Estimating High-Dimensional Directed Acyclic Graphs with the PC-Algorithm

Theresa Meier, 13.01.2023

Seminar Modeling under Dependence

How to find conditional independence (CI) relationships in a DAG?

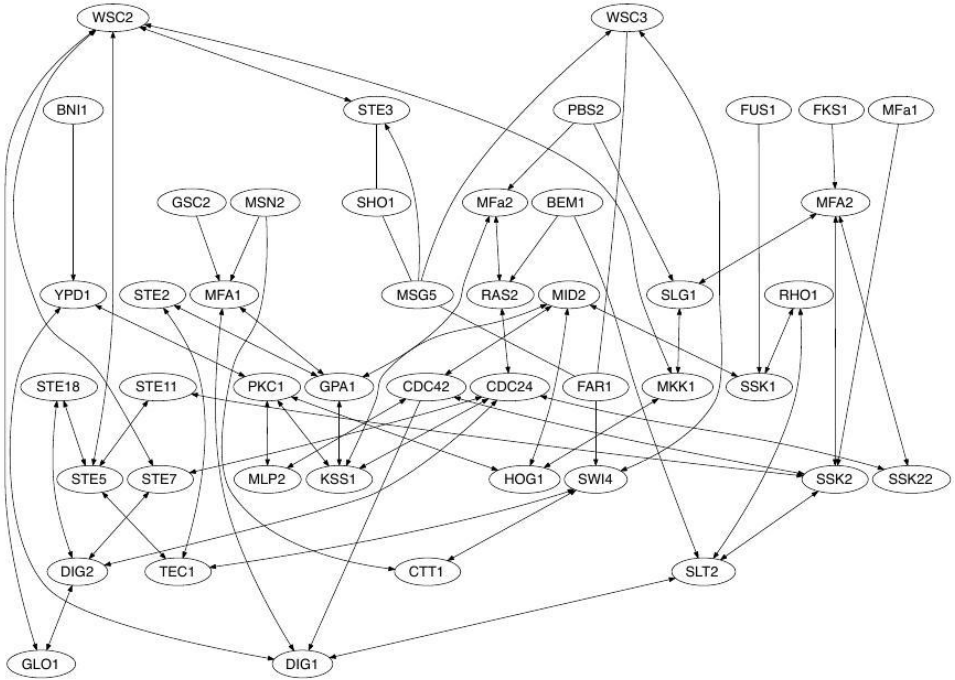

Figure 1: Output of the rank PC-algorithm for yeast gene expression data (Harris and Drten, 2013).

Agenda

1) Basic Definitions
2) Introduction to the PC-Algorithm
3) Limitations of the PC-Algorithm
4) The stable PC-Algorithm
5) The parallel PC-Algorithm
6) Simulation Study in R
7) Final Notes and Discussion

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Directed Acyclic Graphs (DAGs)

All following definitions are taken from Harris and Drton (2013), Le et al. (2014) and Koller and Friedman (2009).

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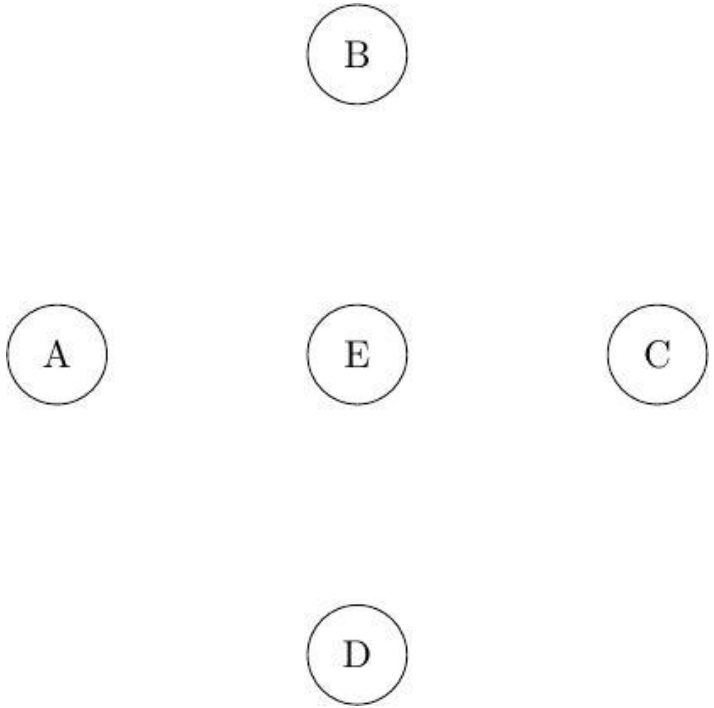
Let $\mathcal{G} = (\mathcal{N}, \mathcal{E})$ be a graph consisting of:

