### Ancestral Causal Inference

### Sara Magliacane, Tom Claassen, Joris M. Mooij

s.magliacane@uva.nl



5<sup>th</sup> December, 2016

# Part I

# Introduction

Sara Magliacane (VU, UvA)

Ancestral Causal Inference



### Causal inference: learning causal relations from data

#### Definition

X causes  $Y (X \rightarrow Y) = intervening upon$  (changing) X changes Y

• We can represent causal relations with a causal DAG (hidden vars):

$$X \longrightarrow Y$$
 E.g.  $X =$ Smoking,  $Y =$ Cancer

#### Definition

X causes  $Y (X \rightarrow Y) = intervening upon$  (changing) X changes Y

• We can represent causal relations with a causal DAG (hidden vars):

$$X \longrightarrow Y$$
 E.g.  $X =$ Smoking,  $Y =$ Cancer

• Causal inference = structure learning of the causal DAG

#### Definition

X causes  $Y (X \rightarrow Y) = intervening upon$  (changing) X changes Y

• We can represent causal relations with a causal DAG (hidden vars):

$$X \longrightarrow Y$$
 E.g.  $X =$ Smoking,  $Y =$ Cancer

• Causal inference = structure learning of the causal DAG

- Traditionally, causal relations are inferred from interventions.
- Sometimes, interventions are unethical, unfeasible or too expensive

### Holy Grail of Causal Inference

Learn as much causal structure as possible from observations, integrating background knowledge and experimental data.

#### Holy Grail of Causal Inference

Learn as much causal structure as possible from observations, integrating background knowledge and experimental data.

- **Constraint-based causal discovery**: use statistical independences to express constraints over possible causal models
- Intuition: Under certain assumptions, independences in the data correspond with d-separations in a causal DAG

### Holy Grail of Causal Inference

Learn as much causal structure as possible from observations, integrating background knowledge and experimental data.

- **Constraint-based causal discovery**: use statistical independences to express constraints over possible causal models
- Intuition: Under certain assumptions, independences in the data correspond with d-separations in a causal DAG
- Issues:
  - **0** Vulnerability to errors in statistical independence tests
  - O No estimation of confidence in the causal predictions

### Causal inference as an optimization problem (e.g. HEJ)

- Weighted list of statistical independence results:  $I = \{(i_j, w_j)\}$ :
  - E.g.  $I = \{ (Y \perp Z \mid X, 0.2), (Y \not\perp X, 0.1) \}$

#### HEJ [Hyttinen et al., 2014]

### Causal inference as an optimization problem (e.g. HEJ)

• Weighted list of statistical independence results:  $I = \{(i_j, w_j)\}$ :

• E.g. 
$$I = \{ (Y \perp Z \mid X, 0.2), (Y \not\perp X, 0.1) \}$$

• For any possible causal structure *C*, we define the loss function:

$$\mathcal{Loss}(C, I) := \sum_{(i_j, w_j) \in I: \ i_j \text{ is not satisfied in } C} w_j$$

• " $i_j$  is not satisfied in C" = defined by causal reasoning rules

## Causal inference as an optimization problem (e.g. HEJ)

• Weighted list of statistical independence results:  $I = \{(i_j, w_j)\}$ :

• E.g. 
$$I = \{ (Y \perp Z \mid X, 0.2), (Y \not\perp X, 0.1) \}$$

• For any possible causal structure *C*, we define the loss function:

$$\mathcal{Loss}(C, I) := \sum_{(i_j, w_j) \in I: i_j \text{ is not satisfied in } C} w_j$$

- " $i_j$  is not satisfied in C" = defined by causal reasoning rules
- Causal inference = Find causal structure minimizing loss function

$$C^* = \arg\min_{C \in \mathcal{C}} \mathcal{Loss}(C, I)$$

• Problem: Scalability

HEJ [Hyttinen et al., 2014]

# Part II

# Ancestral Causal Inference

### A more coarse grained representation

• Can we improve scalability of the most accurate state-of-the-art method (HEJ)?

### A more coarse grained representation

• Can we improve scalability of the most accurate state-of-the-art method (HEJ)?

#### Ancestral Causal Inference: Main Idea

Instead of representing direct causal relations use a more coarse-grained representation of causal information, e.g., an ancestral structure (a set of "indirect" causal relations).



### A more coarse grained representation

• Can we improve scalability of the most accurate state-of-the-art method (HEJ)?

#### Ancestral Causal Inference: Main Idea

Instead of representing direct causal relations use a more coarse-grained representation of causal information, e.g., an ancestral structure (a set of "indirect" causal relations).



