HPI Hasso Plattner Institut
Digital Engineering · Universität Potsdam

Causal Inference
Theory and Applications in Enterprise Computing

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May 19, 2020

Agenda

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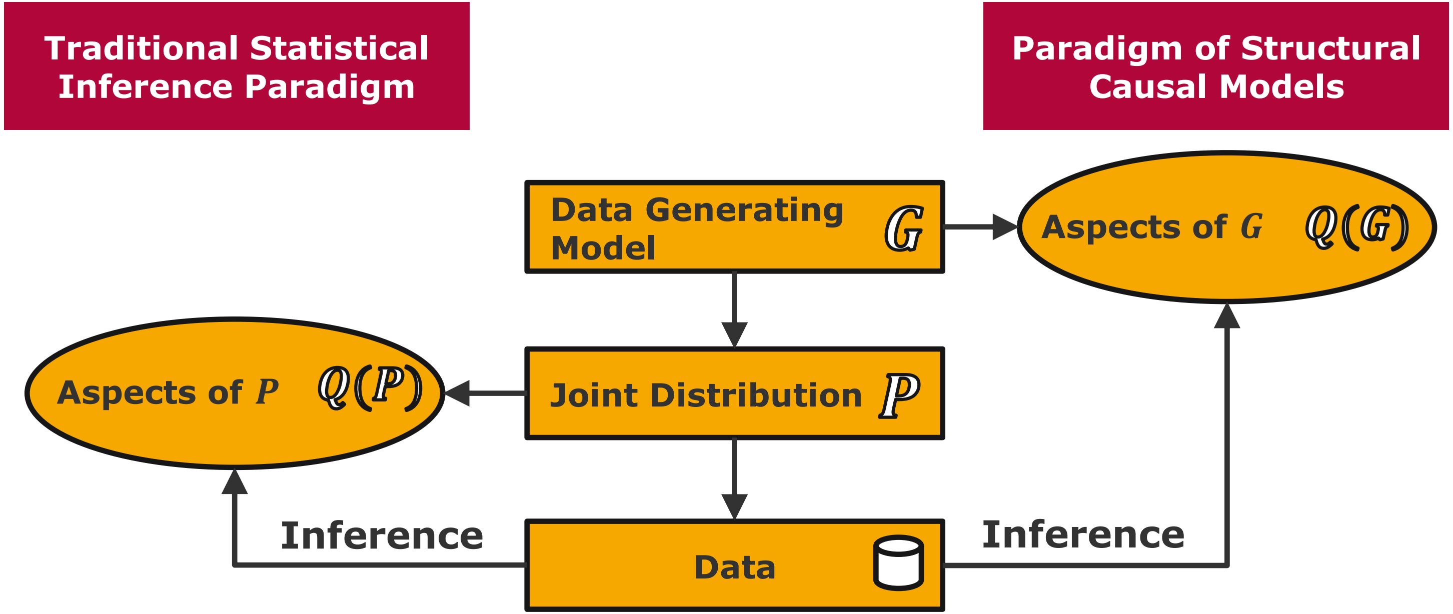
- **Embedding: Causal Inference in a Nutshell**
- **Introduction to Causal Structure Learning**

Embedding: Causal Inference in a Nutshell

Embedding: Causal Inference in a Nutshell
Concept


Traditional Statistical Inference Paradigm
Paradigm of Structural Causal Models
Data Generating Model G
Aspects of G $Q(G)$
Joint Distribution P
Aspects of P $Q(P)$
Inference
Data
Inference

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

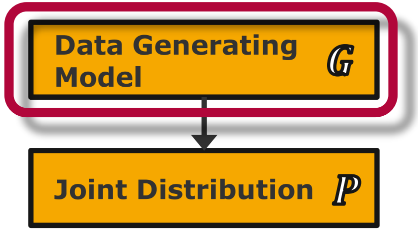
$$Q(P) = P(recovery|lemons)$$

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

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

Recap: Causal Inference in a Nutshell

Causal Graphical Models



Data Generating Model $\mathbb{G}$
Joint Distribution $\mathbb{P}$

Causal Graphical Model

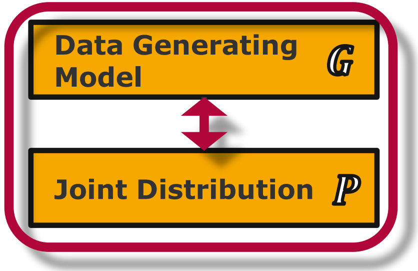
- *Directed Acyclic Graph (DAG)* $G = (V, E)$
  - □ *Vertices* $V_1, \dots, V_n$
  - □ *Directed edges* $E = (V_i, V_j)$, i.e., $V_i \rightarrow V_j$
  - □ *No cycles*
- *Directed Edges* encode direct causes via
  - □ $V_j = f_j\left(\mathrm{Pa}\left(\mathrm{V_j}\right), \mathrm{N_j}\right)$ with independent noise $N_1, \dots, N_n$

Causal Sufficiency

- All relevant variables are included in the DAG G

Recap: Causal Inference in a Nutshell

Connecting G and P



Data Generating Model $\mathbb{G}$
Joint Distribution $\mathbb{P}$

$$(X \perp\!\!\!\perp Y|Z)_G \Rightarrow (X \perp\!\!\!\perp Y|Z)_P$$

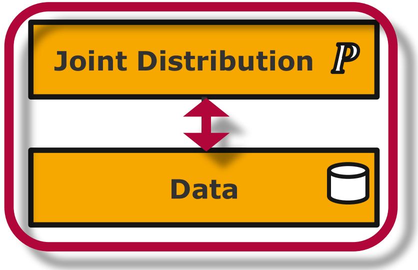
- Key Postulate: *(Local) Markov Condition*
- Essential mathematical concept: *d-Separation*
  - Idea: *Blocking* of paths
  - Implication: *Global Markov Condition*