- set of nodes $\mathcal{N}$



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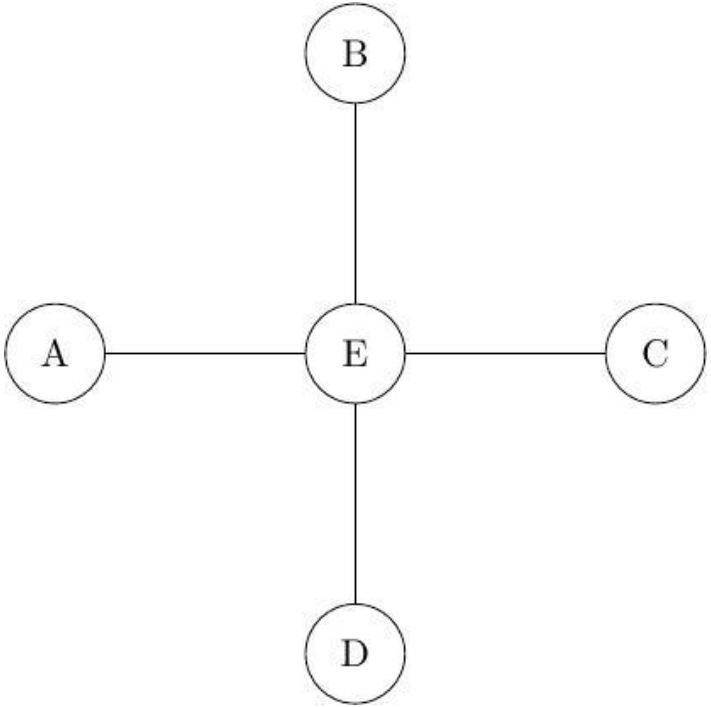

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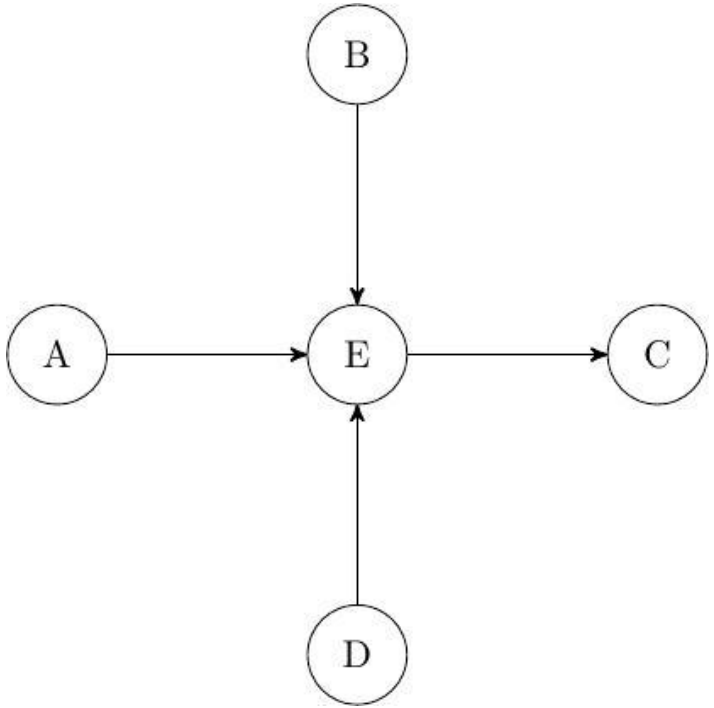

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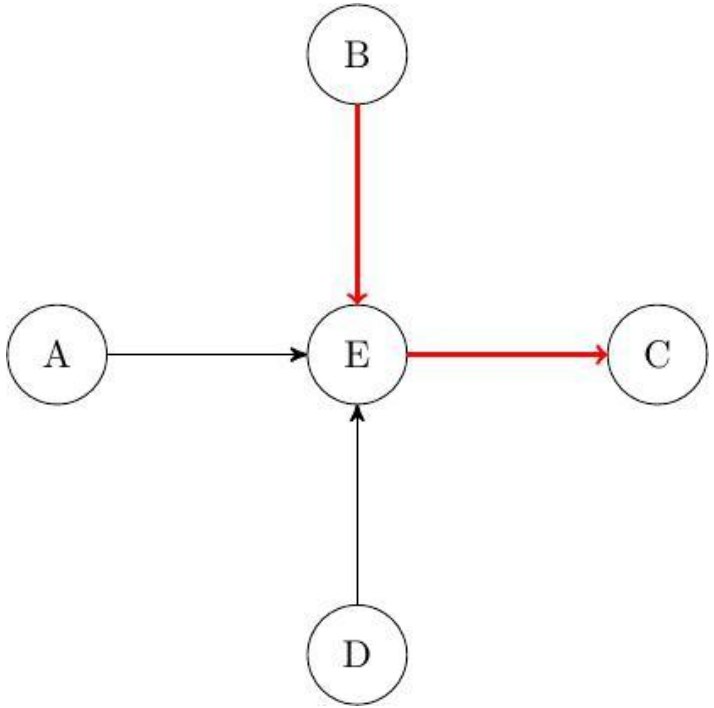

