



### **Agenda**

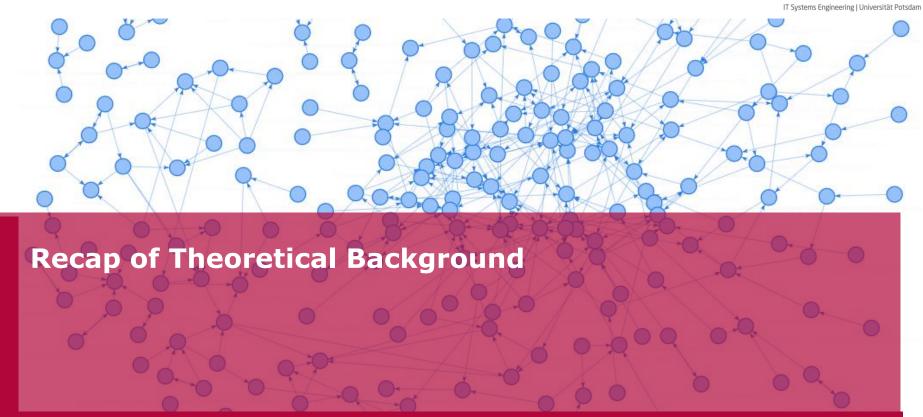
## April 24, 2019



- Recap of Theoretical Background
- Constraint-Based Causal Structure Learning
  - 1. Introduction
  - Constraint-Based Causal Structure Learning
  - 3. PC Algorithm
  - 4. PC Algorithm in the Cooling House Example
  - 5. Extensions of the PC Algorithm
  - 6. Excursion: Other Causal Structure Learning Concepts
  - Causal Inference in Application
  - Outlook: Group Work on Research Topics

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

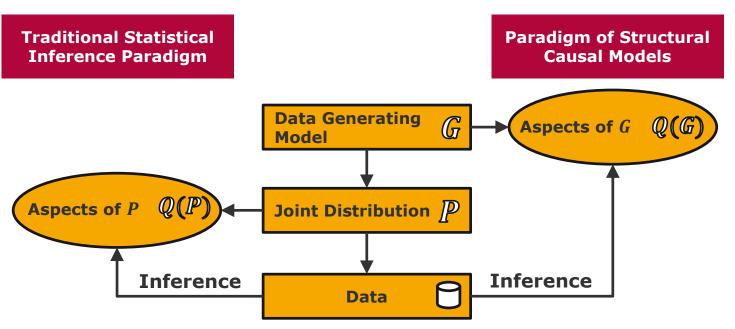




# **Recap of Theoretical Background**

Causal Inference in a Nutshell





E.g., what is the sailors' probability of recovery when **we see** a treatment with lemons?

Q(P) = P(recovery|lemons)

E.g., what is the sailors' probability of recovery if **we do** treat them with lemons?

Q(G) = P(recovery|do(lemons))

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

# **Recap of Theoretical Background**

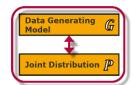
Causal Graphical Models



- Causal Structures formalized by *DAG* (directed acyclic graph) G with random variables  $V_1, ..., V_n$  as vertices.
- Causal Sufficiency, Causal Faithfulness and Global Markov Condition imply  $(X \perp Y \mid Z)_G \Leftrightarrow (X \perp Y \mid Z)_P$ .
- Local Markov Condition states that the density  $p(v_1, ..., v_n)$  then factorizes into

$$p(v_1, \dots, v_n) = \prod_{i=1}^n p(v_i | Pa(v_i)).$$

• Causal conditional  $p(v_i|Pa(v_i))$  represent causal mechanisms.



Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

# Recap of Theoretical Background



- *Null Hypothesis*  $H_0$  is the claim that is initially assumed to be true
- Alternative Hypothesis  $H_1$  is a claim that contradicts the  $H_0$
- How to test a hypothesis?