$$(X \perp\!\!\!\perp Y|Z)_G \Leftarrow (X \perp\!\!\!\perp Y|Z)_P$$

- Key Postulate: *Causal Faithfulness*

Recap: Causal Inference in a Nutshell

Connecting P and 🛢

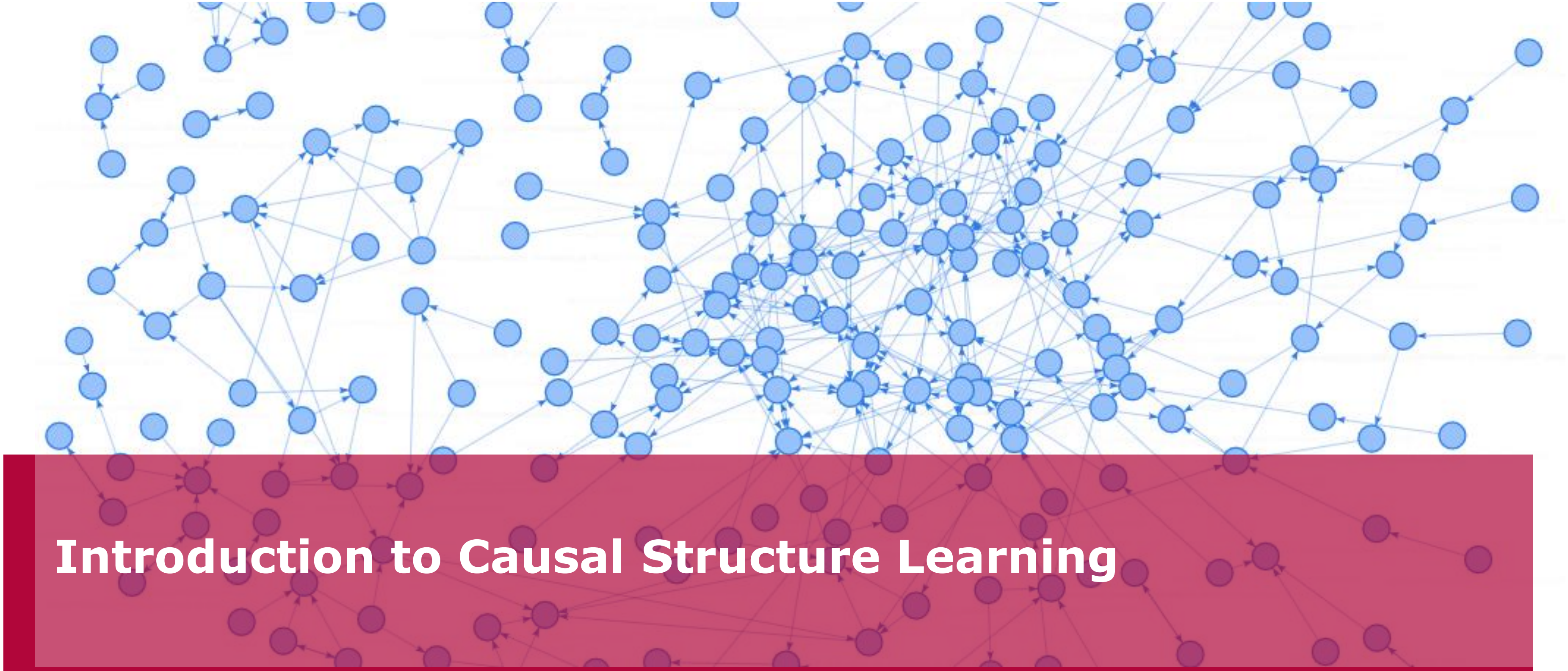


Statistical Inference

- Essential concept: *Point estimator $\hat{\Theta}$*
  - □ *Statistic* $g(X_1,\dots,X_n)$ of *random samples* $X_1,\dots,X_n$ to estimate *population parameter Θ*
- Inference: *Statistical Hypothesis Test*
  - □ *Null Hypothesis H_0*, claim on a population's property initially assumed to be true
  - □ *Alternative Hypothesis H_1*, a claim that contradicts H_0
  - □ Rejection criteria for H_0: c-value $T(x) > c$ or equivalently p-value $P_{H_0}\big(T(X) > T(x)\big) < \alpha$

$$(\boldsymbol{X} \perp\!\!\!\perp \boldsymbol{Y} | \boldsymbol{Z})_{\boldsymbol{P}} \Leftarrow \text{🛢}$$

- Key idea: *Conditional Independence Test*
  - □ Distribution of $\boldsymbol{V} = \{V_1,\dots,V_N\} \Rightarrow$ dependence measure $T(V_i,V_j,\boldsymbol{S})$ ⇒ hypothesis $H_0\!: t = 0$

