Differentiable Causal Discovery
with observational and interventional data


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Outline

Introduction and Motivation

The limits of statistical association

Consider the relationships between altitude (A) and temperature (T)

Example taken from [Peters et al., 2017]

$$P(A, T) = P(A|T)P(T)$$
$$= P(T|A)P(A)$$

If altitude $\uparrow$ then temperature $\downarrow$

The limits of statistical association

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Will cooling house #1 make it climb the mountain?

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Will pushing house #2 down the mountain change its temperature?

Why care about causal relationships: Simpson's paradox

Recovery of kidney stone patients

	Overall
Treatment a: Open surgery	78% (273/350)
Treatment b: Percutaneous nephrolithotomy	**83%** (289/350)

Example taken from Julious & Mullee [1994]

Overall: treatment **b** more effective.

- Small stones: treatment **a** more effective
- Large stones: treatment **a** more effective

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Recovery of kidney stone patients

	Overall	Patients with small stones	Patients with large stones
Treatment a: Open surgery	78% (273/350)	**93%** (81/87)	**73%** (192/263)
Treatment b: Percutaneous nephrolithotomy	**83%** (289/350)	87% (234/270)	69% (55/80)

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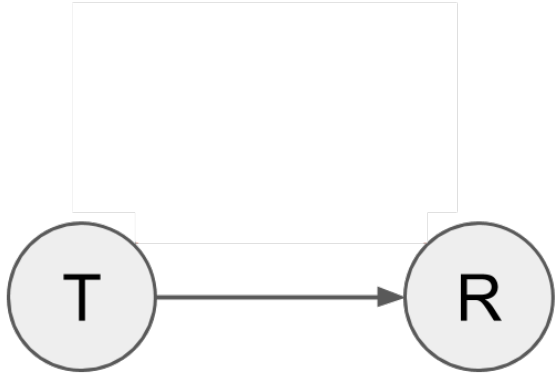
Simpson's paradox: what's really going on?

T = Treatment $\in \{A, B\}$

R = Patient recovered $\in \{0, 1\}$



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We are assuming the wrong model!

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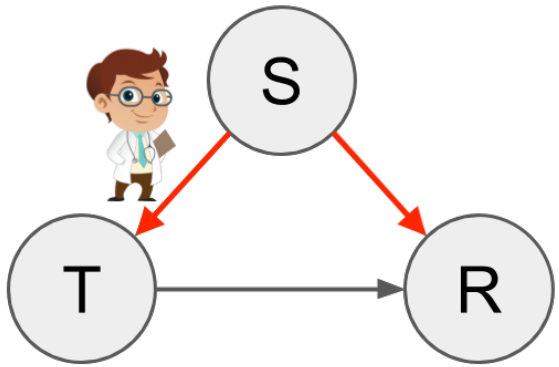

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Confounding: patients with small stones are more likely to receive treatment b and also more likely to have a good outcome.

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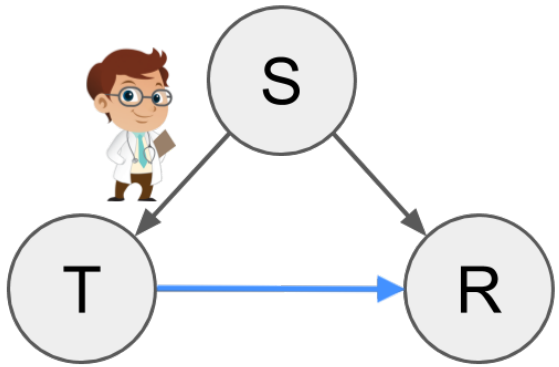

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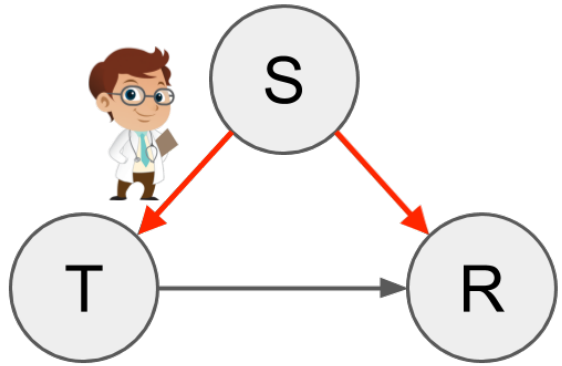
Causal vs non-causal questions

- Non-causal: What is my probability of recovery if I receive treatment A?
  $\hookrightarrow P(R = 1 \mid T = A)$



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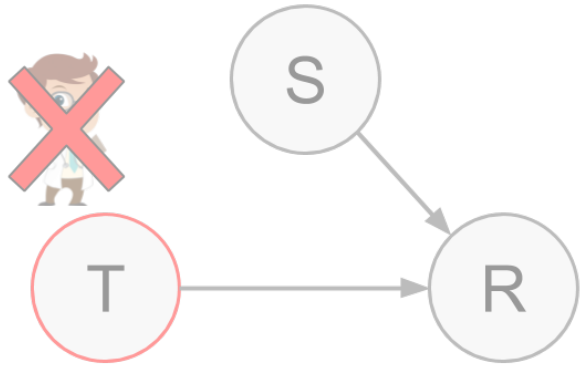

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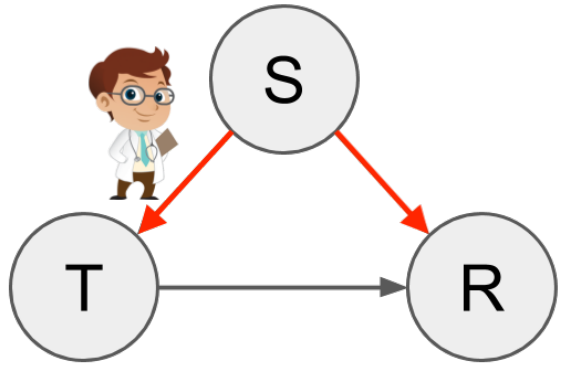

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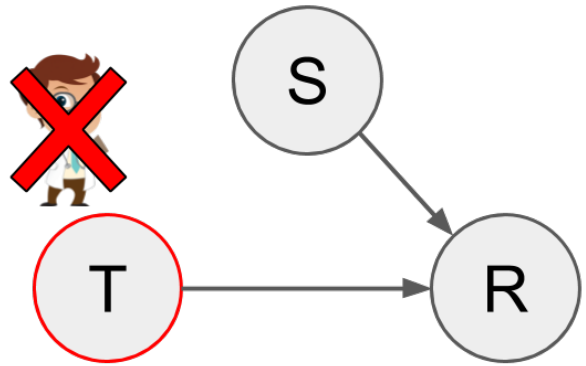

Causal Bayesian networks

- Random vector $X = (X_1, ..., X_d)$
- Let $\mathcal{G}$ be a directed acyclic graph (DAG)
  - d vertices (one per X_i)
  - edges indicate causal relationships
- Encodes (conditional) independence constraints (via *d-separation*, see Koller & Friedman [2009])
- Distribution P_X: $p(X) = \prod_{i=1}^{d} p(X_i | X_{\pi_i^{\mathcal{G}}})$, where $\pi_i^{\mathcal{G}}$ = parents of i in $\mathcal{G}$

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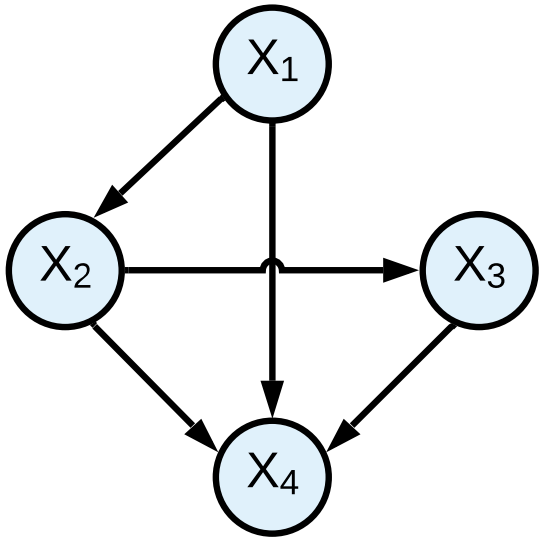

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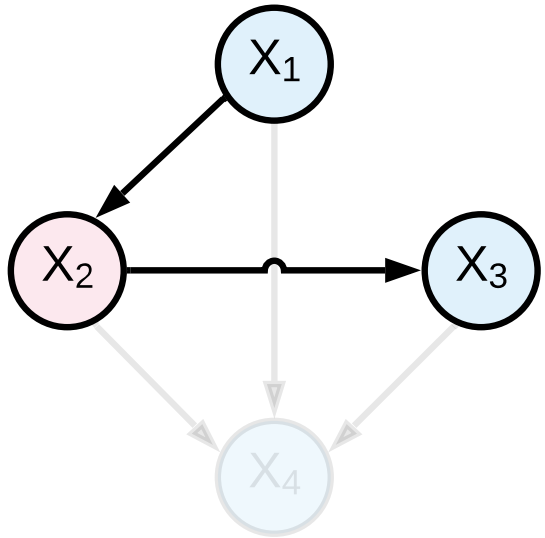

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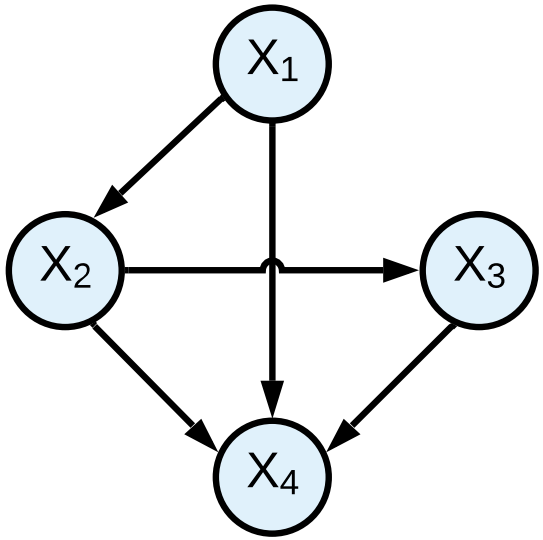
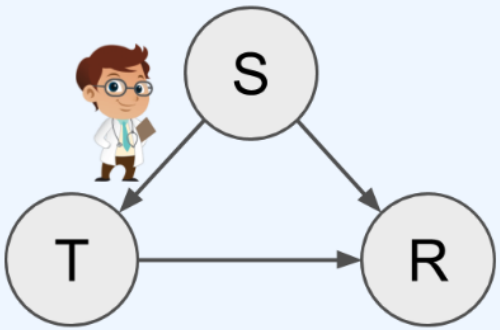


Interventions: manipulating causal bayesian networks

Intervening on the treatment T

$T =$ Treatment $\in \{A, B\}$
$S =$ Stone size $\in \{\text{small}, \text{large}\}$
$R =$ Patient recovered $\in \{0, 1\}$

Observations



$$p(S)p(T \mid S)p(R \mid S, T)$$

Observational data: may contain biases

$$P(R = 1 \mid T = A) \neq P(R = 1 \mid do(T = A))$$

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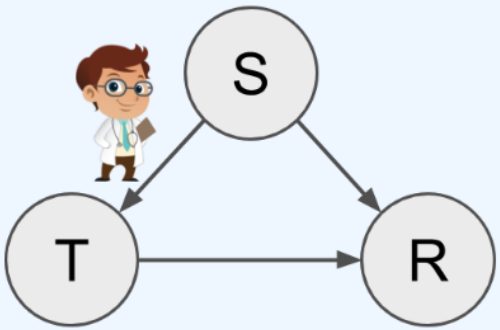
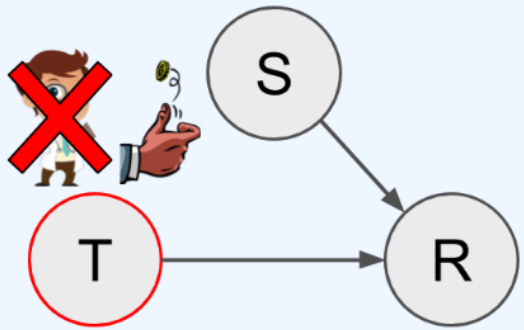


$p(S)p(T \mid S)p(R \mid S, T)$

Perfect intervention



$p(S)\tilde{p}(T)p(R \mid S, T)$

Perfect intervention: edges into T are removed (e.g., via randomization)

$$P(R = 1 \mid T = A) = P(R = 1 \mid do(T = A))$$

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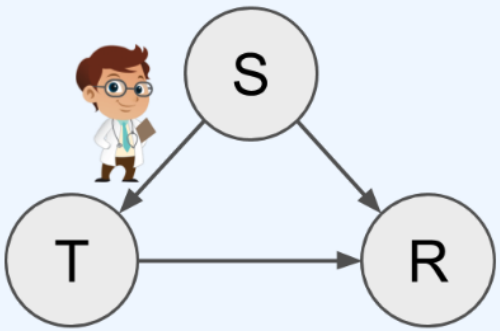

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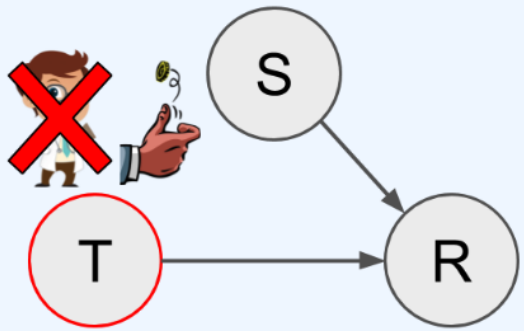

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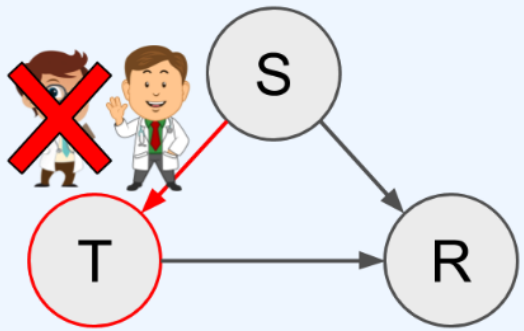
Imperfect intervention



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Imperfect intervention: incoming edges are preserved, conditionals are changed.

