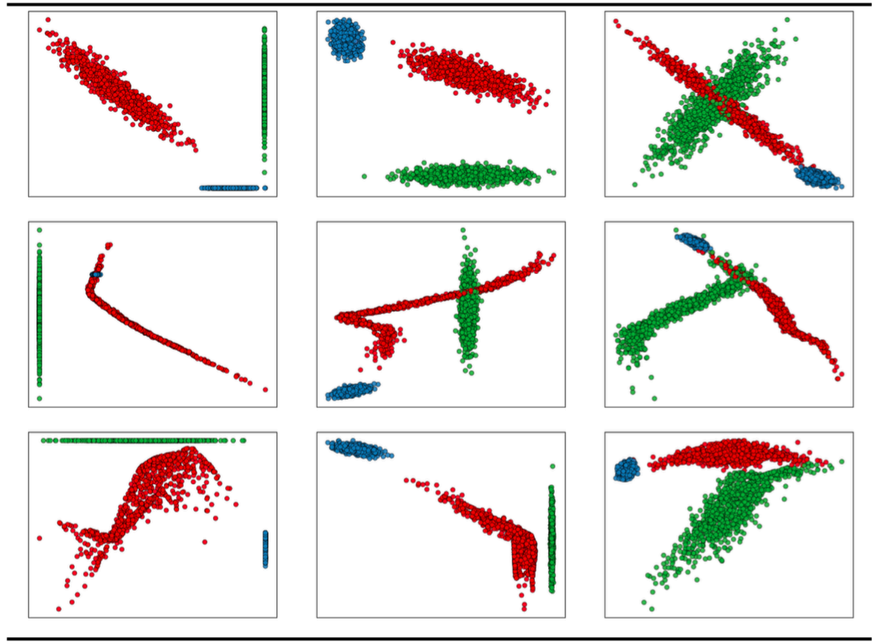
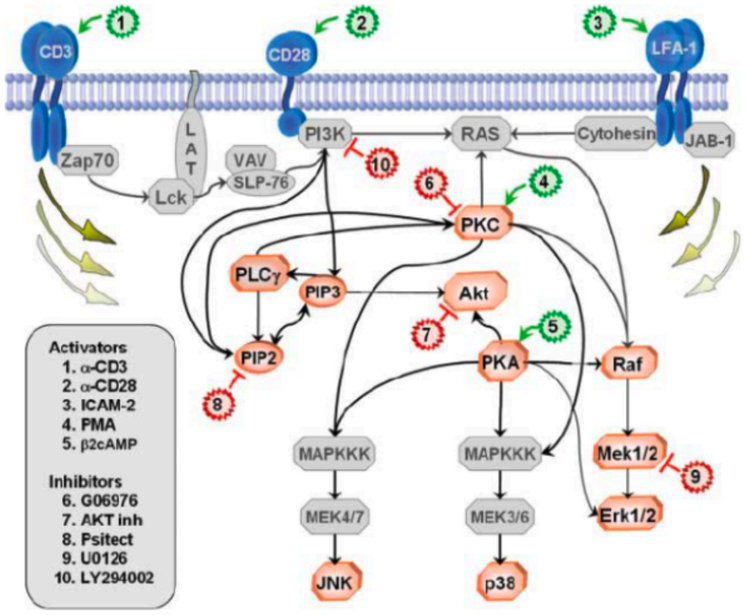
Table 4.1: Hamming distances on synthetic 10 variable SCMs.



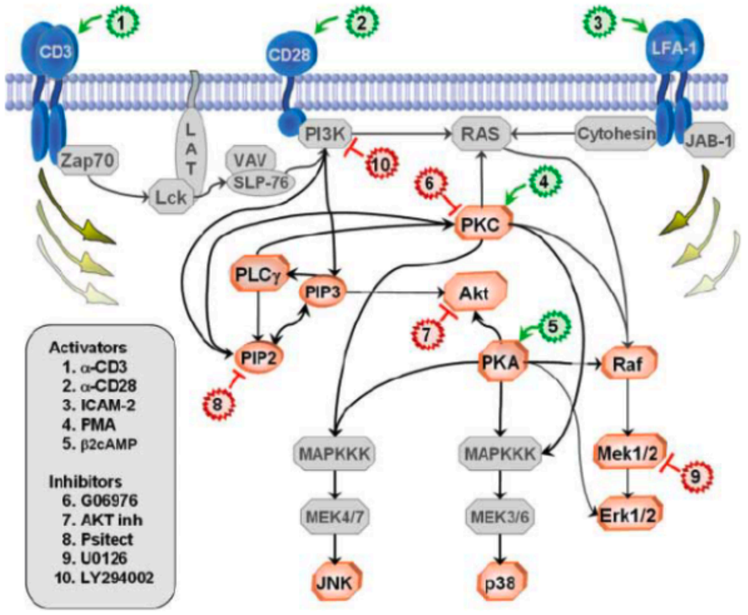
Experiments on real data



ground truth causal model.