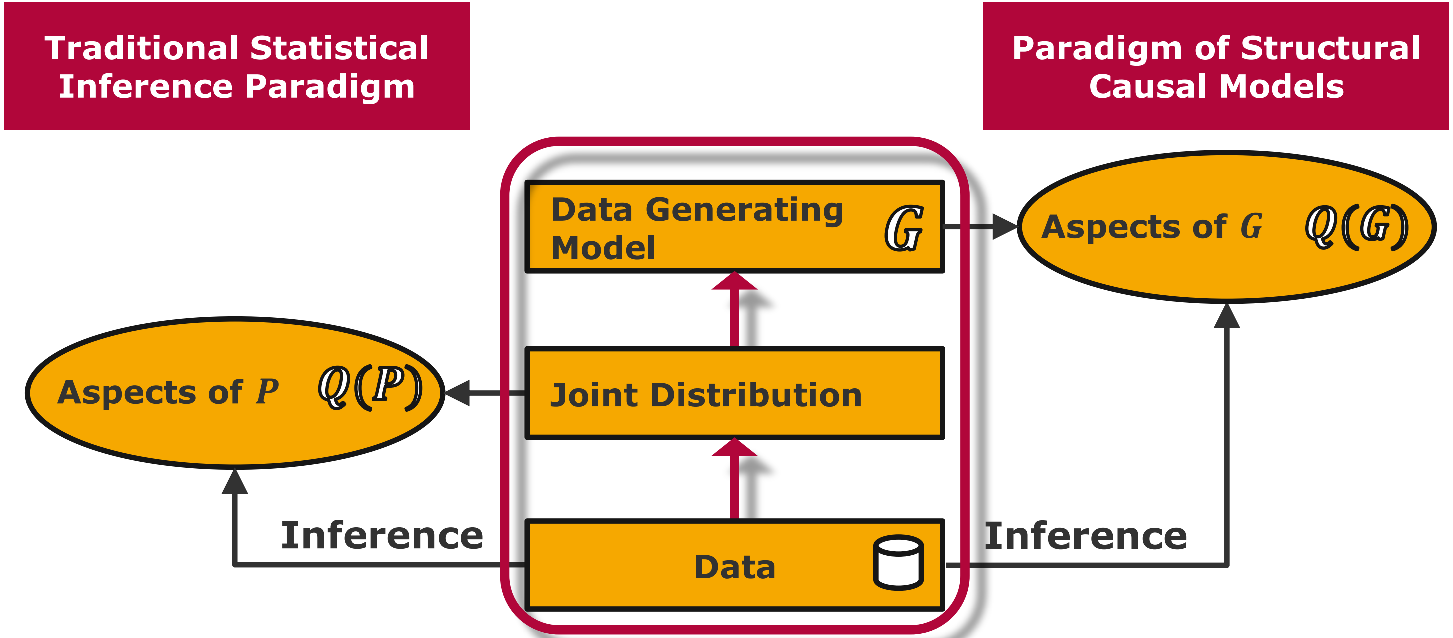


Introduction to Causal Structure Learning

Introduction to Causal Structure Learning
Content

1. Introduction
2. Constraint-Based Causal Structure Learning
   - Foundation
   - Algorithmic Construction
3. PC Algorithm
   - The Idea
   - Skeleton Discovery
   - Edge Orientation
   - Review
   - Cooling House Example
   - Extensions of the PC Algorithm
4. Other Methods of Causal Structure Learning

1. Introduction
Causal Inference in a Nutshell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$$Q(G) = P(recovery|do(lemons))$$

1. Introduction

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

- **Assumptions:**
  - □ *Causal Sufficiency*
  - □ *Markov Condition*
  - □ *Causal Faithfulness*

- **Causal Structure Learning:**
  - □ Accept only those DAG’s G as causal hypothesis for which
    $$(X \perp\!\!\!\perp Y | \, Z)_G \Leftrightarrow (X \perp\!\!\!\perp Y | \, Z)_P.$$
  - □ 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)*

2. Constraint-Based Causal Structure Learning

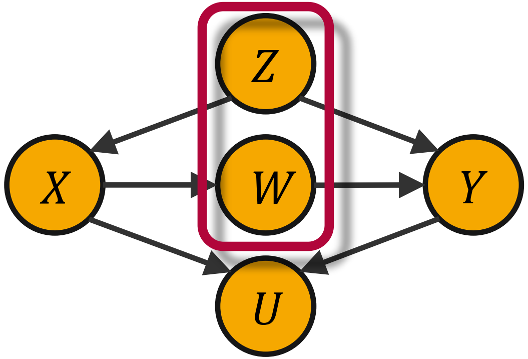
Basis

Theorem

Assume Markov condition and faithfulness holds. Then V_i and V_j are linked by an edge if and only if there is no set $S(V_i, V_j)$ such that

$$\left(V_i \perp\!\!\!\perp V_j \middle| S(V_i, V_j)\right)_P.$$

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

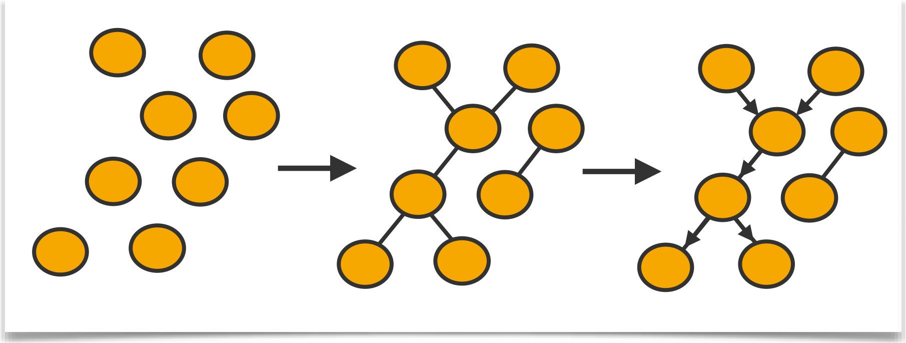


- $X \perp\!\!\!\perp Y | \{Z, W\}$
- But:
  - $X \not\perp\!\!\!\perp Y | U$
  - $X \not\perp\!\!\!\perp Y | \{Z, W, U\}$

…but not by conditioning on all other variables!

- $S(V_i, V_j)$ is called *separation set of V_i and V_j*

2. Constraint-Based Causal Structure Learning
Algorithmic Construction



Idea:

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

➡ *IC algorithm* by Verma and Pearl (1990) to reconstruct CPDAG G from P

3. PC Algorithm
The Idea

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

- Check $V_\mathrm{i} \perp\!\!\!\perp V_j \mid S(V_i, V_j)$ for all possible separation sets $S(V_i, V_j) \subseteq \boldsymbol{V} \setminus \{V_i, V_j\}$
  - □ Computationally infeasible for large V

- Efficient construction of the skeleton C
  - □ Iteration over size of the separation sets S:
    1. Remove all edges $V_i - V_j$ with $V_i \perp\!\!\!\perp V_j$
    2. Remove all edges $V_i - V_j$