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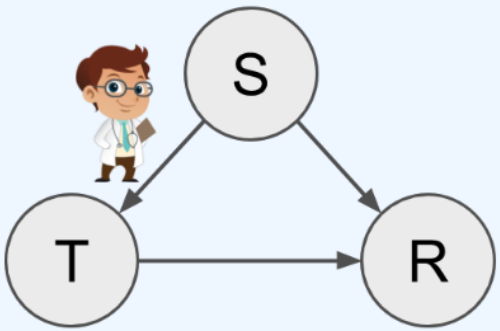

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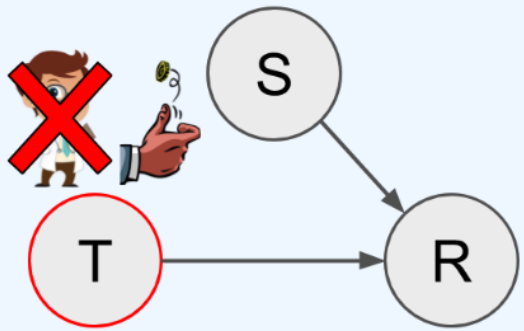

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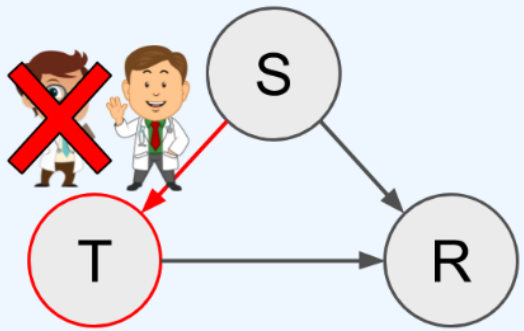

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⚠ **Important:** notice how conditionals that are not under intervention are invariant across distributions (a.k.a, modularity/autonomy).

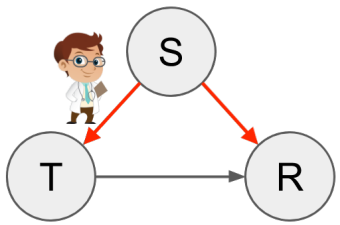
Causal inference from observational data

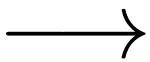
- **Objective:** estimate the effect of an intervention: $P(R = 1 \mid do(T = A))$

  ↳ randomization is not always possible

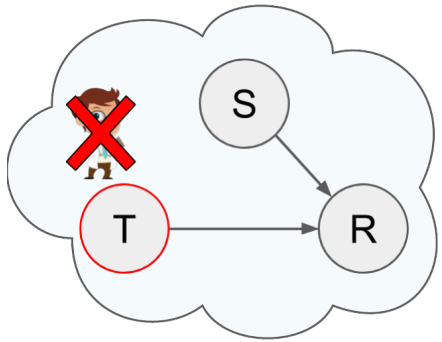
  e.g., life threatening, detrimental to the economy, etc.

Observational distribution





Interventional distribution



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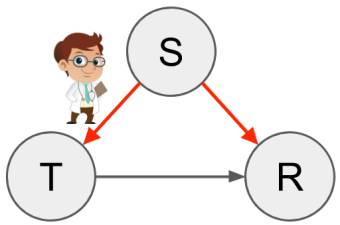

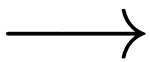

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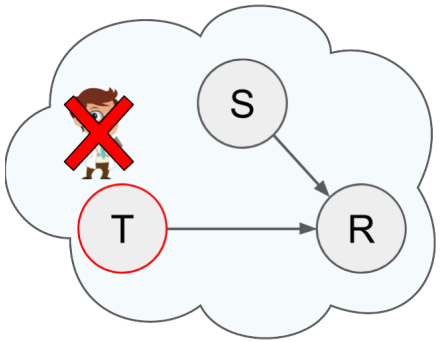

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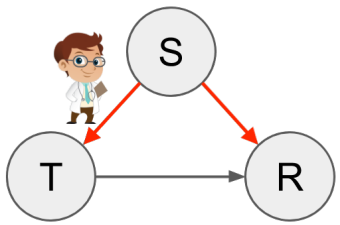

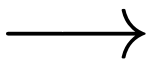

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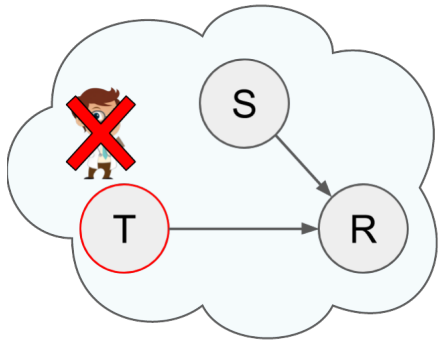

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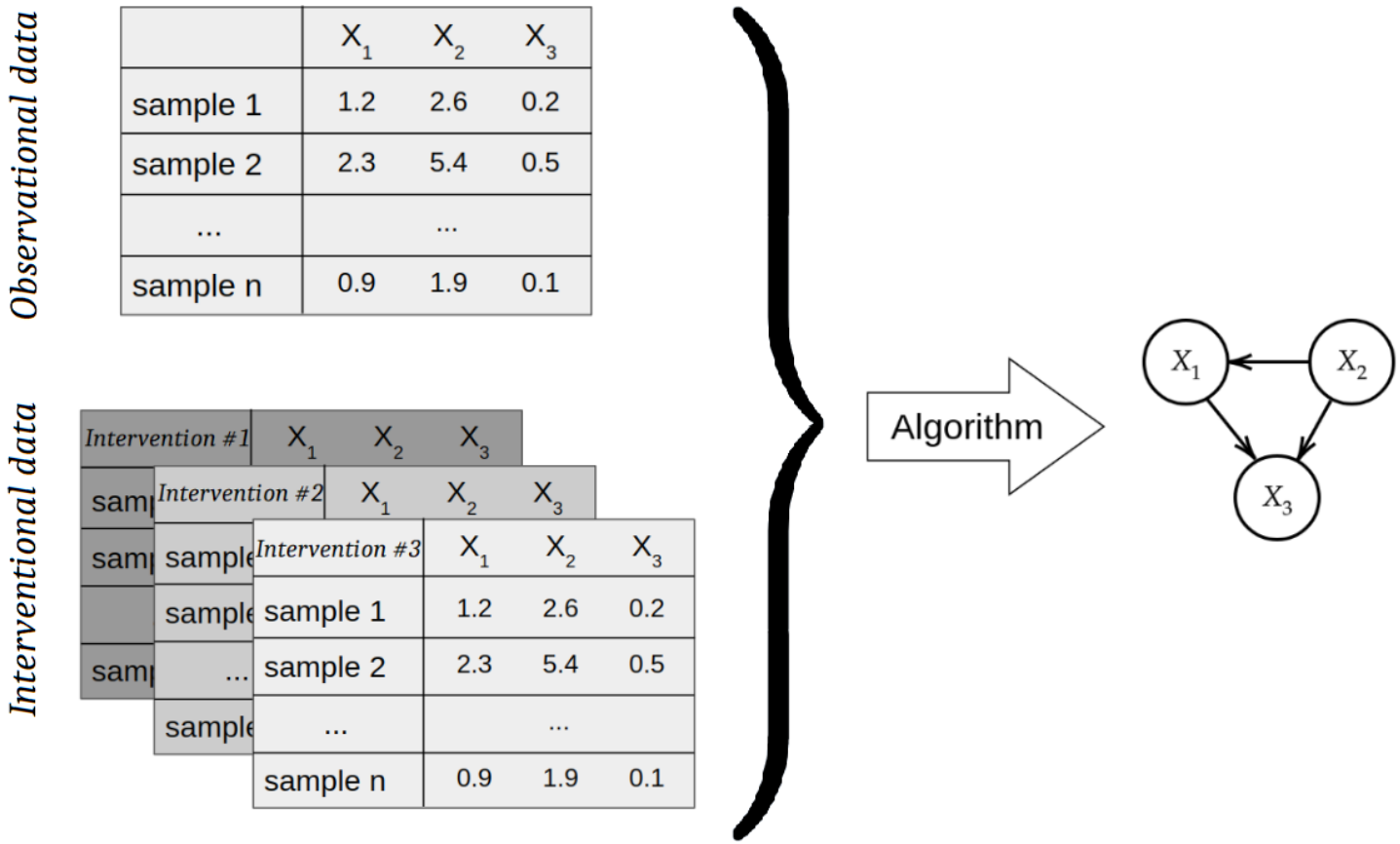
What if you don't know the causal graph?

Causal Discovery

Problem statement



Common assumptions

To make this possible, we need to make assumptions

- **Causal sufficiency:** no hidden confounding variables
- **Markov property:** *d-separation* in the graph implies *conditional independence*

  $X_1 \perp\!\!\!\perp_{\mathcal{G}} X_2 \,|\, Z \Longrightarrow X_1 \perp\!\!\!\perp_{P_X} X_2 \,|\, Z$
- **Faithfulness:** *conditional independence* implies *d-separation* in the graph

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- **Markov property:** *d-separation* in the graph implies *conditional independence*

  $X_1 \perp\!\!\!\perp_{\mathcal{G}} X_2 \,|\, Z \implies X_1 \perp\!\!\!\perp_{P_X} X_2 \,|\, Z$
- **Faithfulness:** *conditional independence* implies *d-separation* in the graph

  $X_1 \perp\!\!\!\perp_{P_X} X_2 \,|\, Z \implies X_1 \perp\!\!\!\perp_{\mathcal{G}} X_2 \,|\, Z$

These last two assumptions guarantee an equivalence between properties of the data and properties of the graph

Score-based causal discovery

- **Idea:** find the DAG that maximizes a score function ($\mathcal{S}$)
  - E.g., data likelihood + sparsity prior
  - Consistency: need to demonstrate that the score leads to the true solution

$$\hat{\mathcal{G}} \in \underset{\mathcal{G} \in DAG}{\arg\max}\, \mathcal{S}(\mathcal{G})$$

- **Problem:** search space grows superexponentially with variables

p	number of DAGs with p nodes
1	1
2	3
3	25
4	543
5	29281
6	3781503
7	1138779265
8	783702329343
9	1213442454842881
10	4175098976430598143
11	31603459396418917607425
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13	18676600744432035186664816926721
14	1439428141044398334941790719839535103
15	237725265553410354992180218286376719253505
16	83756670773733202876990304799641223522313830 3
17	62707921196923889899446452602494921906963551482675201
18	99421195322159515895228914592354524516555026878588305014783
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- **Examples:** Greedy Equivalence Search [Chickering, 2003], DAG with NO TEARS [Zheng et al., 2018]