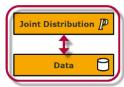
Statistical Inference

- Approximate T under  $H_0$  by a known distribution
- Different distributions yield to different tests, e.g., T-test,  $\chi^2$ -test, etc.
- Derive rejection criteria for  $H_0$ 

  - c-value: reject  $H_0$  if  $T(x_n) > c$  for a  $c \in \mathbb{R}$  p-value: reject  $H_0$  if  $P_{H_0}(T(X) > T(x)) < \alpha$  are equivalent
- (Conditional) Independence Test

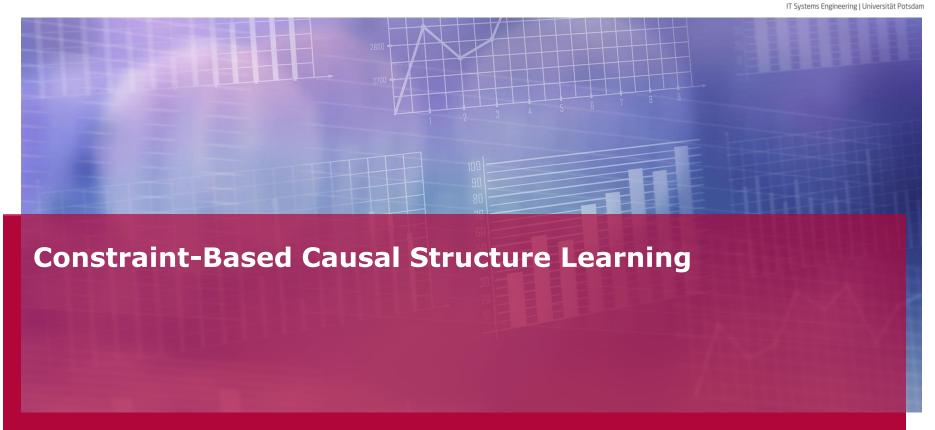
Distribution of  $V_1, ..., V_N \Rightarrow$  dependence measures  $T(V_i, V_i, S) \Rightarrow$  test  $H_0: t = 0$ 

Allows for constraint-based causal structure learning



Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

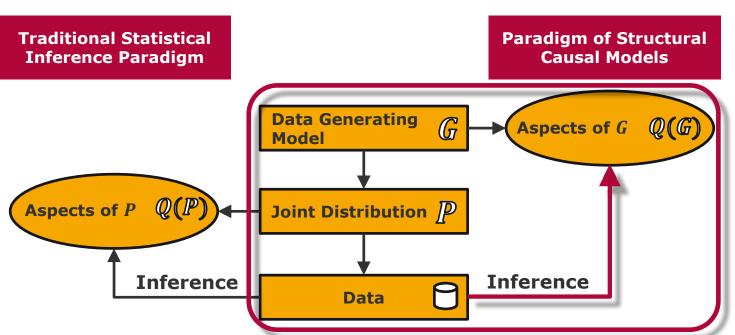




### 1. Introduction

# The Concept





E.g., what is the sailors' probability of recovery when **we see** a treatment with lemons?

Q(P) = P(recovery|lemons)

E.g., what is the sailors' probability of recovery if **we do** treat them with lemons?

Q(G) = P(recovery|do(lemons))

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

### 1. Introduction

Recap: Basis of Causal Structure Learning (Pearl et al.)



### Assumptions:

- Causal Sufficiency
- Global Markov Condition
- Causal Faithfulness

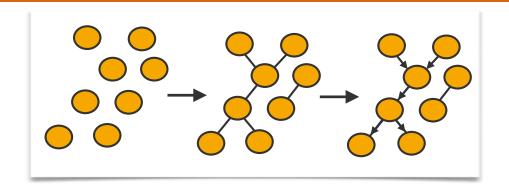
### Causal Structure Learning:

- Accept only those DAG's G as causal hypothesis for which  $(X \perp Y \mid Z)_G \Leftrightarrow (X \perp Y \mid Z)_P$ .
- Identifies causal DAG up to Markov equivalence class
   (DAGs that imply the same conditional independencies)
- The Markov equivalence class of a DAG G includes all DAGs G' that have the same  $skeleton\ C$  and the same v-structures
- Markov equivalence class of the true DAG G that can be uniquely described by a completed partially directed acyclic graph (CPDAG)

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

# **2. Constraint-Based Causal Structure Learning** Algorithmic Construction (I/II)





#### Idea:

- Construct skeleton C
- 2. Find *v*-structures
- 3. Direct further edges that follow from
  - Graph is acyclic
  - $\Box$  All v-structures have been found in 2