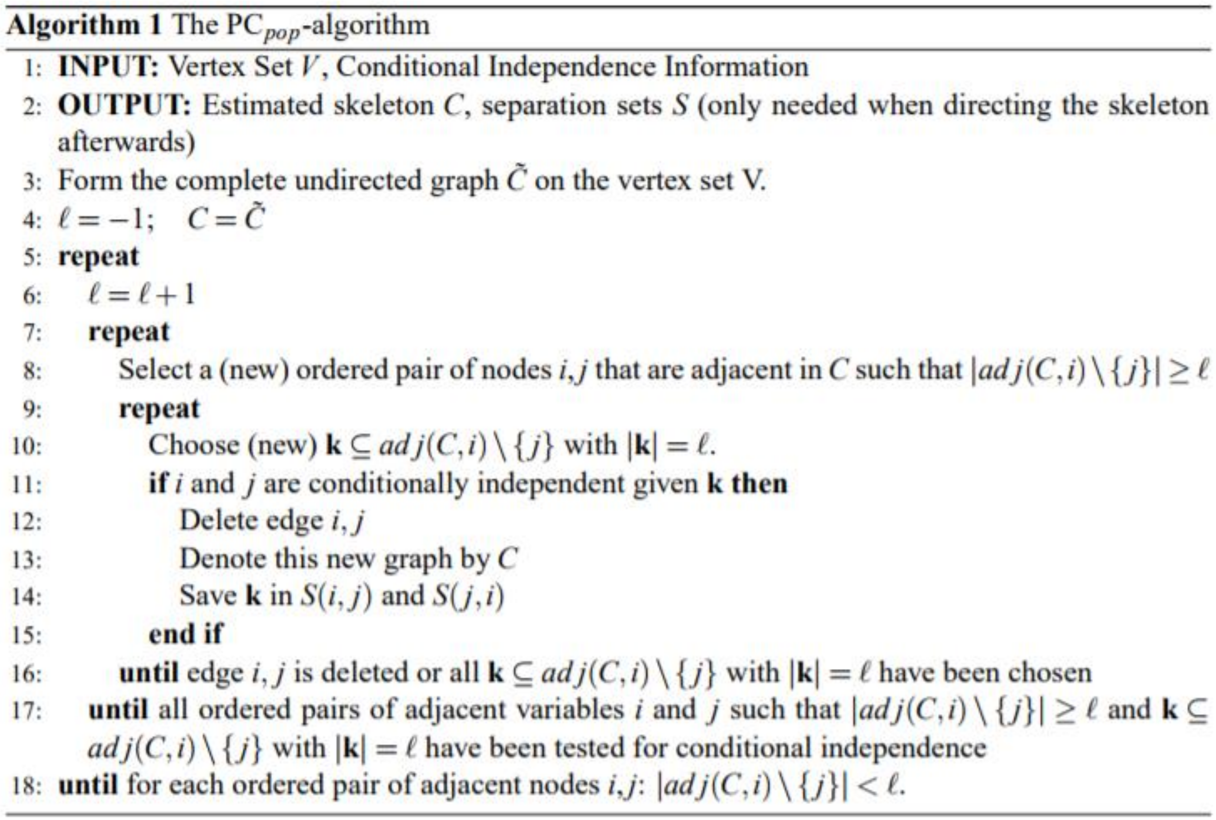
       for which there is an adjacent $V_k \neq V_j$ of V_i with $V_i \perp\!\!\!\perp V_j \mid V_k$
    3. Remove all edges $\mathrm{V_i} - V_j$

       for which there are two adjacent $\mathrm{V_k}, V_\mathrm{l} \neq V_j$ of V_i with $\mathrm{V_i} \perp\!\!\!\perp V_j \mid \{V_k, V_l\}$
    4. …

➡ *PC algorithm* by Spirtes et al. (1993) to reconstruct CPDAG G from P

3. PC Algorithm

Skeleton Discovery: Pseudocode



Algorithm 1 The PC$_{pop}$-algorithm

```
INPUT: Vertex Set $V$, Conditional Independence Information
OUTPUT: Estimated skeleton $C$, separation sets $S$ (only needed when directing the skeleton afterwards)
Form the complete undirected graph $\tilde{C}$ on the vertex set V.
$\ell = -1$;   $C = \tilde{C}$
repeat
    $\ell = \ell + 1$
    repeat
        Select a (new) ordered pair of nodes $i, j$ that are adjacent in $C$ such that $|adj(C,i) \setminus \{j\}| \geq \ell$
        repeat
            Choose (new) $\mathbf{k} \subseteq adj(C,i) \setminus \{j\}$ with $|\mathbf{k}| = \ell$.
            if $i$ and $j$ are conditionally independent given $\mathbf{k}$ then
                Delete edge $i, j$
                Denote this new graph by $C$
                Save $\mathbf{k}$ in $S(i,j)$ and $S(j,i)$
            end if
        until edge $i, j$ is deleted or all $\mathbf{k} \subseteq adj(C,i) \setminus \{j\}$ with $|\mathbf{k}| = \ell$ have been chosen
    until all ordered pairs of adjacent variables $i$ and $j$ such that $|adj(C,i) \setminus \{j\}| \geq \ell$ and $\mathbf{k} \subseteq$
    $adj(C,i) \setminus \{j\}$ with $|\mathbf{k}| = \ell$ have been tested for conditional independence
until for each ordered pair of adjacent nodes $i, j$: $|adj(C,i) \setminus \{j\}| < \ell$.
```

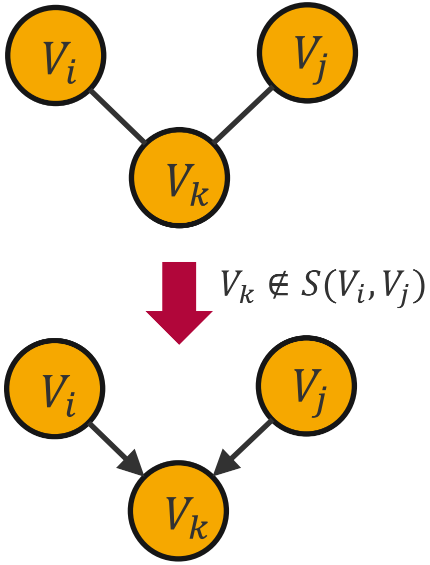
3. PC Algorithm
Edge Orientation: v-Structures

- Assume the skeleton is given by:
  - Given $V_i - V_k - V_j$ with V_i and V_j nonadjacent
  - Given $S(V_i, V_j)$ with $V_i \perp\!\!\!\perp V_j \mid S(V_i, V_j)$

- A priori, there are 4 possible orientations

$$\left.\begin{array}{l} \square\ V_i \to V_k \to V_j \\ \square\ V_i \leftarrow V_k \to V_j \\ \square\ V_i \leftarrow V_k \leftarrow V_j \end{array}\right\} V_k \in S(V_i, V_j)$$

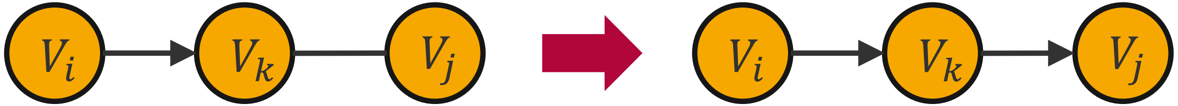
$$\left.\begin{array}{l} \square\ V_i \to V_k \leftarrow V_j \end{array}\right\} V_k \notin S(V_i, V_j)$$



v-Structures:
If $\mathrm{V_k} \notin S(V_i, V_j)$ then replace $\mathrm{V_i} - V_k - V_j$ by $\mathrm{V_i} \to V_k \leftarrow V_j$.