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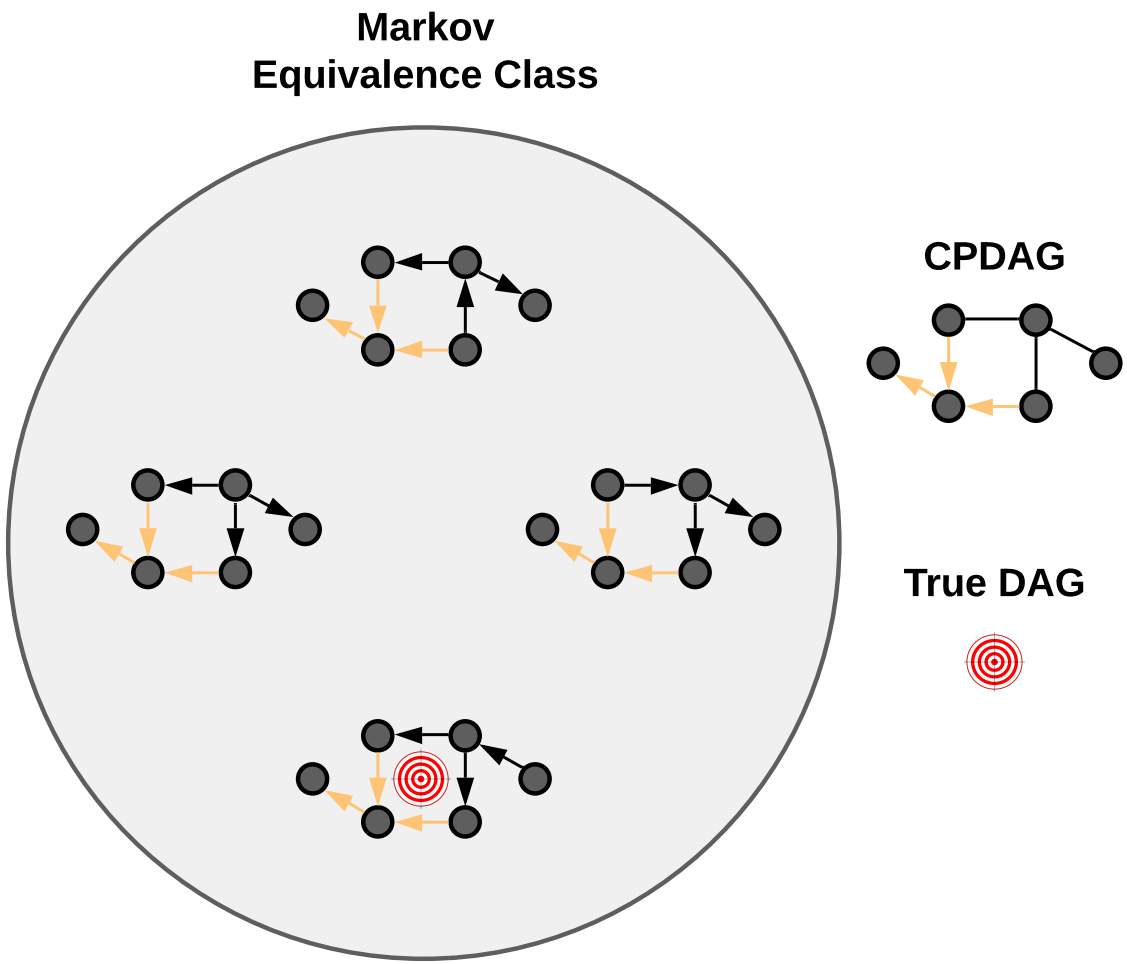
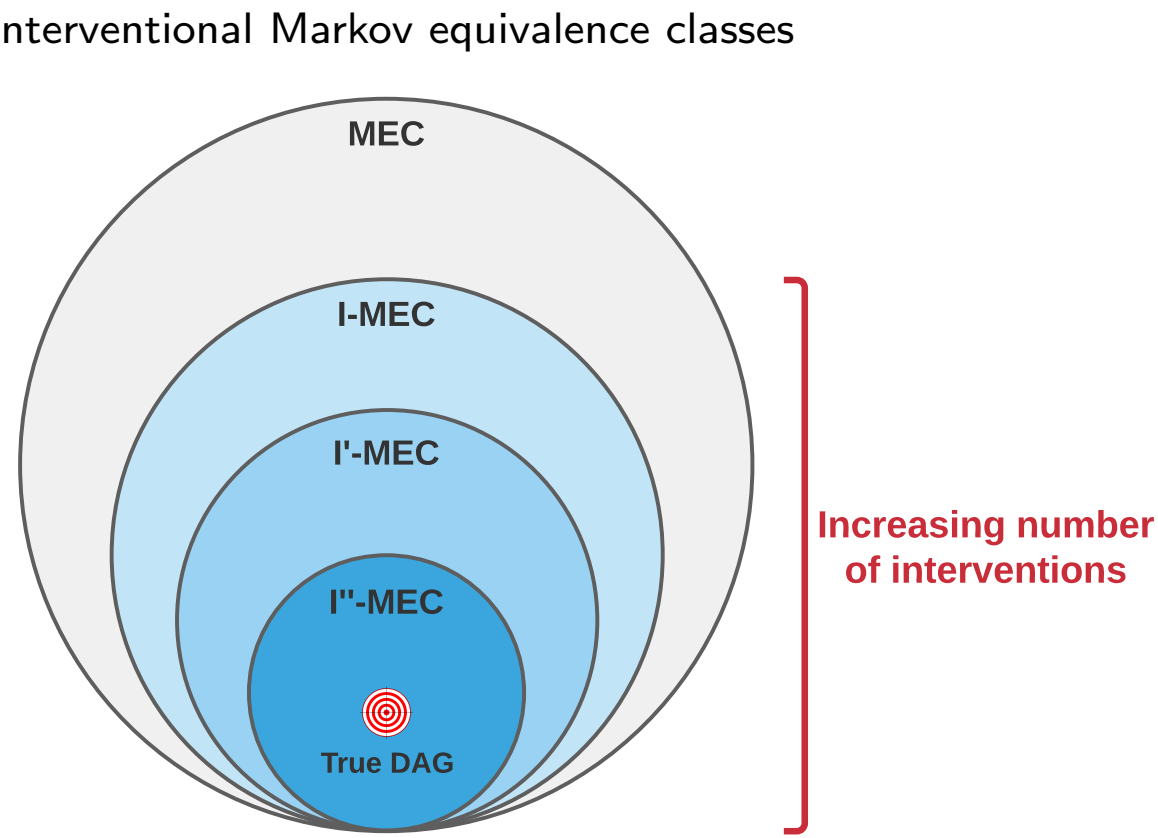
Identifiability of the DAG



Without making more assumptions, observational data only allows identification up to a Markov equivalence class (MEC) [Verma & Pearl, 1991]

Can you shrink the equivalence class?



- An I-MEC is a subset of the MEC (see Eberhardt et al. [2005])
- **Example:** gene knockout/knockdown experiments in biology [Dixit et al., 2016]

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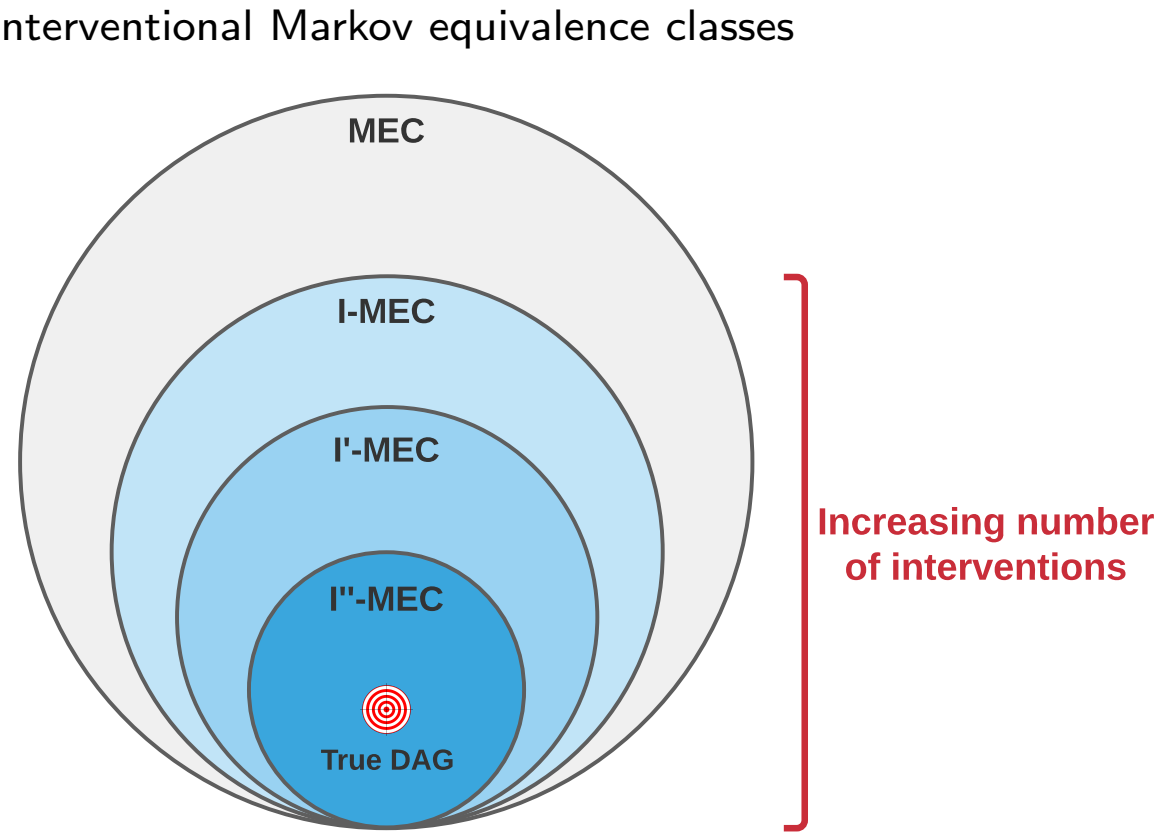

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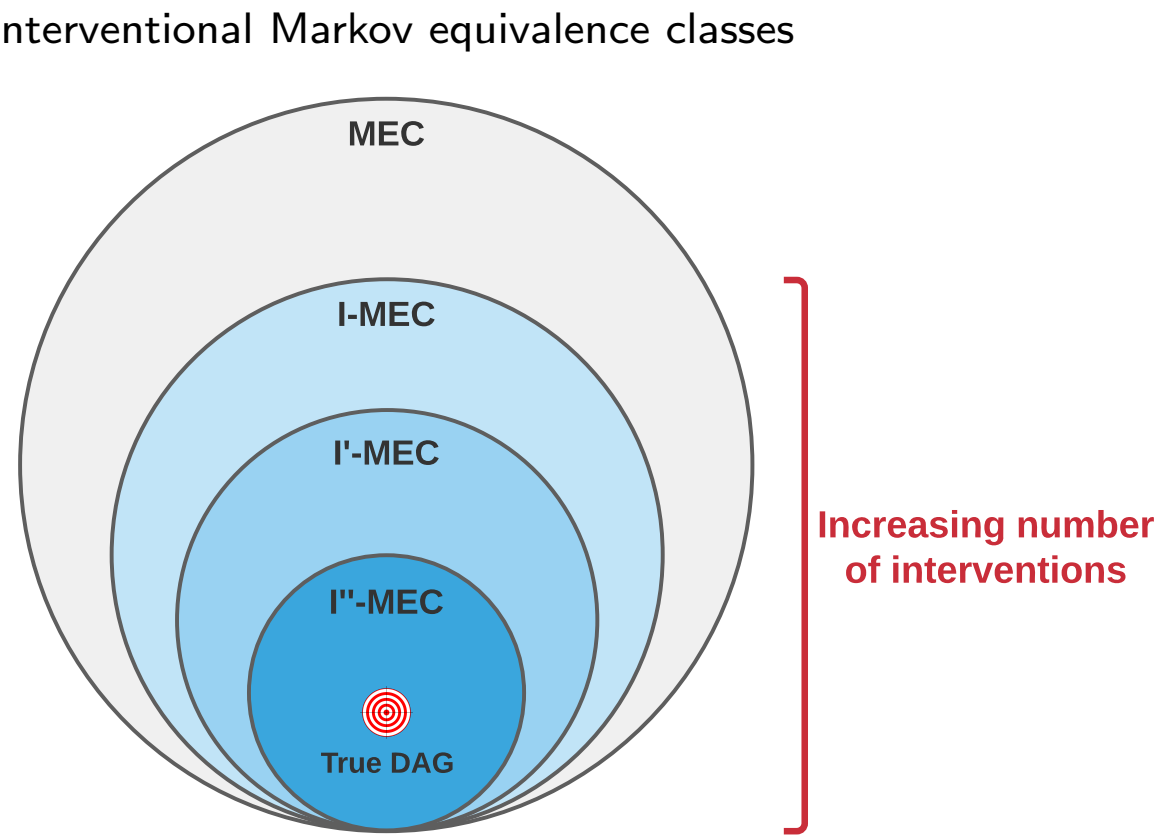