- Ancestral structures reduce drastically search space
- $\bullet\,$  For 7 variables:  $2.3\times10^{15}\rightarrow6\times10^{6}$

### Causal inference as an optimization problem (Reprise)

- Weighted list of inputs:  $I = \{(i_j, w_j)\}$ :
  - E.g.  $I = \{ (Y \perp Z \mid X, 0.2), (Y \not\perp X, 0.1) \}, (U \rightarrow Z, 0.8) \}$
  - Any consistent weighting scheme, e.g. frequentist, Bayesian

### Causal inference as an optimization problem (Reprise)

- Weighted list of inputs:  $I = \{(i_j, w_j)\}$ :
  - E.g.  $I = \{ (Y \perp Z \mid X, 0.2), (Y \not\perp X, 0.1) \}, (U \longrightarrow Z, 0.8) \}$
  - Any consistent weighting scheme, e.g. frequentist, Bayesian
- For any possible ancestral structure *C*, we define the loss function:

$$\mathcal{Loss}(C, I) := \sum_{(i_j, w_j) \in I: \ i_j \text{ is not satisfied in } C} w_j$$

• Here: " $i_j$  is not satisfied in C" = defined by ancestral reasoning rules

### Causal inference as an optimization problem (Reprise)

- Weighted list of inputs:  $I = \{(i_j, w_j)\}$ :
  - E.g.  $I = \{ (Y \perp Z \mid X, 0.2), (Y \not\perp X, 0.1) \}, (U \longrightarrow Z, 0.8) \}$
  - Any consistent weighting scheme, e.g. frequentist, Bayesian
- For any possible ancestral structure *C*, we define the loss function:

$$\mathcal{Loss}(C, I) := \sum_{(i_j, w_j) \in I: \ i_j \ \text{is not satisfied in } C} w_j$$

- Here: "*i*<sub>j</sub> is not satisfied in C" = defined by ancestral reasoning rules
- Causal inference = Find ancestral structure minimizing loss function

$$C^* = \arg\min_{C \in \mathcal{C}} \mathcal{Loss}(C, I)$$

### Ancestral reasoning rules: Example

• ACI rules: 7 ancestral reasoning rules that given (in)dependences constrain possible (non) ancestral relations

### Ancestral reasoning rules: Example

• ACI rules: 7 ancestral reasoning rules that given (in)dependences constrain possible (non) ancestral relations

#### Example

For X, Y, W disjoint (sets of) variables:

$$(X \perp Y \mid \boldsymbol{W}) \land (X \not \to \boldsymbol{W}) \implies X \not \to Y$$

- $X \perp Y \mid W = "X$  is independent of Y given a set of variables W"
- $X \rightarrow W = X$  does not cause any variable in the set W
- $\implies$  = "then"
- $X \rightarrow Y = "X$  does not cause Y"

• Score the confidence in a predicted statement s (e.g.  $X \rightarrow Y$ ) as:

$$C(f) = \min_{C \in \mathcal{C}} \mathcal{Loss}(C, \ I + (\neg s, \infty))$$
$$- \min_{C \in \mathcal{C}} \mathcal{Loss}(C, \ I + (s, \infty))$$

• pprox MAP approximation of the log-odds ratio of s

• Score the confidence in a predicted statement s (e.g.  $X \rightarrow Y$ ) as:

$$C(f) = \min_{C \in \mathcal{C}} \mathcal{Loss}(C, \ I + (\neg s, \infty))$$
$$- \min_{C \in \mathcal{C}} \mathcal{Loss}(C, \ I + (s, \infty))$$

- pprox MAP approximation of the log-odds ratio of s
- Asymptotically consistent, when consistent input weights
- Can be used with any method that solves an optimization problem

# Part III

# **Evaluation**



### Simulated data accuracy: example Precision Recall curve



• ACI is as accurate as HEJ + our scoring method

Sara Magliacane (VU, UvA)

### Simulated data execution time



- ACI is orders of magnitude faster than HEJ
- The difference grows exponentially in the number of variables
- HEJ is not feasible for more than 8 variables

Sara Magliacane (VU, UvA)

Ancestral Causal Inference

## Application: Reconstructing a Protein Signalling Network



- Black edges = overlap
- Consistent with score-based method [Mooij and Heskes, 2013]

- Ancestral Causal Discovery (ACI), a causal discovery method as accurate as the state-of-the-art but much more scalable
- A method for scoring causal relations by confidence

- Source code: http://github.com/caus-am/aci
- Poster: WIML, 1.30pm 2.30pm, poster 3
- Poster: NIPS, Tuesday 6pm 9.30pm, poster 81
- Talk on extensions of ACI at "What If?" NIPS workshop, Saturday

#### Claassen, T. and Heskes, T. (2011).

A logical characterization of constraint-based causal discovery. In Proceedings of the 27th Conference on Uncertainty in Artificial Intelligence (UAI 2011), pages 135–144.

Entner, D., Hoyer, P., and Spirtes, P. (2013).

Data-driven covariate selection for nonparametric estimation of causal effects. In Proceedings of the Sixteenth International Conference on Artificial Intelligence and Statistics (AISTATS 2013).