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

Slide 10

 $\rightarrow$  IC algorithm by Verma and Pearl (1990) to reconstruct CPDAG G from P

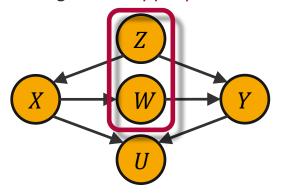
# 2. Constraint-Based Causal Structure Learning Algorithmic Construction (II/II)



#### **Theorem**

Assume Markov condition and faithfulness holds. Then X and Y are linked by an edge if and only if there is no set S(X,Y) such that  $(X \perp Y | S(X,Y))_{P}$ .

 I.e., dependence mediated by other variables can be screened off by conditioning on an appropriate set



- $X \perp Y \mid \{Z, W\}$
- But not:
  - $X \perp Y \mid U$
  - $X \perp Y \mid \{Z, W, U\}$

...but not by conditioning on all other variables!

• S(X,Y) is called separation set of X and Y

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

### The Idea



### **Question:**

How to find the appropriate separation sets  $S(V_i, V_i)$  for all variables  $V_i$  and  $V_i$ ?

- Check  $V_i \perp V_j \mid S(V_i, V_j)$  for all possible separation sets  $S(V_i, V_j) \subseteq V \setminus \{V_i, V_j\}$ 
  - Computationally infeasible for large V
- Efficient construction of the skeleton C

Iteration over size of the separation sets *S*:

- **1.** Remove all edges X Y with  $X \perp Y$
- 2. Remove all edges X Y for which there is an adjacent  $Z \neq Y$  of X with  $X \perp Y \mid Z$
- 3. Remove all edges X Y for which there are two adjacent  $Z_1, Z_2 \neq Y$  of X with  $X \perp Y \mid \{Z_1, Z_2\}$
- 4. ...

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

Slide 12

 $\rightarrow$  PC algorithm by Spirtes et al. (1993) to reconstruct CPDAG G from P

# Skeleton Discovery: Pseudocode



#### Algorithm 1 The PCpop-algorithm

- 1: INPUT: Vertex Set V, Conditional Independence Information
- 2: **OUTPUT:** Estimated skeleton C, separation sets S (only needed when directing the skeleton afterwards)
- 3: Form the complete undirected graph  $\tilde{C}$  on the vertex set V.

```
4: \ell = -1; C = \tilde{C}
```

5: repeat

$$\ell = \ell + 1$$

7: repeat

8: Select a (new) ordered pair of nodes i, j that are adjacent in C such that  $|adj(C, i) \setminus \{j\}| \ge \ell$ 

9: repeat

10: Choose (new)  $\mathbf{k} \subseteq adj(C,i) \setminus \{j\}$  with  $|\mathbf{k}| = \ell$ .

if i and j are conditionally independent given k then

12: Delete edge i, j

13: Denote this new graph by C

14: Save **k** in S(i, j) and S(j, i)

15: end if

16: **until** edge i, j is deleted or all  $\mathbf{k} \subseteq adj(C, i) \setminus \{j\}$  with  $|\mathbf{k}| = \ell$  have been chosen

17: **until** all ordered pairs of adjacent variables i and j such that  $|adj(C,i) \setminus \{j\}| \ge \ell$  and  $k \subseteq adj(C,i) \setminus \{j\}$  with  $|\mathbf{k}| = \ell$  have been tested for conditional independence

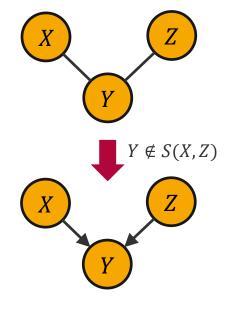
18: **until** for each ordered pair of adjacent nodes  $i, j: |adj(C, i) \setminus \{j\}| < \ell$ .

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

# Edge Orientation: *v*-Structures



- Assume the skeleton is given by:
  - □ Given X Y Z with X and Z nonadjacent
  - Given S(X,Z) with  $X \perp Z \mid S(X,Z)$
- A priori, there are 4 possible orientations



Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

Slide 14

#### *v*-Structures:

If  $Y \notin S(X,Z)$  then replace X - Y - Z by  $X \to Y \leftarrow Z$ .