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Differentiable Causal Discovery with Interventional Data

Differentiable Causal Discovery from Interventional Data

Philippe Brouillard*
Mila, Université de Montréal

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Alexandre Lacoste
Element AI

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Mila, Université de Montréal
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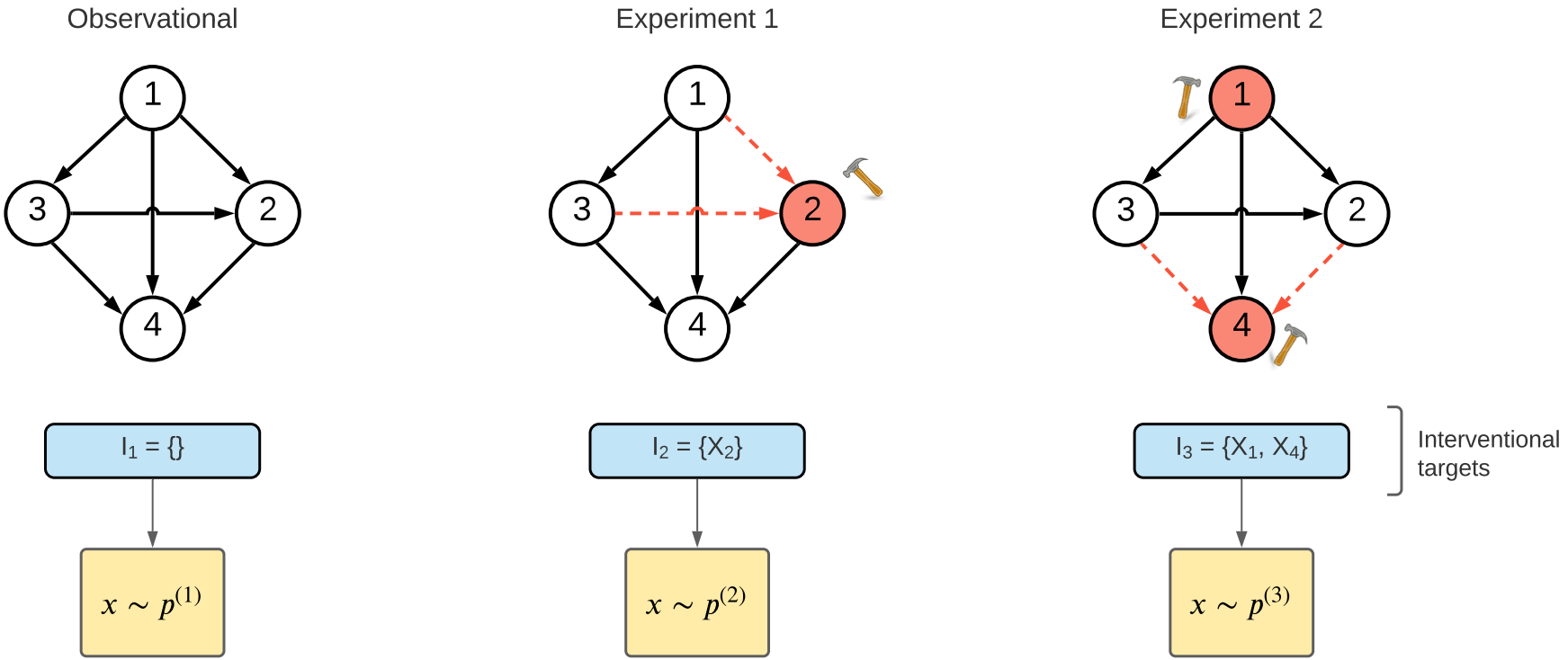
Alexandre Drouin
Element AI

34th Conference on Neural Information Processing Systems (NeurIPS 2020), Vancouver, Canada.

DCDI Fact Sheet:

- **Type:** score-based
- **Search strategy:** continuous-constrained optimization [Zheng et al., 2018]
- **Data:** observational and interventional (perfect/imperfect)
- **Theoretical guarantees:** consistency in the limit of infinite data

Interventional distributions and the invariance property



$$p^{(1)}(x_1, ..., x_4) := p^{(1)}(x_1)p^{(1)}(x_3|\ x_1)p^{(1)}(x_2|x_1, x_3)p^{(1)}(x_4|\ x_1, x_2, x_3)$$

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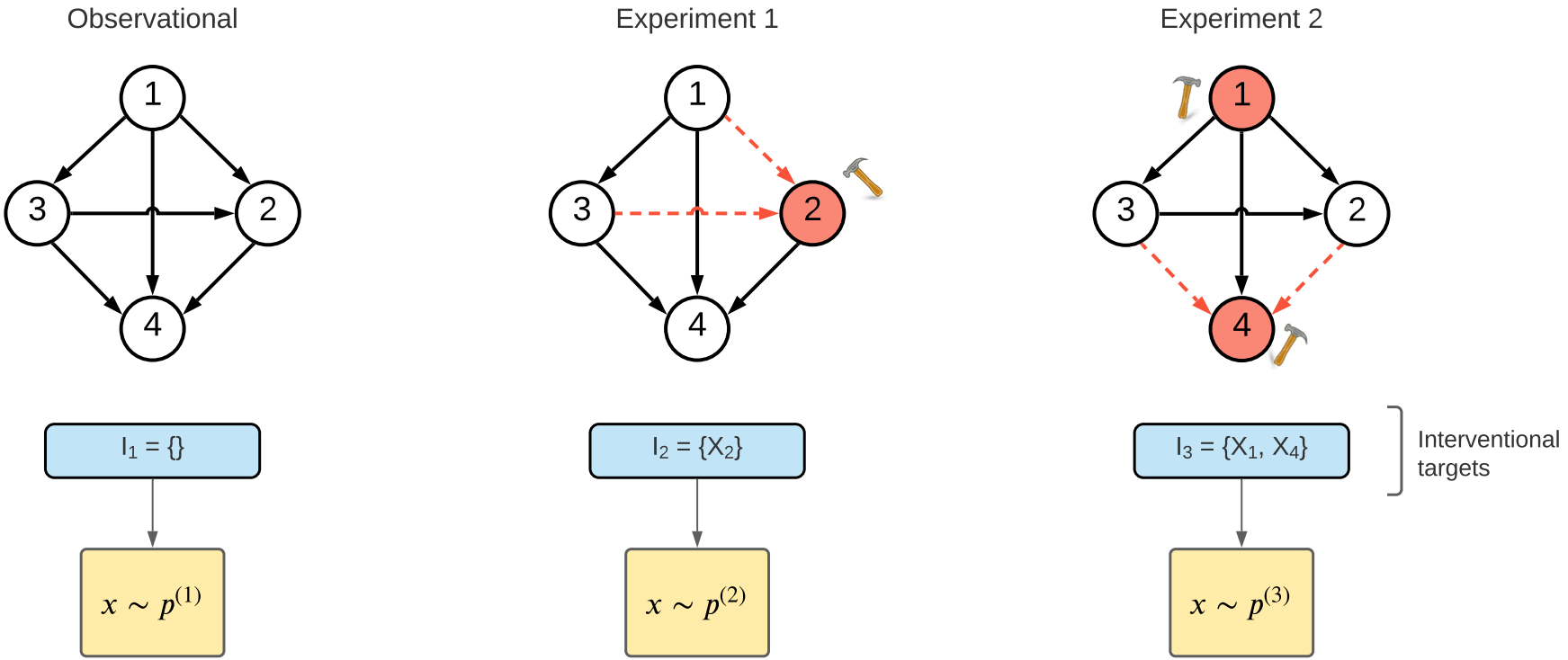

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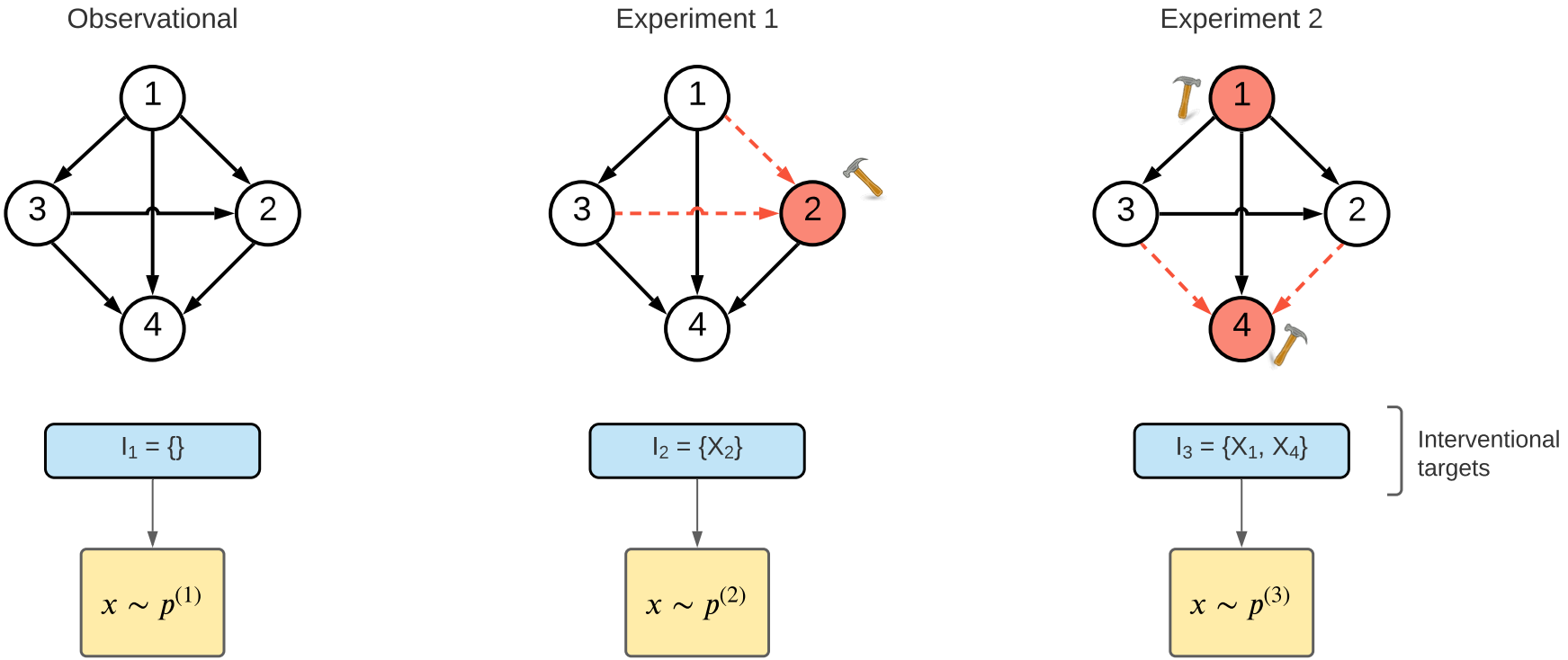