	HD	tp	fn	fp	rev	F_1 score
GIES (Hauser and Bühlmann, 2012)	38	10	0	41	7	0.33
CAM (Bühlmann et al., 2014)	35	12	1	30	4	0.51
IGSP (Wang et al., 2017)	18	4	6	5	7	0.42
DCDI-G (Brouillard et al., 2020)	36	6	2	25	9	0.31
DCDI-DSF (Brouillard et al., 2020)	33	6	2	22	9	0.33
FCI (Spirtes et al., 1993)	35	4	12	21	5	0.22
Imperfect Linear Gaussian **(ours)**	33	7	11	22	3	0.30
Imperfect Non-Linear Gaussian **(ours)**	19	7	11	8	0	0.42
Imperfect Normalizing Flow **(ours)**	30	9	9	21	1	0.38
Perfect Linear Gaussian **(ours)**	23	8	10	13	3	0.41
Perfect Non-Linear Gaussian **(ours)**	24	11	7	17	1	0.48
Perfect Normalizing Flow **(ours)**	23	7	11	12	2	0.38

Experiments on real data



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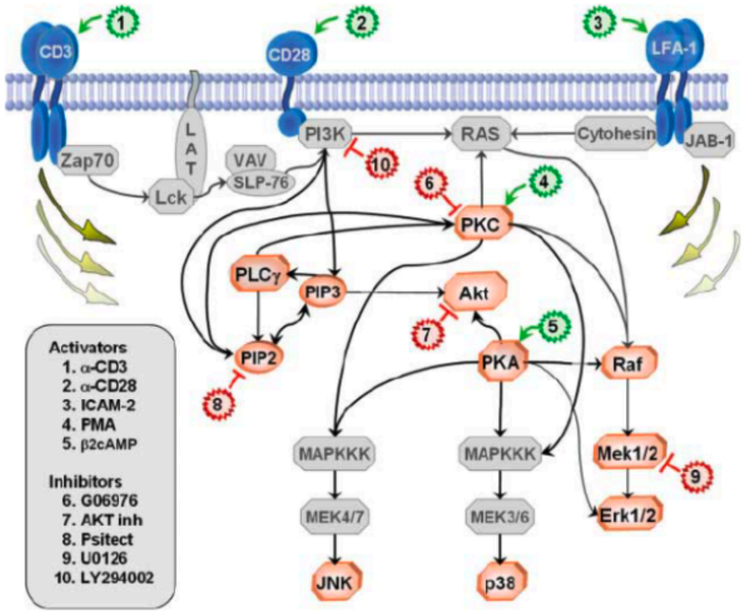

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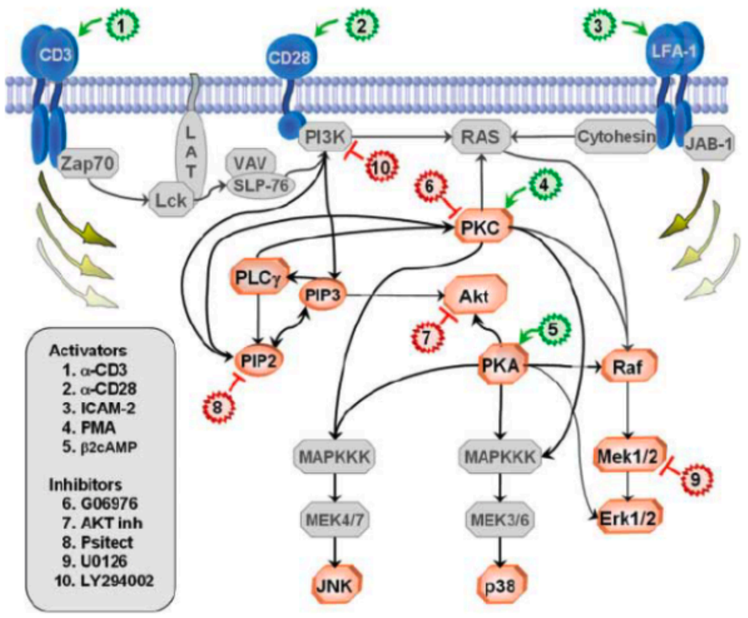
Experiments on real data



ground truth causal model.

Edges in the wrong direction

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Conclusion

- Make heterogeneity or non-stationarity your friend.
- Causal Discovery under Latent Interventions

Causal discovery and Deep Learning

Faria et. al. 2022; Pearl et. al. 2018; Neal et. al. 2022; Schölkopf et. al. 2019; Bengio et. al. 2020; Peters et. al. 2017, Ke et. al. 2020, Brouillard et. al. 2020

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Deep Learning Sessions Portugal