Edge Orientation: Rule 1





(Otherwise we get a new v-structure)

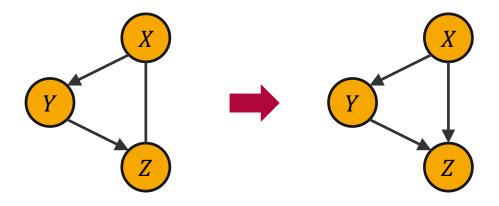
### Rule 1:

Orient Y - Z to  $Y \to Z$  whenever there is an arrow  $X \to Y$  s.t. X and Z are nonadjacent

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

Edge Orientation: Rule 2





(Otherwise we get a cycle)

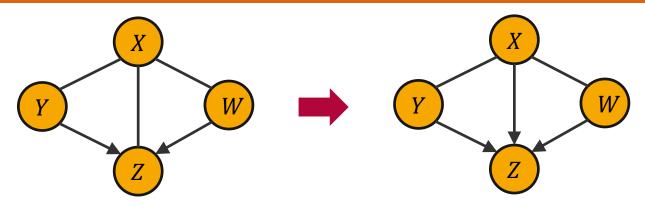
#### Rule 2:

Orient X - Z to  $X \to Z$  whenever there is a chain  $X \to Y \to Z$ 

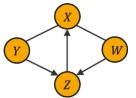
Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

Edge Orientation: Rule 3





(Could not be completed without creating a cycle or a new *v*-structure)



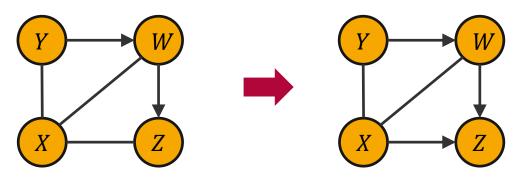
### Rule 3:

Orient X - Z to  $X \to Z$  whenever there are two chains  $X - Y \to Z$  and  $X - W \to Z$  s.t. Y and W are nonadjacent

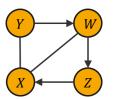
Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

Edge Orientation: Rule 4





(Could not be completed without creating a cycle or a new *v*-structure)



#### Rule 4:

Orient X - Z to  $X \to Z$  whenever there are two chains  $X - Y \to W$  and  $Y \to W \to Z$  s.t. Y and Z are nonadjacent

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

## Edge Orientation: Pseudocode



### Algorithm 2 Extending the skeleton to a CPDAG

**INPUT:** Skeleton  $G_{skel}$ , separation sets S

**OUTPUT:** CPDAG G

for all pairs of nonadjacent variables i, j with common neighbour k do

if  $k \notin S(i, j)$  then

Replace i - k - j in  $G_{skel}$  by  $i \rightarrow k \leftarrow j$ 

end if

end for

In the resulting PDAG, try to orient as many undirected edges as possible by repeated application of the following three rules:

**R1** Orient j - k into  $j \to k$  whenever there is an arrow  $i \to j$  such that i and k are nonadjacent.

**R2** Orient i - j into  $i \rightarrow j$  whenever there is a chain  $i \rightarrow k \rightarrow j$ .

**R3** Orient i - j into  $i \to j$  whenever there are two chains  $i - k \to j$  and  $i - l \to j$  such that k and l are nonadjacent.

**R4** Orient i - j into  $i \to j$  whenever there are two chains  $i - k \to l$  and  $k \to l \to j$  such that k and j are nonadjacent.

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

### A Review



### **Advantages**

- Testing all sets S(X,Y) containing the adjacencies of X is sufficient
- Many edges can be removed already for small sets
- Depending on sparseness, the algorithm only requires independence tests with small conditioning sets S(X,Y)
- Polynomial complexity for graph of N vertices of bounded degree k, i.e.,

$$\frac{N^2(N-1)^{k-1}}{(k-1)!}$$

Asymptotic consistency (under technical assumptions), i.e.,

$$\Pr(\widehat{G} = G) \to 1 \quad (n \to \infty)$$

### **Disadvantages**

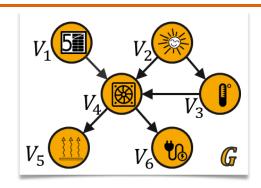
- In the worst case, complexity exponential to number of vertices N
- Assumes causal sufficiency, faithfulness and Markov conditions