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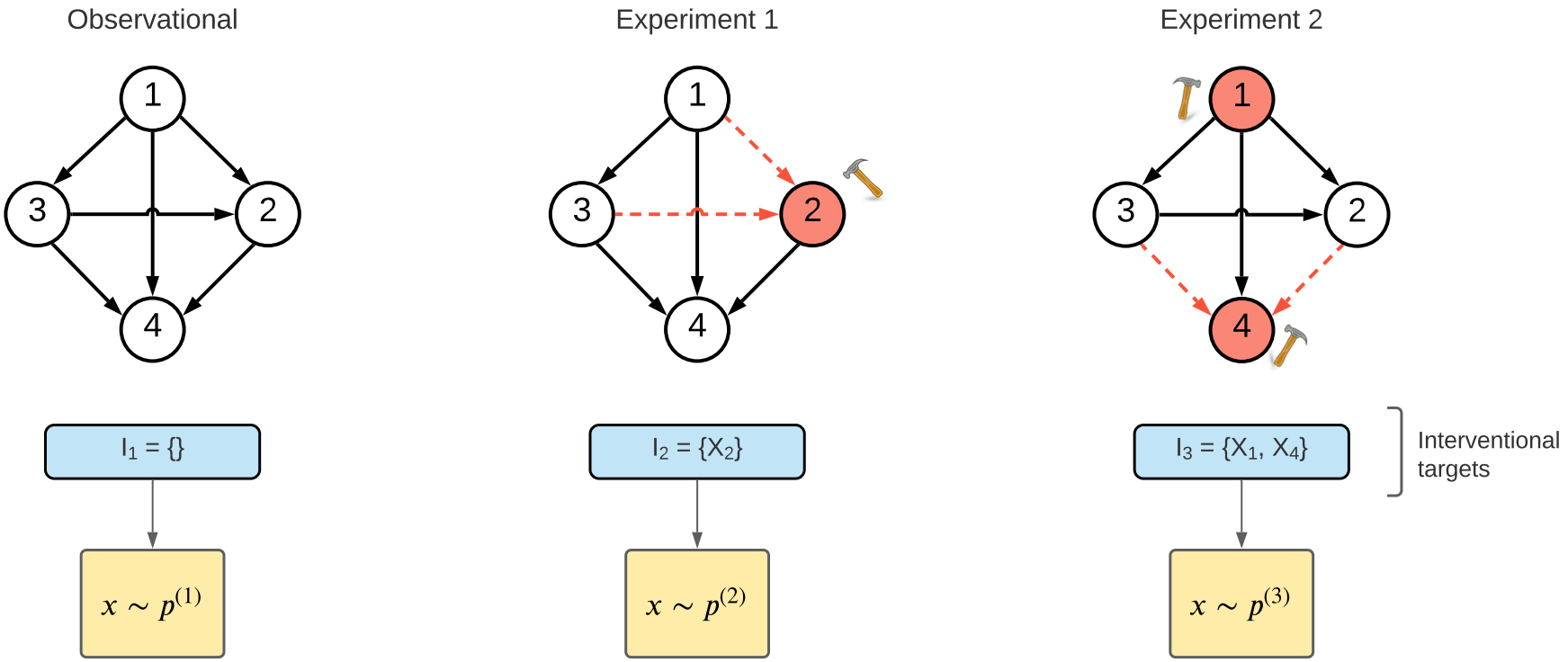
Interventional distributions and the invariance property

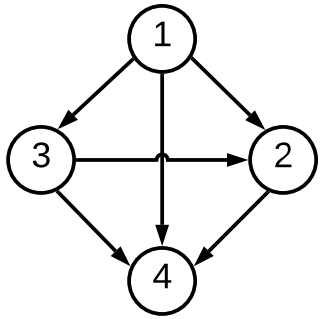


$$p^{(k)}(x_1, ..., x_d) := \prod_{j \notin I_k} p_j^{(1)}(x_j | x_{\pi_j^{\mathcal{G}}}) \prod_{j \in I_k} p_j^{(k)}(x_j | x_{\pi_j^{\mathcal{G}}})$$

DCDI: problem setting and notation

- We define a binary adjacency matrix over d variables:

$$\text{Causal DAG} = \underbrace{G = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{\text{Adjacency matrix}} \in \{0,1\}^{d \times d}$$



- We observe K experiments and their target variables

$$\underbrace{I = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}}_{\text{Intervention matrix}} \in \{0,1\}^{K \times d}$$

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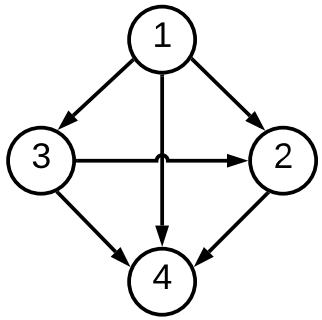

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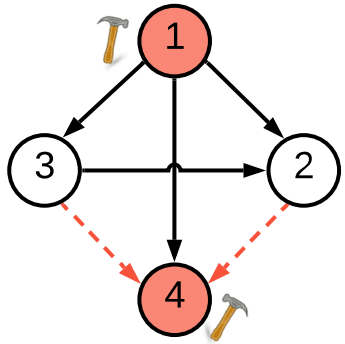
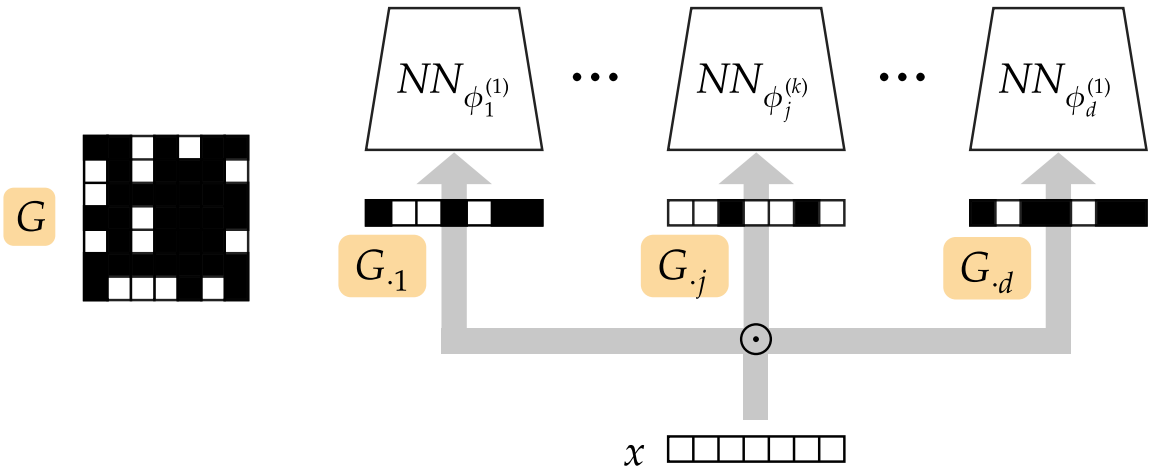
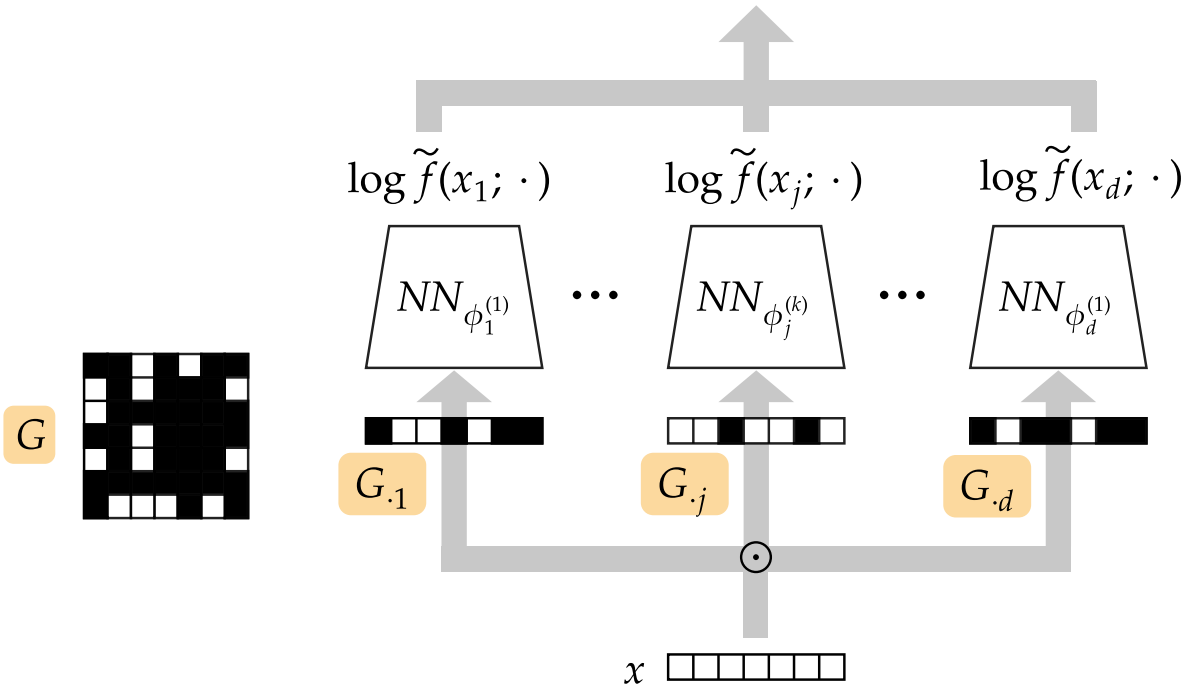


DCDI: model architecture



The graph adjacency matrix acts as a mask that filters the input variables.

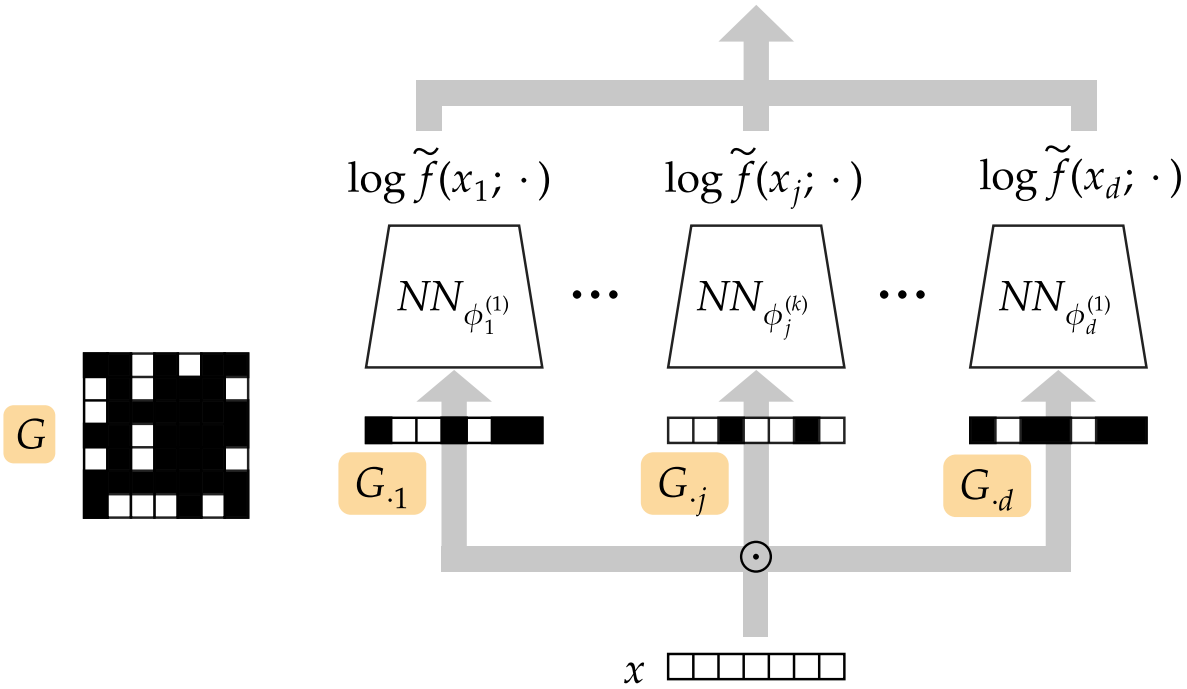
DCDI: model architecture



Each conditional distribution is estimated by a distinct neural network.