3. PC Algorithm

Edge Orientation: Rule 1

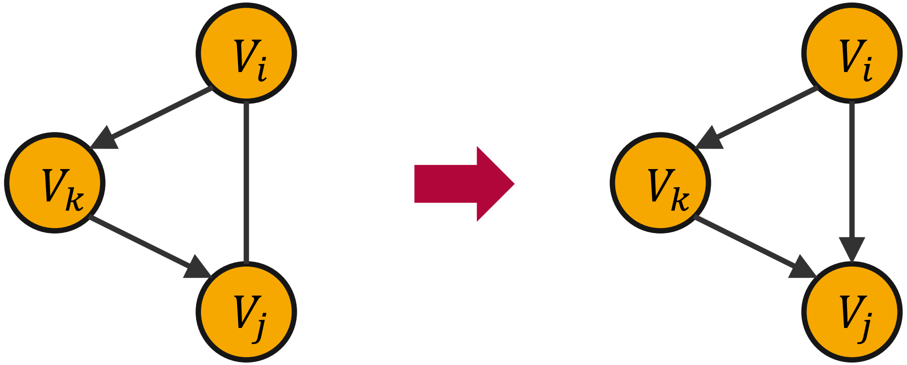


(Otherwise we get a new v-structure)

Rule 1:
Orient $V_k - V_j$ to $V_k \rightarrow V_j$ whenever
there is an arrow $V_i \rightarrow V_k$ s.t. V_k and V_j are nonadjacent

3. PC Algorithm

Edge Orientation: Rule 2

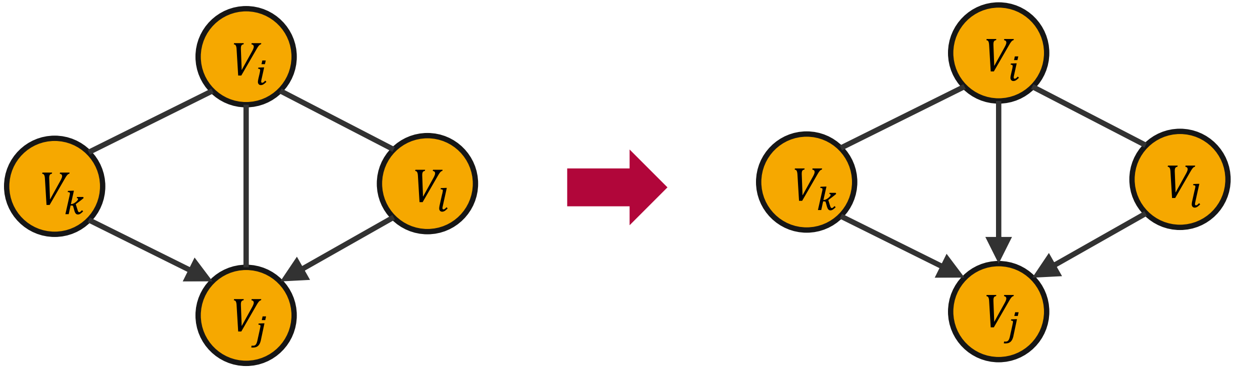


(Otherwise we get a cycle)

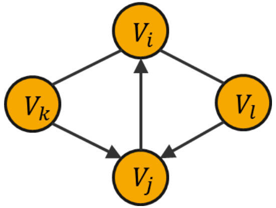
Rule 2:
Orient $V_i - V_j$ to $V_i \rightarrow V_j$ whenever
there is a chain $V_i \rightarrow V_k \rightarrow V_j$

3. PC Algorithm

Edge Orientation: Rule 3



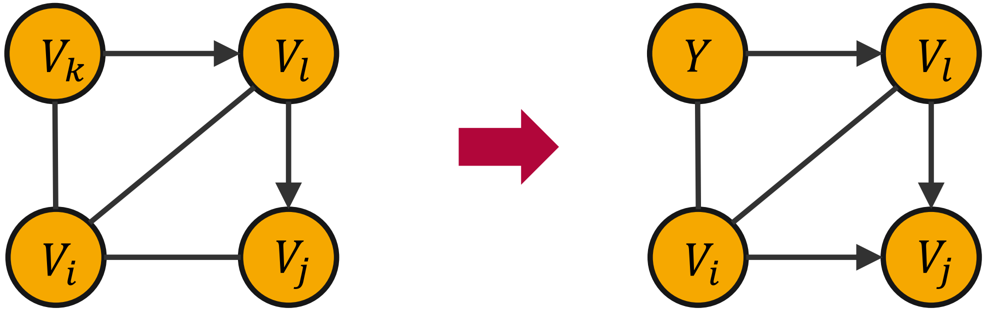
(Could not be completed without creating a cycle or a new v-structure)



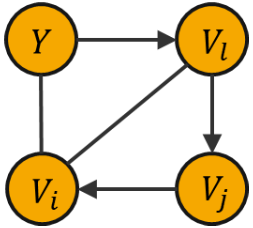
Rule 3:
Orient $V_i - V_j$ to $V_i \rightarrow V_j$ whenever
there are two chains $V_i - V_k \rightarrow V_j$, $V_i - V_l \rightarrow V_j$ s.t. V_k and V_l are nonadjacent