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

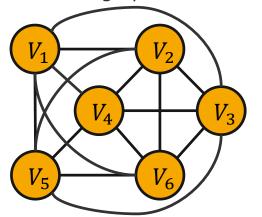
# **4. PC Algorithm in the Cooling House Example**Cooling House Example (I/V)



Assume the true DAG G is given by:



We start with a fully connected undirected graph:

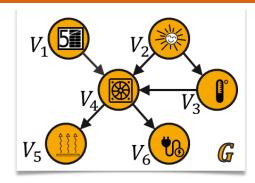


Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

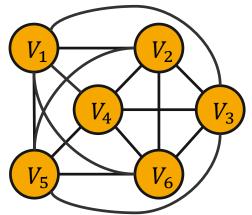
Cooling House Example (II/V)



Assume the true DAG G is given by:



- Remove all edges X Y that are directly independent, i.e.,  $X \perp Y \mid \emptyset$ 
  - $\circ$   $V_1 \perp V_2$
  - $\circ$   $V_1 \perp V_3$

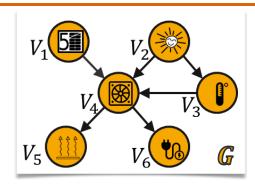


Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

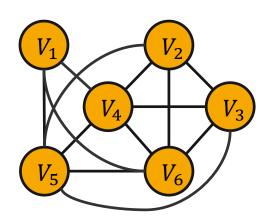
# Cooling House Example (III/V)



Assume the true DAG G is given by:



- Remove all edges X Y having separation sets of size 1, i.e.,  $X \perp Y \mid Z$ 
  - $\circ$   $V_1 \perp V_5 \mid V_4$
  - $\circ$   $V_1 \perp V_6 \mid V_4$
  - $\circ$   $V_2 \perp V_5 \mid V_4$
  - $\circ$   $V_2 \perp V_6 \mid V_4$
  - $\circ$   $V_3 \perp V_5 \mid V_4$
  - $\circ$   $V_3 \perp V_6 \mid V_4$
  - $\circ$   $V_5 \perp V_6 \mid V_4$

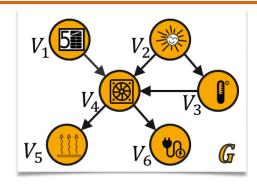


Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

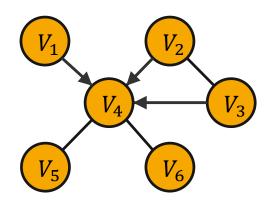
# Cooling House Example (IV/V)



Assume the true DAG G is given by:



- Find v-structures, i.e., orient X Y Z to  $X \to Y \leftarrow Z$  if  $Y \notin S(X,Z)$ 
  - $\circ$   $V_4 \notin S(V_1, V_2)$
  - $\circ V_4 \notin S(V_1, V_3)$

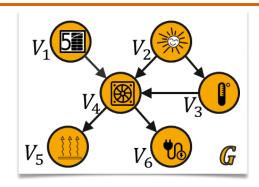


Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

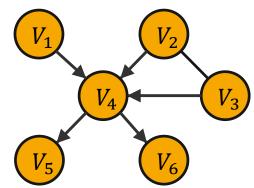
Cooling House Example (V/V)



Assume the true DAG G is given by:



- Orient further edges (such that no further v-structures arise)
  - $\circ$   $V_1 \rightarrow V_4 V_5$  (Rule 1)
  - $\circ \quad V_1 \to V_4 V_6 \text{ (Rule 1)}$



• No further edges can be oriented, i.e.,  $V_2 - V_3$  remain undirected

Causal Inference
Theory and Applications
in Enterprise Computing
Uflacker, Huegle,
Schmidt