DCDI: model architecture

$$f^{(k)}(x; G, I, \phi) := \prod_{j=1}^{d} \tilde{f}(x_j; \mathrm{NN}(G_j \odot x; \overbrace{\phi_j^{(1)}}^{\text{Observational parameter}}))$$



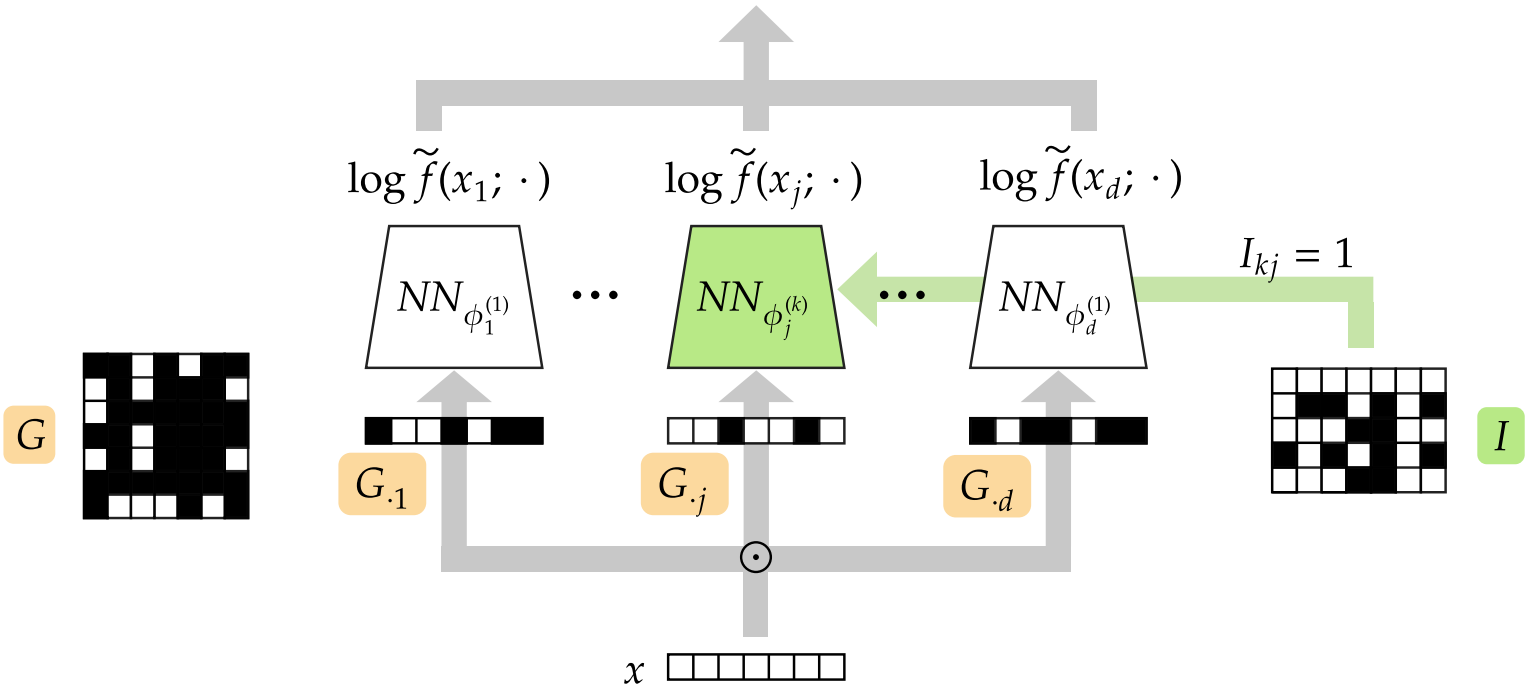
The joint likelihood is calculated as the product of conditional distributions (obs/int)

DCDI: model architecture

Observational parameter

Interventional parameter

$$f^{(k)}(x; G, I, \phi) := \prod_{j=1}^{d} \tilde{f}(x_j; \mathrm{NN}(G_j \odot x; \overbrace{\phi_j^{(1)}}))^{1-I_{kj}} \tilde{f}(x_j; \mathrm{NN}(G_j \odot x; \overbrace{\phi_j^{(k)}}))^{I_{kj}}$$



The intervention matrix I activates the right set of parameters.

DCDI: graph scoring function (discrete)

- We suggest maximizing this score over the space of DAGs:

$$\mathcal{S}_{I^*}(G) := \sup_{\phi} \sum_{k=1}^{K} \underbrace{\mathbb{E}_{X \sim p^{(k)}}}_{k\text{th ground truth intervention}} \log f^{(k)}(X; G, I^*, \phi) - \underbrace{\lambda \|G\|_0}_{\text{Sparsity regularization}}$$

- **Search:** discrete search over DAGs $\rightarrow$ continuous-constrained opt. problem [Zheng et al., 2018]

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$\downarrow$ Relaxation where $G_{ij} \sim \text{Bernoulli}(\sigma(\Lambda_{ij}))$, with $\sigma(\cdot) :=$ sigmoid function

$$\hat{\mathcal{S}}_{I^*}(\Lambda) := \sup_{\phi} \mathop{\mathbb{E}}_{G \sim \sigma(\Lambda)} \left[\sum_{k=1}^{K} \mathop{\mathbb{E}}_{X \sim p^{(k)}} \log f^{(k)}(X; G, I^*, \phi) - \lambda ||G||_0 \right]$$

$\downarrow$ Optimize for Λ under acyclicity constraint

$$\sup_{\Lambda} \hat{\mathcal{S}}_{I^*}(\Lambda) \quad s.t. \quad \underbrace{\text{Tr}\left(e^{\sigma(\Lambda)}\right) - d = 0}_{\text{Acyclicity constraint}}$$

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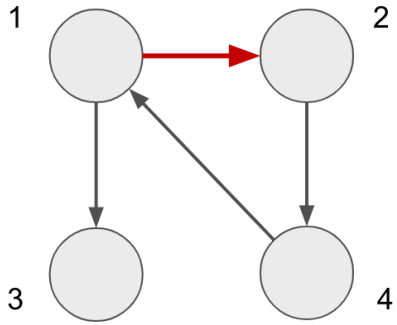
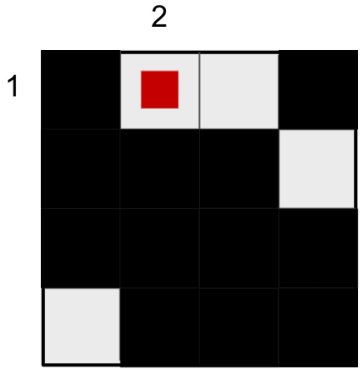
The acyclicity constraint explained

If $A^k_{ij} \neq 0$, it means that there is a path of length k from i to j



A =



- $Tr(A^k) \neq 0 \iff$ presence of cycle of length k
- Thus, $Tr(A) + Tr(A^2) + \cdots + Tr(A^d) = 0 \iff$ no cycle
- We can expand $Tr(e^A)$ as: $\sum_{k=0}^{\infty} \frac{1}{k!} Tr(A^k)$

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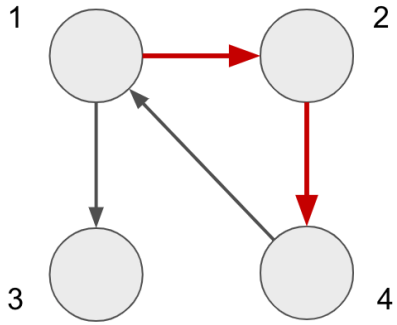

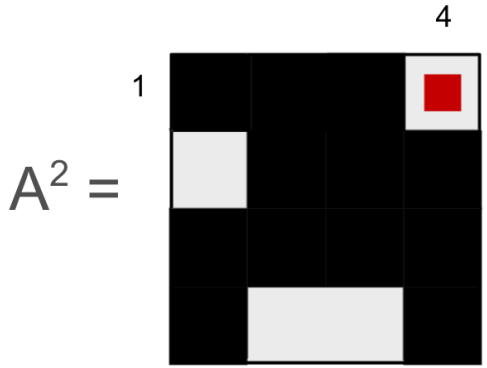

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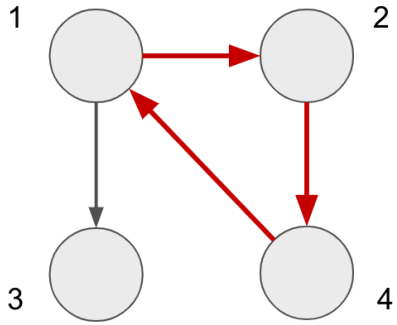
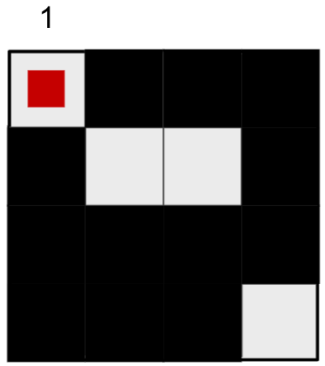


$A^3 =$



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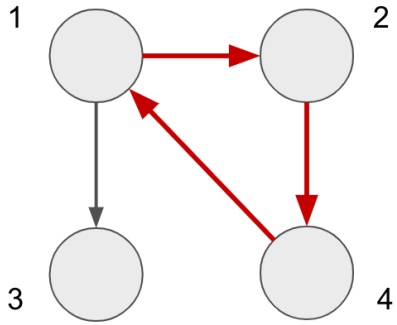
If $A^k_{ij} \neq 0$, it means that there is a path of length k from i to j



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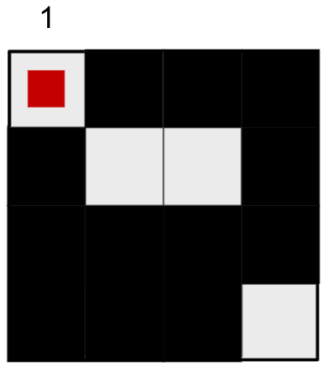

- $Tr(A^k) \neq 0 \iff$ presence of cycle of length k
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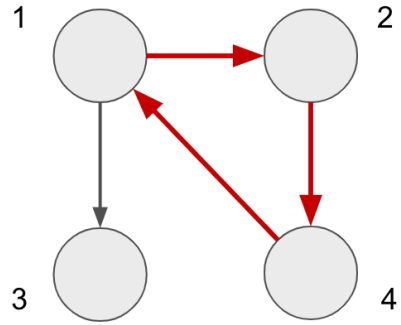

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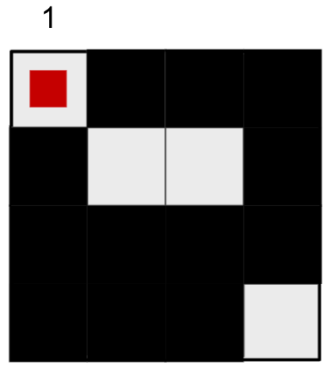

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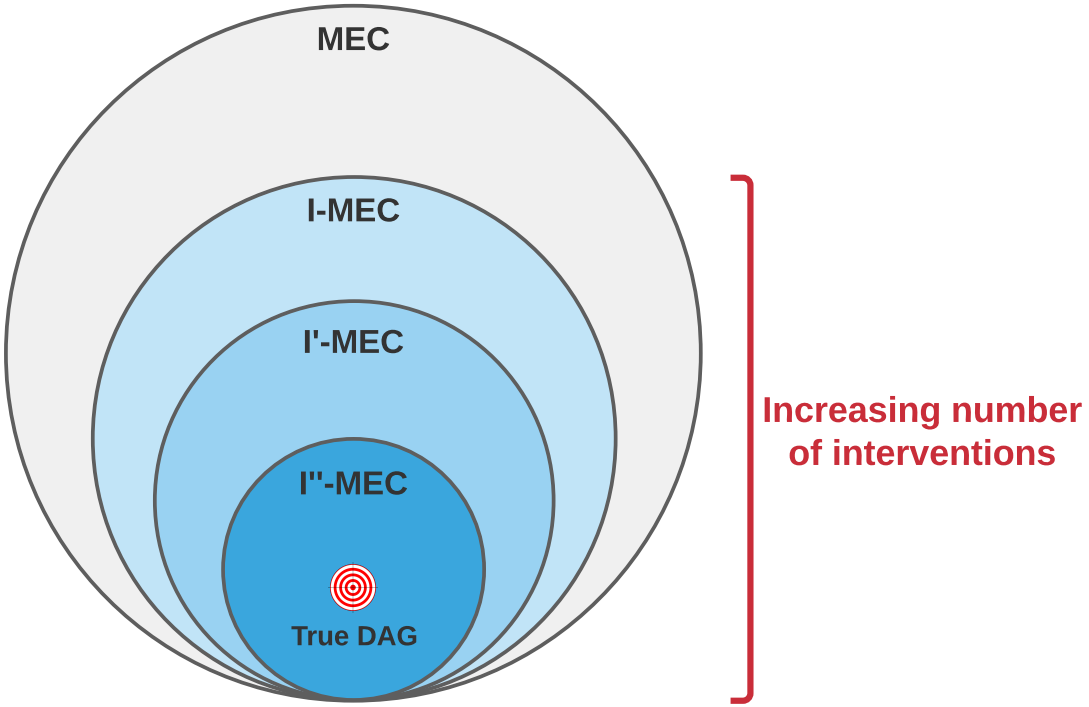