3. PC Algorithm

Edge Orientation: Rule 4

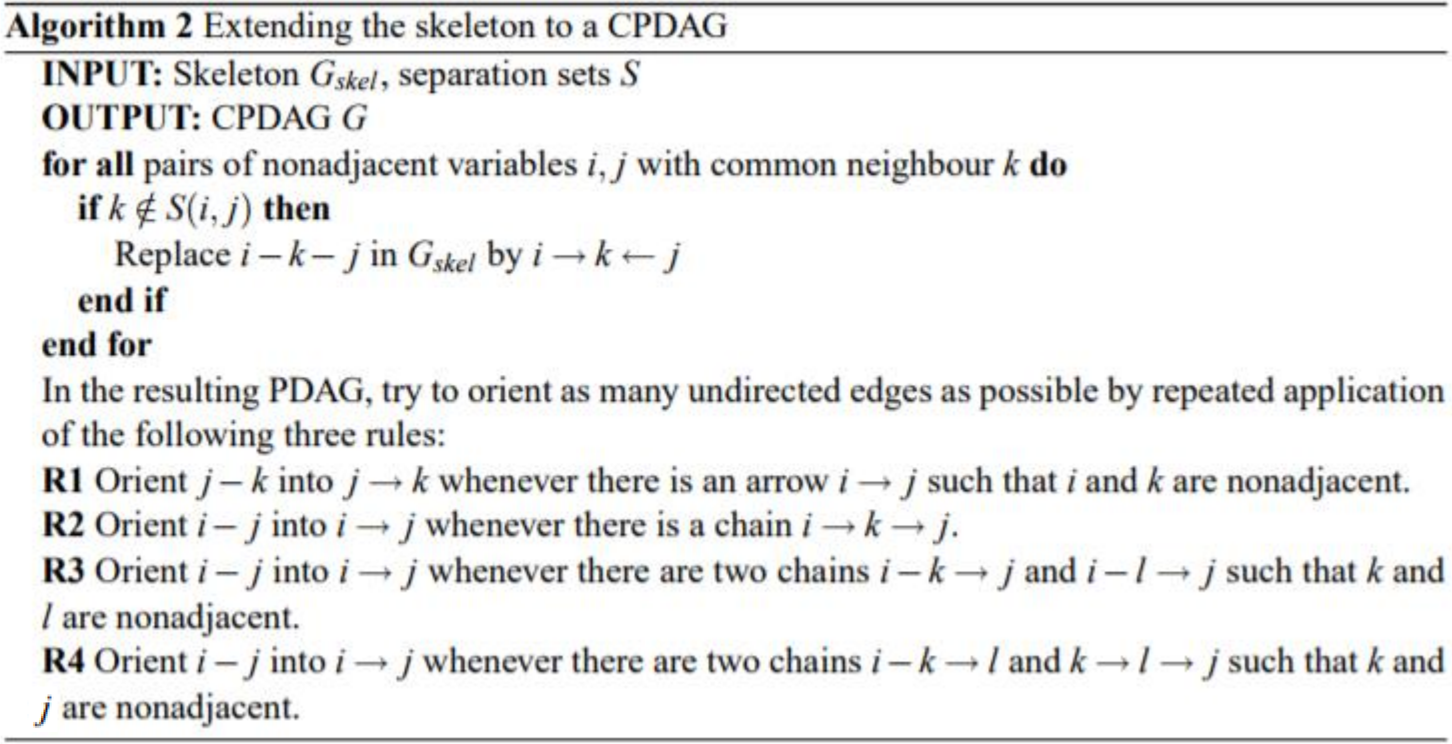


(Could not be completed without creating a cycle or a new v-structure)



Rule 4:
Orient $V_i - V_j$ to $V_i \rightarrow V_j$ whenever
there are two chains $V_i - V_k \rightarrow V_l$, $V_k \rightarrow V_l \rightarrow V_j$ s.t. V_k and V_l are nonadjacent