## 5. Extensions of the PC Algorithm

# Order Independence (Colombo et al. 2014)



### **PC** algorithm

Order of  $V_1, ..., V_N$  affects estimation of

- 1. Skeleton C
- 2. Separating sets  $S(V_i, V_j)$
- 3. Edge orientation

### **PC-stable algorithm**

For each level l

- □ Compute and store the adjacency set  $a(V_i)$  of all vertices  $V_i$
- $\Box$  Use  $a(V_i)$  for search of separation sets
- Edge deletion longer affects which conditional independencies are checked for other pairs of variables at this level *l*

```
Algorithm 4.1 Step 1 of the PC-stable algorithm (oracle version)
Require: Conditional independence information among all variables in V, and an ordering
    order(V) on the variables
1: Form the complete undirected graph \mathcal{C} on the vertex set \mathbf{V}
 2: Let ℓ = −1:
       for all vertices X_i in C do
         Let a(X_i) = adj(C, X_i)
       end for
          Select a (new) ordered pair of vertices (X_i, X_i) that are adjacent in C and satisfy
          |a(X_i) \setminus \{X_i\}| \ge \ell, using order(V);
         repeat
            Choose a (new) set \mathbf{S} \subseteq a(X_i) \setminus \{X_i\} with |\mathbf{S}| = \ell, using order(V);
11:
            if X_i and X_j are conditionally independent given S then
13:
               Delete edge X_i - X_j from C;
               Let sepset(X_i, X_i) = \text{sepset}(X_i, X_i) = \mathbf{S};
         until X_i and X_j are no longer adjacent in \mathcal{C} or all \mathbf{S} \subseteq a(X_i) \setminus \{X_j\} with |\mathbf{S}| = \ell
          have been considered
     until all ordered pairs of adjacent vertices (X_i, X_i) in \mathcal{C} with |a(X_i) \setminus \{X_i\}| \geq \ell have
18: until all pairs of adjacent vertices (X_i, X_i) in \mathcal{C} satisfy |a(X_i) \setminus \{X_i\}| \leq \ell
19: return C, sepset.
```

Causal Inference
Theory and Applications
in Enterprise Computing
Uflacker, Huegle,
Schmidt

### 5. Extensions of the PC Algorithm

Parallelization (Le et al. 2016)



### **PC** algorithm

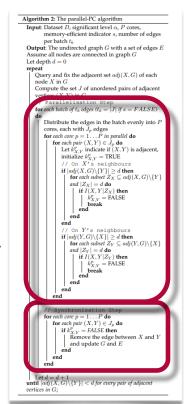
#### Limitations:

- 1. Order-dependent (→*PC-stable*)
- 2. Sequential execution does not utilize modern hardware
- Long runtime hinders its application on high dimensional datasets

### parallelPC algorithm

PC-stable allows for easy parallelization at each level l, i.e.,

- 1. CI tests are distributed evenly among the cores
- 2. Each core performs its own sets of CI tests in parallel with the others
- 3. Synchronize test results into the global skeleton  ${\cal C}$
- ⇒ Efficient in high dimensional datasets and consistent with PC-stable algorithm



Causal Inference
Theory and Applications
in Enterprise Computing

Uflacker, Huegle, Schmidt

## 5. Extensions of the PC Algorithm

Theoretical Extensions (A Selection)



#### Weaker form of faithfulness

- Learn a Markov equivalence class of DAGs under a weaker-than-standard causal faithfulness assumption
- Assumes Adjacency-Faithfulness to justify the step of recovering adjacencies in constraint-based algorithms
- Conservative PC (CPC) by Ramsey et al. (1995)

#### Allow for latent and selection variables

- Learn a Markov equivalence class of DAGs with latent and selection variables
- Follows maximal ancestral graph (MAG) models
- ⇒ Fast causal inference (FCI) by Spirtes et al. (1999)

### Allow for cycles

- Learn Markov equivalence classes of directed (not necessarily acyclic)
   graphs under the assumption of causal sufficiency.
- ⇒ Cyclic causal discovery (CCD) by Richardson (1996)

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

### 6. Excursion:

# Other Causal Structure Learning Concepts



#### Score-based methods

- "search-and-score approach", i.e.,
  - 1. Assume causal structure G and functional restrictions (e.g., linear relations and independent Gaussian noise)
  - 2. Optimize some score (e.g., likelihood or BIC) given these restrictions
  - 3. Change G and compute new optimal score value
  - 4. Repeat this for many G and return  $G^{opt}$  with the best (optimized) score
- ⇒ E.g., Greedy-Equivalent-Search (GES) by Chickering (2002)