- General case: identifies the smallest interventional Markov equivalence class
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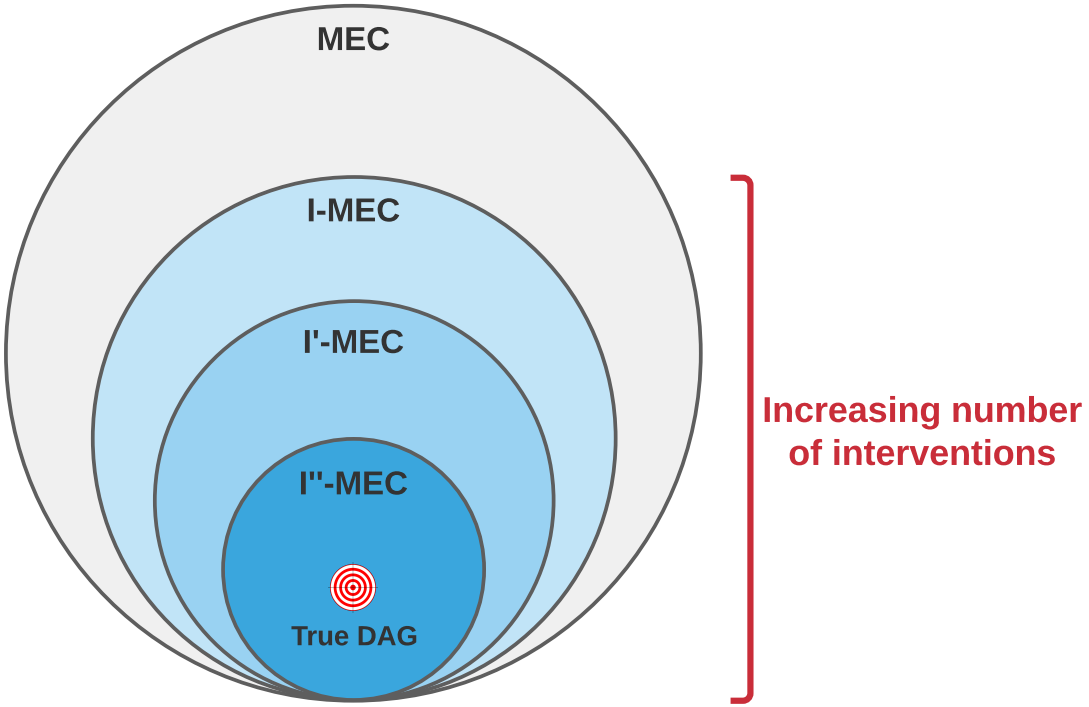

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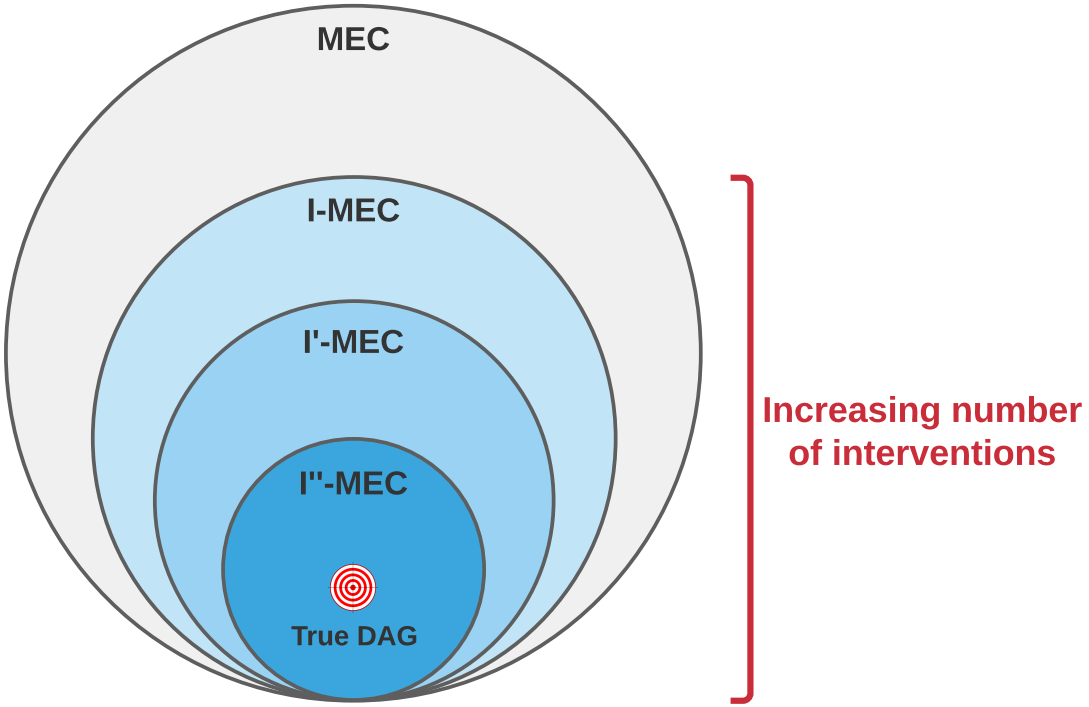

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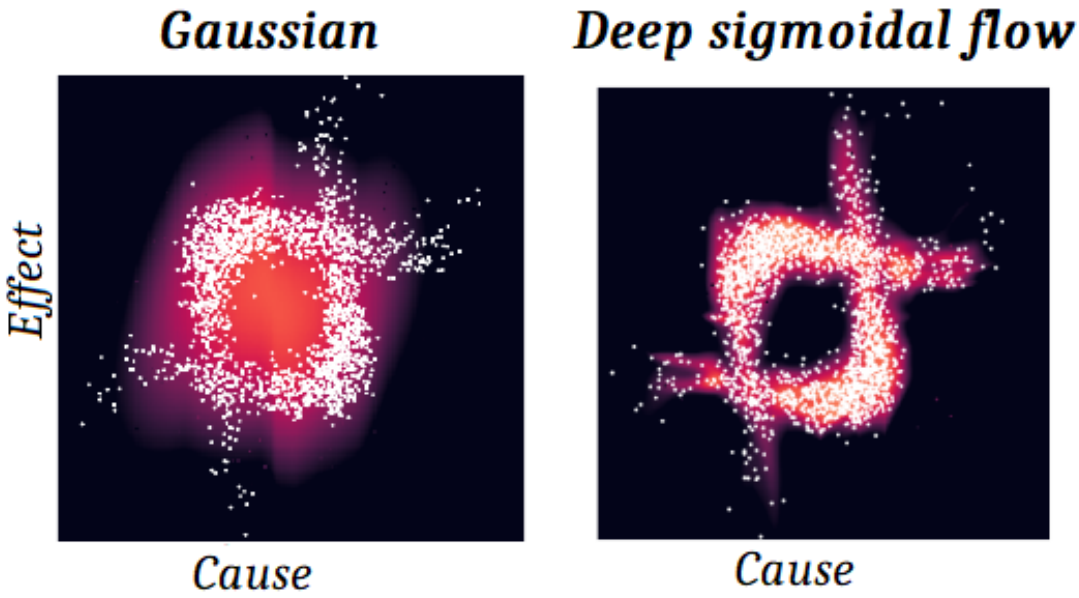
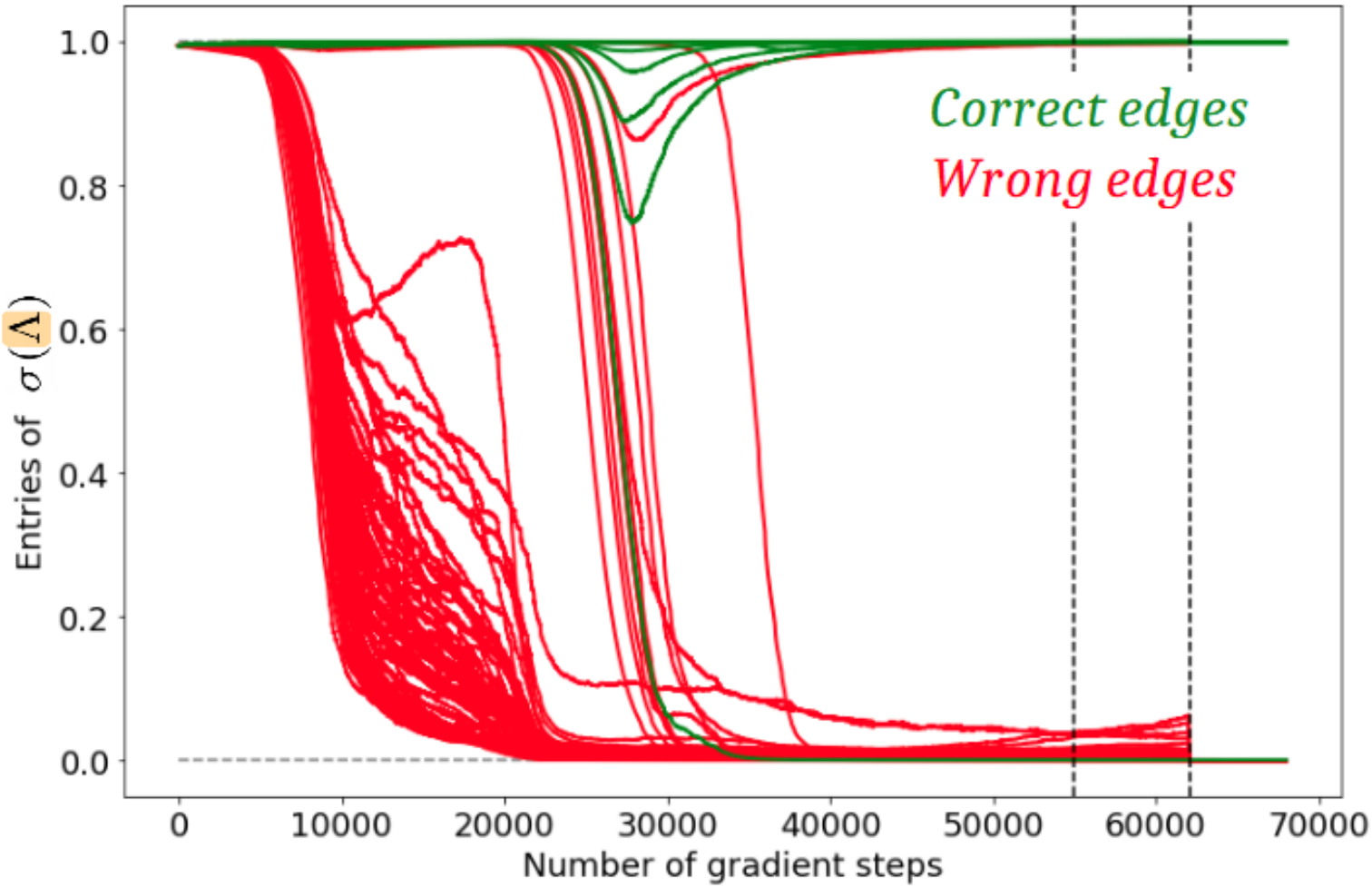
DCDI: choice of density function $\tilde{f}$



Density estimator	Assumption	Identification
Gaussian [Peters et al., 2014]	non-linear + additive noise	✓
Deep sigmoidal flow [Huang et al., 2018]	None	✓

Result: structure learning via continuous optimization



Optimizing the objective gradually prunes anti-causal edges from the graph

Results – Structural Hamming Distance (lower is better)

DCDI-G = DCDI with Gaussian density
DCDI-DSF = DCDI with deep sigmoidal flow

ANM = nonlinear with additive noise
NN = nonlinear (no additive noise)
e = average number of parents

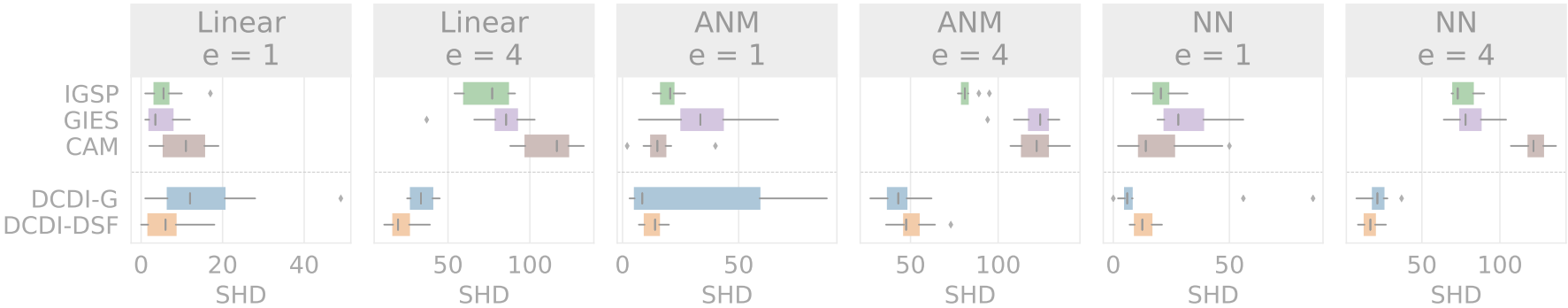


Figure: **Known target** interventions (20 nodes)