3. PC Algorithm
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 $j \rightarrow k$ whenever there is an arrow $i \rightarrow j$ 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 $i \rightarrow j$ whenever there are two chains $i - k \rightarrow j$ and $i - l \rightarrow j$ such that $k$ and
$l$ are nonadjacent.
R4 Orient $i - j$ into $i \rightarrow j$ whenever there are two chains $i - k \rightarrow l$ and $k \rightarrow l \rightarrow j$ such that $k$ and
$j$ are nonadjacent.
```

3. PC Algorithm
A Review

Advantages

- Testing all sets $S(X, Y)$ containing the adjacencies of X is sufficient
- Many edges can be removed already for small separation 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.,

$$\Pr\left(\hat{G} = G\right) \to 1 \quad (n \to \infty)$$

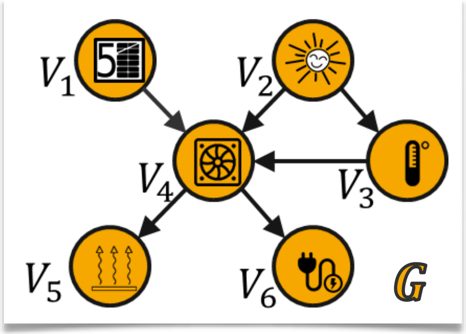
Disadvantages

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

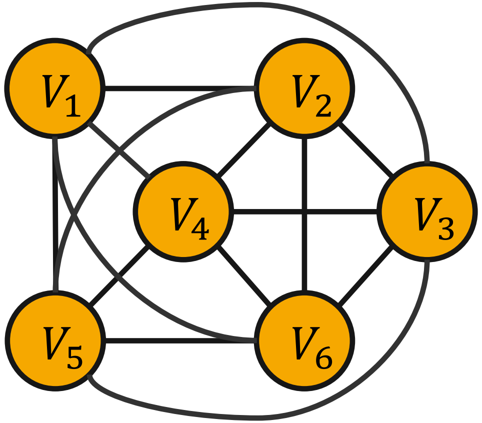
4. PC Algorithm in the Cooling House Example

Cooling House Example (I/V)

- Assume the true DAG G is given by:



- We start with a fully connected undirected graph:



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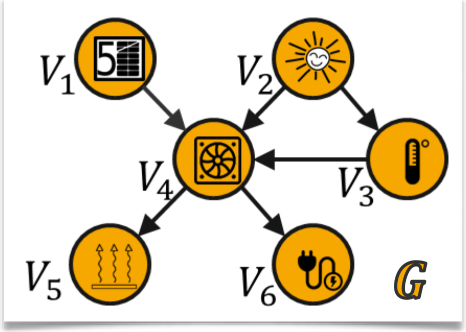
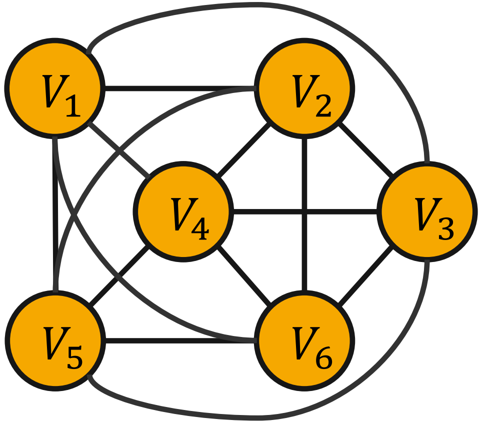
4. PC Algorithm in Application
Cooling House Example (II/V)

- Assume the true DAG G is given by:



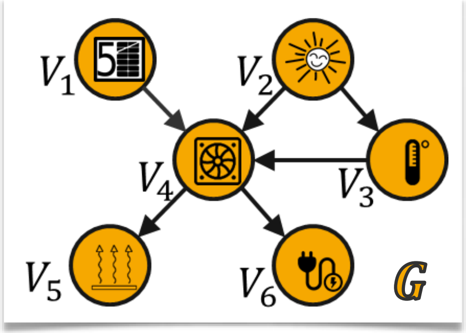
- Remove all edges $V_i - V_j$ that are directly independent, i.e., $V_i \perp\!\!\!\perp V_j \mid \emptyset$
  - $V_1 \perp\!\!\!\perp V_2$
  - $V_1 \perp\!\!\!\perp V_3$



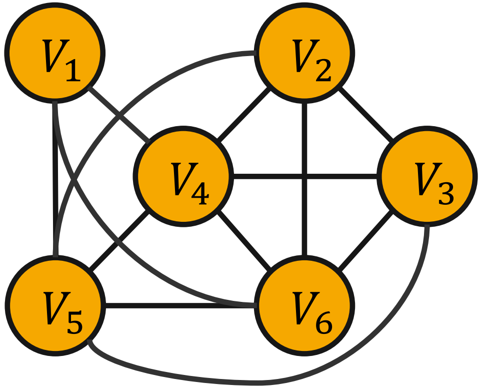
4. PC Algorithm in Application

Cooling House Example (III/V)

- Assume the true DAG G is given by:



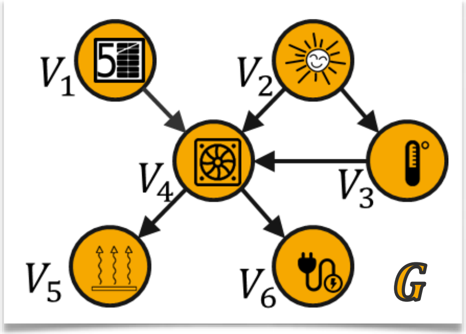
- Remove all edges $V_i - V_j$ having separation sets of size 1, i.e., $V_i \perp\!\!\!\perp V_j \mid V_k$
  - $V_1 \perp\!\!\!\perp V_5 \mid V_4$
  - $V_1 \perp\!\!\!\perp V_6 \mid V_4$
  - $V_2 \perp\!\!\!\perp V_5 \mid V_4$
  - $V_2 \perp\!\!\!\perp V_6 \mid V_4$
  - $V_3 \perp\!\!\!\perp V_5 \mid V_4$
  - $V_3 \perp\!\!\!\perp V_6 \mid V_4$
  - $V_5 \perp\!\!\!\perp V_6 \mid V_4$



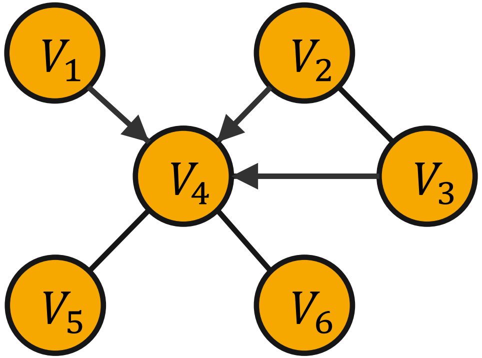
4. PC Algorithm in Application

Cooling House Example (IV/V)

- Assume the true DAG G is given by:

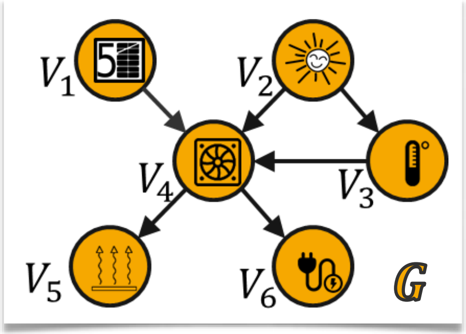


- Find v-structures, i.e., orient $V_i - V_k - V_j$ to $V_i \rightarrow V_k \leftarrow V_j$ if $V_k \notin S(V_i, V_j)$
  - $V_4 \notin S(V_1, V_2)$
  - $V_4 \notin S(V_1, V_3)$

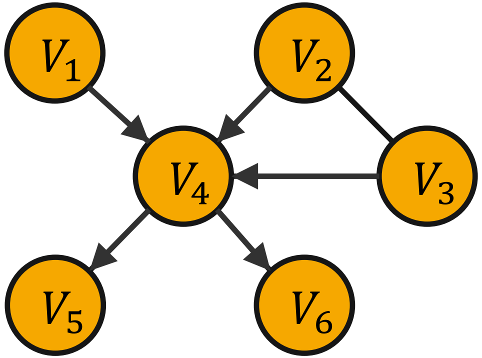


4. PC Algorithm in Application
Cooling House Example (V/V)

- Assume the true DAG G is given by:



- Orient further edges (such that no further v-structures arise)
  - $V_1 \rightarrow V_4 - V_5$ *(Rule 1)*
  - $V_1 \rightarrow V_4 - V_6$ *(Rule 1)*



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

5. Extensions of the PC Algorithm
Order Independence (Colombo et al. 2014)

PC algorithm

Order of $\boldsymbol{V} = \{V_1, \dots, V_N\}$ affects estimation of

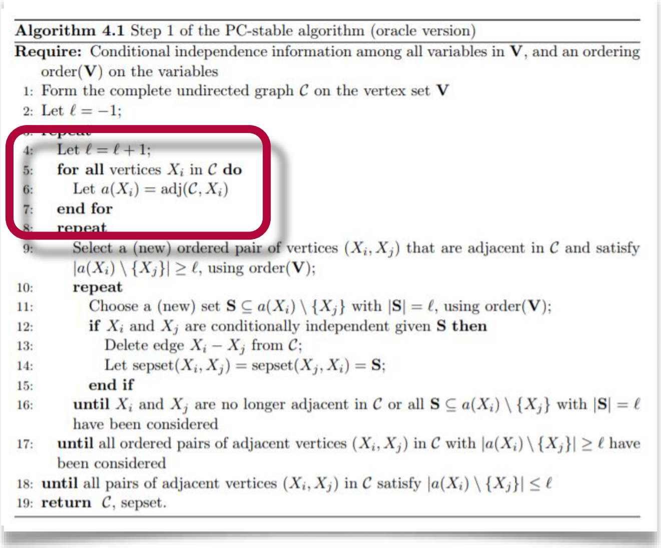
1. Skeleton C
2. Separating sets $S(V_i, V_j)$
3. Edge orientation

PC-stable algorithm

For each level l

- □ Compute and store the adjacency set $a(V_i)$ of all vertices V_i
- □ 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 $\mathbf{V}$, and an ordering
    order($\mathbf{V}$) on the variables
Form the complete undirected graph $\mathcal{C}$ on the vertex set $\mathbf{V}$
Let $\ell = -1$;
repeat
    Let $\ell = \ell + 1$;
    for all vertices $X_i$ in $\mathcal{C}$ do
        Let $a(X_i) = \text{adj}(\mathcal{C}, X_i)$
    end for
    repeat
        Select a (new) ordered pair of vertices $(X_i, X_j)$ that are adjacent in $\mathcal{C}$ and satisfy
        $|a(X_i) \setminus \{X_j\}| \geq \ell$, using order($\mathbf{V}$);
        repeat
            Choose a (new) set $\mathbf{S} \subseteq a(X_i) \setminus \{X_j\}$ with $|\mathbf{S}| = \ell$, using order($\mathbf{V}$);
            if $X_i$ and $X_j$ are conditionally independent given $\mathbf{S}$ then
                Delete edge $X_i - X_j$ from $\mathcal{C}$;
                Let sepset$(X_i, X_j)$ = sepset$(X_j, X_i) = \mathbf{S}$;
            end if
        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 $(X_i, X_j)$ in $\mathcal{C}$ with $|a(X_i) \setminus \{X_j\}| \geq \ell$ have
    been considered
until all pairs of adjacent vertices $(X_i, X_j)$ in $\mathcal{C}$ satisfy $|a(X_i) \setminus \{X_j\}| \leq \ell$
return $\mathcal{C}$, sepset.
```