### **Hybrid methods**

- Combines constraint-based and search-and-score methods, i.e.,
  - Constraint-based search to find skeleton
  - 2. Score-based approach to orient edges
- ⇒ E.g., Max-Min Hill-Climbing (MMHC) by Tsamardinos et al. (2006)

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

### References

### Literature



- Pearl, J. (2009). <u>Causal inference in statistics: An overview</u>. Statistics Surveys.
- Pearl, J. (2009). <u>Causality: Models, Reasoning, and Inference</u>. Cambridge University Press.
- Spirtes et al. (2000). Causation, Prediction, and Search. The MIT Press.
- Kalisch et al. (2007). <u>Estimating high-dimensional directed acyclic graphs</u> with the <u>PC-algorithm</u>. Journal of Machine Learning Research.
- Colombo et al. (2014). <u>Order-independent constraint-based causal</u> <u>structure learning</u>. The Journal of Machine Learning Research.
- Le et al. (2016). <u>A fast PC algorithm for high dimensional causal</u> <u>discovery with multi-core PCs</u>. IEEE/ACM transactions on computational biology and bioinformatics.
- Kalisch et al. (2014). <u>Causal structure learning and inference: a selective</u> <u>review</u>. Quality Technology & Quantitative Management

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

### References

## **Implementations**



#### R

- Kalisch et al. (2017), R Package 'pcalq'.
- Le et al. (2015), <u>R Package 'ParallelPC</u>'.
- Scutari (2007), <u>Learning Bayesian Networks with the bnlearn R Package</u>.

### **Python**

Kobayashi (2015), <u>CPDAG Estimation using PC-Algorithm</u>.
 (Note: Unstable version of the PC Algorithm)

#### Other

Carneggie Mellon University, <u>The Tetrad Project</u>

Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt

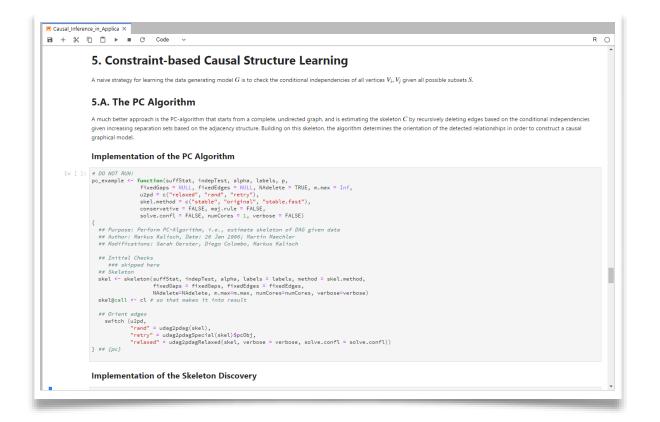




## **Causal Inference in Application**

# Cooling House Example





Causal Inference Theory and Applications in Enterprise Computing Uflacker, Huegle, Schmidt



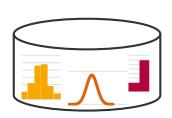


# Outlook: Group Work on Research Topics Overview on Topics



### Data, Distributions, Independence

Work on topics in the application of learnt techniques beyond the examples given in this lecture (e.g., heterogeneous data distributions)



### Causal Structure-Learning

Work on topics in the context of performance improvements of causal structure learning algorithms (e.g., hardware acceleration)

### Applications Scenarios

Work on challenges and opportunities in the application of causal inference techniques on real-world data (e.g., industrial manufacturing)

Causal Inference
Theory and Applications
in Enterprise Computing

Uflacker, Huegle, Schmidt

# Outlook: Group Work on Research Topics Topic Application



### How to work on a topic?

- Understand theoretic basis and your selected topic
- 2. Work on implementation
- 3. Present results
- 4. Write scientific report in a review process

### How to apply for a topic?

- Build groups of around three students
- Send prioritized list of top 3 topics to <u>Johannes Huegle</u> until:
   Fri April 26, 11.59 PM
- Topic Assignments: Tue April 30, 9:00 AM

Causal Inference
Theory and Applications
in Enterprise Computing

Uflacker, Huegle, Schmidt



Thank you for your attention!