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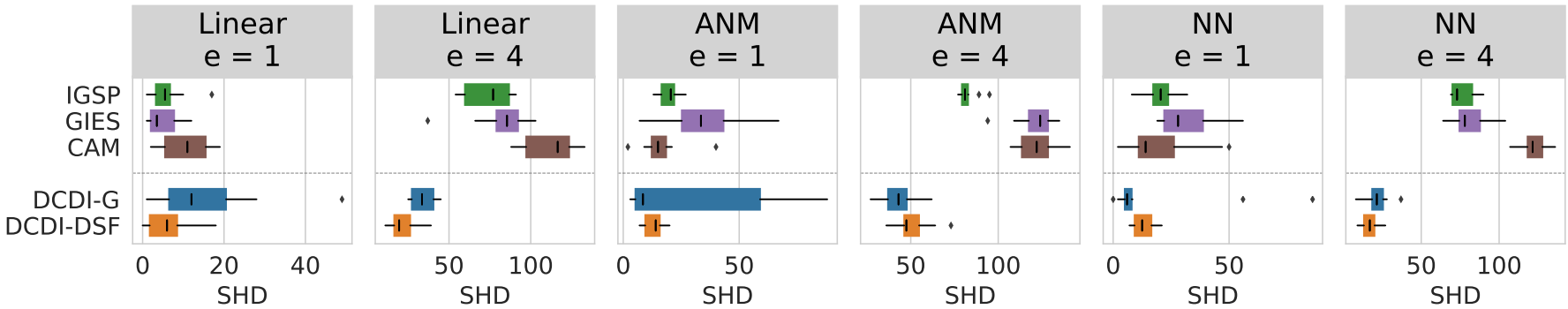

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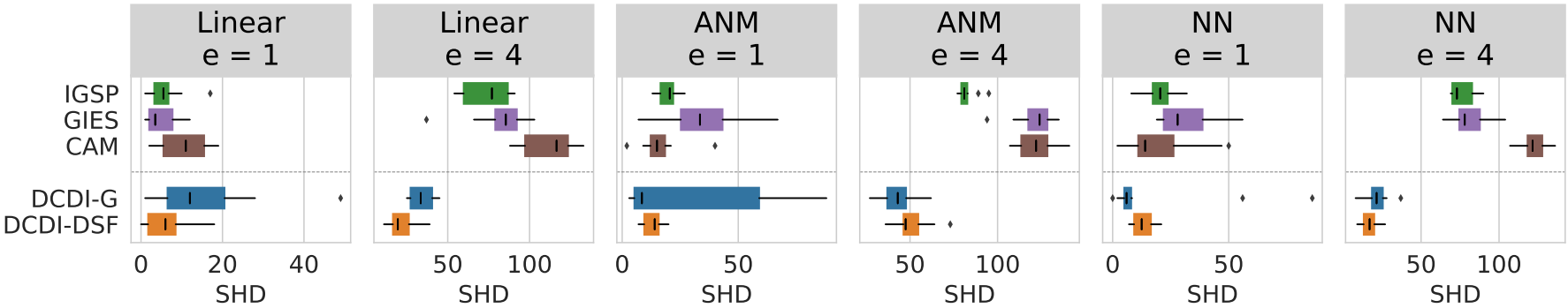

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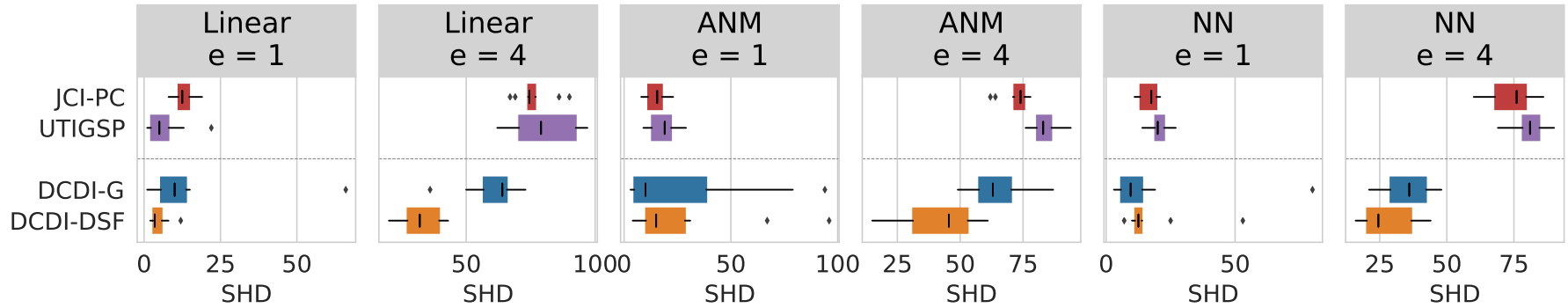

Figure: **Unknown target** interventions (20 nodes)

Conclusions and Future Directions

Conclusion & Future Work

We proposed DCDI, a causal discovery algorithm that:

- is **theoretically grounded**
- supports **perfect**, **imperfect** and **unknown-target** interventions
- **scales well with sample size** (compared to methods using kernel-based independence tests)
- achieves **state-of-the-art** performance, especially on denser graphs

Future work:

- **More extensive evaluation:** beyond synthetic data, violate assumptions [Gentzel et al., 2019]
- **Relax causal sufficiency:** allow for hidden confounders [Bhattacharya et al., 2020]
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Thank you!


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Sébastien Lachapelle *[1]


Alexandre Lacoste [2]


Simon Lacoste-Julien [1]


Alexandre Drouin [2]

[1] Mila & DIRO, Université de Montréal [2] ServiceNow, Element AI * Equal contribution

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DCDI: optimization & gradient estimation

- Optimize jointly Λ and ϕ (NN parameters)

$$\max_{\phi,\Lambda} \mathop{\mathbb{E}}_{G\sim\sigma(\Lambda)} \left[\sum_{k=1}^{K} \mathop{\mathbb{E}}_{X\sim p^{(k)}} \log f^{(k)}(X; G, I^*, \phi) - \lambda ||G||_0 \right] \text{ s.t. } \underbrace{\operatorname{Tr}\left(e^{\sigma(\Lambda)}\right) - d = 0}_{\text{Acyclicity constraint}}$$

- **Optimization:** Augmented Lagrangian Method + RMSprop (as in Lachapelle et al. [2020])
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- What if we don't? (e.g., as in Ke et al. [2019])

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- **Learning:**
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- **Theory:** We showed the same guarantee holds for this score!

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DCDI: theoretical justification

- $\mathcal{G}^*$ = ground-truth DAG
- I^* = ground-truth intervention matrix

$\hat{\mathcal{G}} \in \arg\max_{\mathcal{G} \in \text{DAG}} \mathcal{S}_{I^*}(\mathcal{G})$ is the estimator.

Theorem (Identification via score maximization)

Suppose $I^*_{1,:} = \emptyset$. Given that

1. *Each variable is individually targeted by an intervention;*
2. *The model has enough capacity to express the ground truth;*
3. *The regularization coefficient $\lambda > 0$ is small enough;*
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then

$$\hat{\mathcal{G}} = \mathcal{G}^*$$

More general result

Without the first assumption, we can identify the I^*-Markov equivalence class[a] of $\mathcal{G}^*$.

[a] We use the notion of I^*-Markov equivalence of Yang et al. [2018].

DCDI: theoretical justification

- $\mathcal{G}^*$ = ground-truth DAG
- I^* = ground-truth intervention matrix

$\hat{\mathcal{G}} \in \arg\max_{\mathcal{G} \in \text{DAG}} \mathcal{S}_{I^*}(\mathcal{G})$ is the estimator.

Theorem (Identification via score maximization)

Suppose $I^*_{1,:} = \emptyset$. Given that

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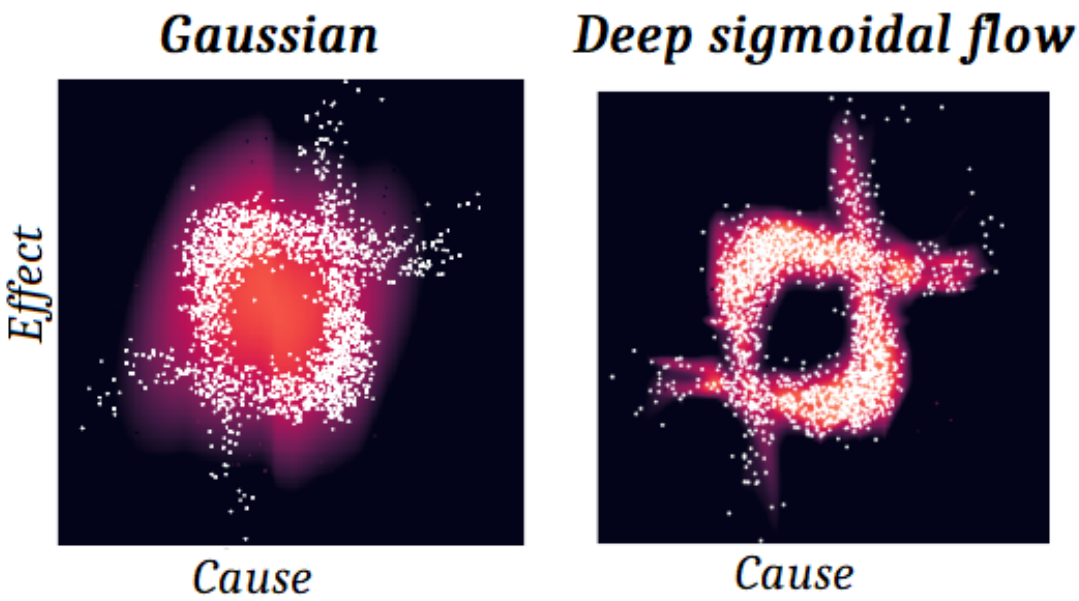

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- **Deep sigmoidal flow**: a type of normalizing flow that was shown to be a universal density approximator [Huang et al., 2018]
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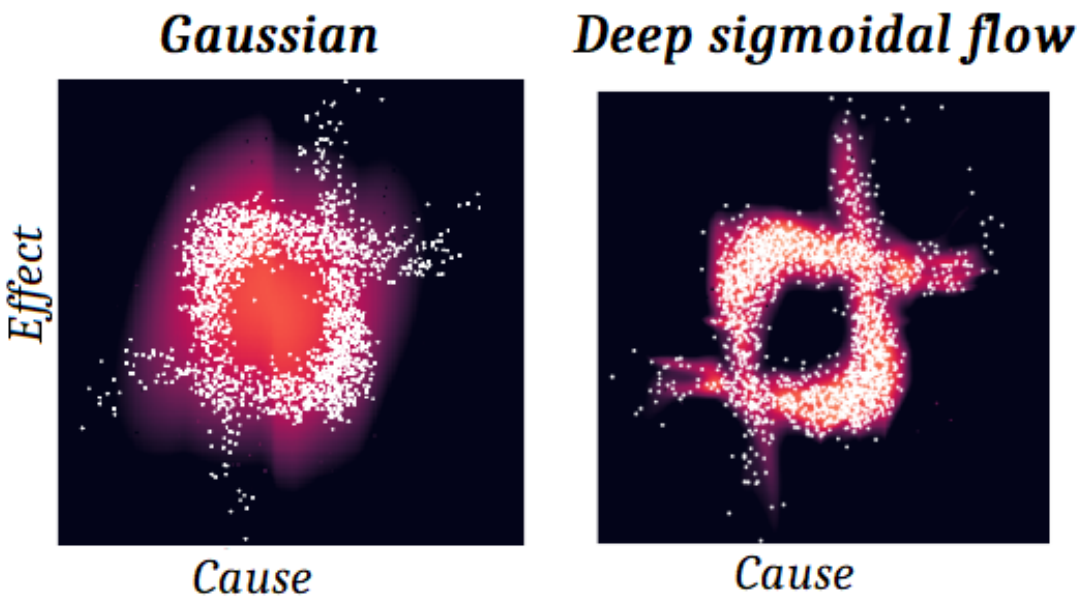

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