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

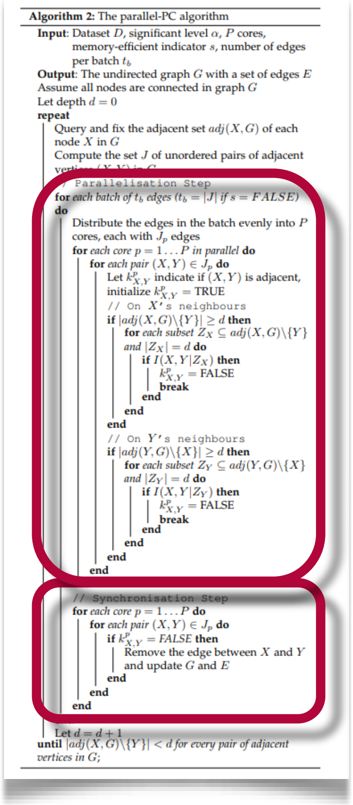
⇨ Long runtime hinders its application on high dimensional datasets

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 C

⇨ Efficient in high dimensional datasets and consistent with PC-stable algorithm



```
Algorithm 2: The parallel-PC algorithm
Input: Dataset $D$, significant level $\alpha$, $P$ cores,
       memory-efficient indicator $s$, number of edges
       per batch $t_b$
Output: The undirected graph $G$ with a set of edges $E$
Assume all nodes are connected in graph $G$
Let depth $d = 0$
repeat
    Query and fix the adjacent set $adj(X, G)$ of each
    node $X$ in $G$
    Compute the set $J$ of unordered pairs of adjacent
    vertices $(X, Y)$ in $G$
    // Parallelisation Step
    for each batch of $t_b$ edges ($t_b = |J|$ if $s = FALSE$)
    do
        Distribute the edges in the batch evenly into $P$
        cores, each with $J_p$ edges
        for each core $p = 1 \dots P$ in parallel do
            for each pair $(X, Y) \in J_p$ do
                Let $k^p_{X,Y}$ indicate if $(X, Y)$ is adjacent,
                initialize $k^p_{X,Y}$ = TRUE
                // On $X$'s neighbours
                if $|adj(X, G) \setminus \{Y\}| \geq d$ then
                    for each subset $Z_X \subseteq adj(X, G) \setminus \{Y\}$
                    and $|Z_X| = d$ do
                        if $I(X, Y | Z_X)$ then
                            $k^p_{X,Y}$ = FALSE
                            break
                        end
                    end
                end
                // On $Y$'s neighbours
                if $|adj(Y, G) \setminus \{X\}| \geq d$ then
                    for each subset $Z_Y \subseteq adj(Y, G) \setminus \{X\}$
                    and $|Z_Y| = d$ do
                        if $I(X, Y | Z_Y)$ then
                            $k^p_{X,Y}$ = FALSE
                            break
                        end
                    end
                end
            end
        end
    // Synchronisation Step
    for each core $p = 1 \dots P$ do
        for each pair $(X, Y) \in J_p$ do
            if $k^p_{X,Y} = FALSE$ then
                Remove the edge between $X$ and $Y$
                and update $G$ and $E$
            end
        end
    end
    Let $d = d + 1$
until $|adj(X, G) \setminus \{Y\}| < d$ for every pair of adjacent
vertices in $G$;
```

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 cycles**
  - □ Learn Markov equivalence classes of directed (not necessarily acyclic) graphs under the assumption of causal sufficiency.

  ⇨ *Cyclic causal discovery (CCD)* by Richardson (1996)

- **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)

6. Other Methods of Causal Structure Learning

Overview

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.,
  1. 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)

References
Literature

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- Kalisch et al. (2014). *Causal structure learning and inference: a selective review*. *Quality Technology & Quantitative Management*

References
Implementations

R

- Kalisch et al. (2017), R Package ‘pcalg’.
- Le et al. (2015), R Package ‘ParallelPC’.
- Scutari (2007), Learning Bayesian Networks with the bnlearn R Package.

Python

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

Other

- Carneggie Mellon University, The Tetrad Project

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Thank you
for your attention!