#### Hyttinen, A., Eberhardt, F., and Järvisalo, M. (2014).

Constraint-based causal discovery: Conflict resolution with answer set programming. In Proceedings of the 30th Conference on Uncertainty in Artificial Intelligence (UAI 2014), pages 340–349.



#### Magliacane, S., Claassen, T., and Mooij, J. M. (2016).

Ancestral causal inference. arXiv.org preprint, arXiv:1606.07035 [cs.LG]. Accepted for Neural Information Processing Systems 2016.

Mooij, J. M. and Heskes, T. (2013).

Cyclic causal discovery from continuous equilibrium data. In Nicholson, A. and Smyth, P., editors, *UAI*, pages 431–439. AUAI Press.

# Part IV

# Backup slides

Sara Magliacane (VU, UvA)

Ancestral Causal Inference



#### ACI is sound for predicting ancestral relations:

#### Theorem

The confidence scores  $C(X \rightarrow Y)$  are sound for oracle inputs with infinite weights, i.e.:

$$C(X \dashrightarrow Y) = \begin{cases} \infty & \text{if } X \dashrightarrow Y \text{ is identifiable,} \\ -\infty & \text{if } X \nrightarrow Y \text{ is identifiable,} \\ 0 & \text{otherwise.} \end{cases}$$

### Finite Weights: Definition and Consistency

We propose two choices for the weights:

- Frequentist Weights: w<sub>j</sub> = |log p<sub>j</sub> log α| where p<sub>j</sub> is the p-value of a statistical test for i<sub>j</sub>, and α a threshold.
- Bayesian Weights:  $w_j = \log p(i_j | data) \log p(\neg i_j | data)$ . Under mild assumptions, such weights are consistent, i.e., as sample size

 $N \rightarrow \infty$ , for the frequentist weights:

$$\log p^{(N)} - \log \alpha^{(N)} \xrightarrow{P} \begin{cases} -\infty & H_1 \\ +\infty & H_0 \end{cases}$$

when  $\alpha^{(N)} \rightarrow 0$  at a suitable rate, or for the Bayesian weights:

$$w_N \xrightarrow{P} \begin{cases} -\infty & \text{ if } i_j \text{ is true} \\ +\infty & \text{ if } i_j \text{ is false.} \end{cases}$$

The probability of a type I and type II errors will then converge to 0.

Sara Magliacane (VU, UvA)

### ACI is consistent for predicting ancestral relations:

#### Theorem

The confidence scores  $C(X \rightarrow Y)$  are asymptotically consistent, i.e.:

$$C(X \dashrightarrow Y) \xrightarrow{P} \begin{cases} \infty & \text{if } X \dashrightarrow Y \text{ is identifiable,} \\ -\infty & \text{if } X \nrightarrow Y \text{ is identifiable,} \\ 0 & \text{otherwise.} \end{cases}$$

### Complete ACI rules

Trivial rules:

For X, Y, W disjoint (sets of) variables:

$$(X \perp Y \mid \boldsymbol{W}) \land (X \not \to \boldsymbol{W}) \implies X \not \to Y$$

- $(X \perp Y \mid \boldsymbol{W} \cup [Z]) \land (X \perp Z \mid \boldsymbol{W} \cup U) \implies (X \perp Y \mid \boldsymbol{W} \cup U)$
- $(Z \not\!\!\perp X \mid \boldsymbol{W}) \land (Z \not\!\!\perp Y \mid \boldsymbol{W}) \land (X \not\!\!\perp Y \mid \boldsymbol{W}) \implies X \not\!\!\perp Y \mid \boldsymbol{W} \cup Z$
- $X \not\to \mathbf{W} \land X \not\to Z \land Z \perp Y \mid \mathbf{W} \cup [X] \implies \\ p(Y|\operatorname{do}(X)) = \int p(Y|X, \mathbf{W}) p(\mathbf{W}) d\mathbf{W}$

[Claassen and Heskes, 2011], [Entner et al., 2013], [Magliacane et al., 2016]

#### Example (Genomics)

How to infer gene regulatory networks from micro-array data?



#### Traditional statistics, machine learning

- Models the distribution of the data
- Focuses on predicting observations
- Useful e.g. in medical diagnosis: given the symptoms, what is the most likely disease?

### **Causal Inference**

- Models the mechanism that generates the data
- Also allows to predict results of interventions
- Useful e.g. in medical treatment: if we treat the patient with a drug, will it cure the disease?

### Constraint-based causal discovery

**Constraint-based**: use statistical independences to express constraints over possible causal models.

... but wait, correlation does not imply causation, see XCKD:



True, but it does imply something:

If A and B are correlated, A causes B or B causes A or they share a latent common cause. (Hans Reichenbach)

**Idea**: Under certain assumptions, independences in the data correspond with d-separations in a causal graph.

Sara Magliacane (VU, UvA)

Ancestral Causal Inference