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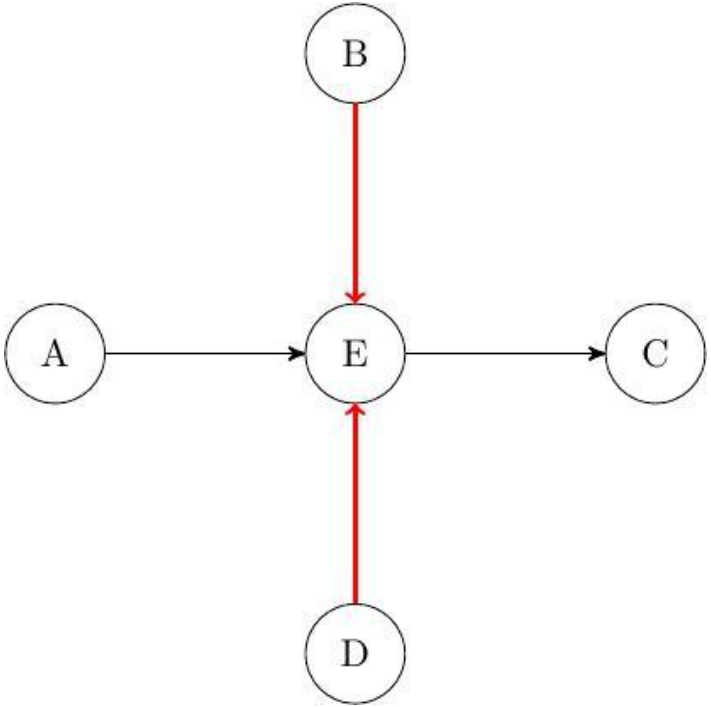

Directed Acyclic Graphs (DAGs)

A **collider** or **v-structure** is a triple of nodes $(A, B, C) \in \mathcal{M}^3$ that induces the subgraph

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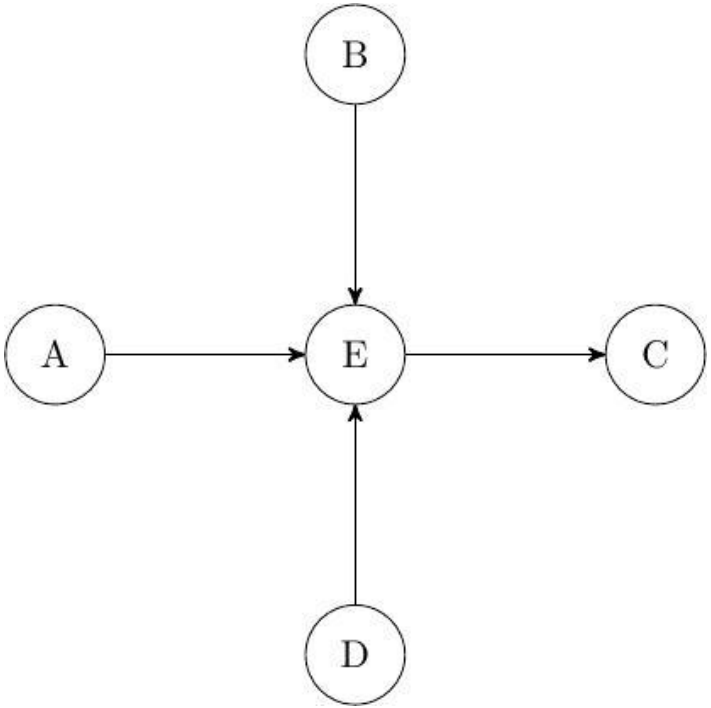
where A and C are not adjacent (i.e. there is no edge between A and C).



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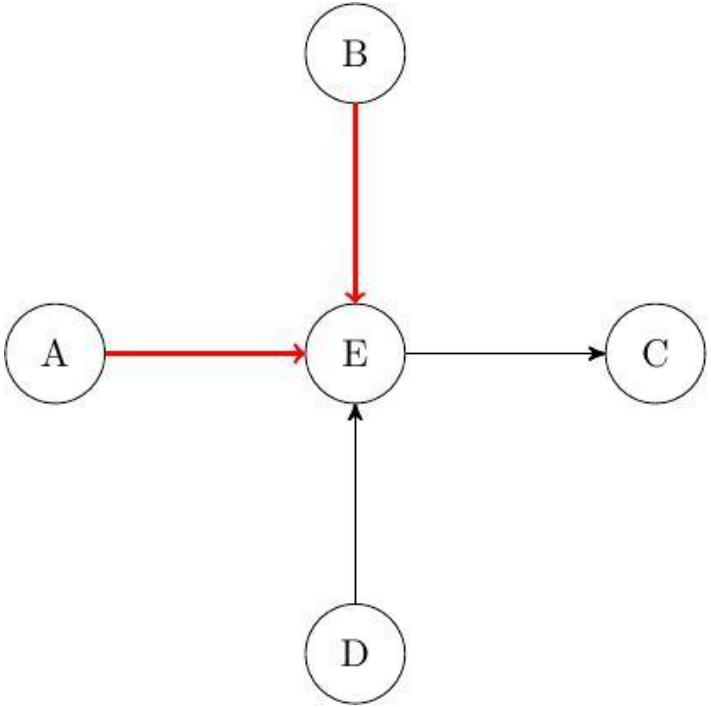

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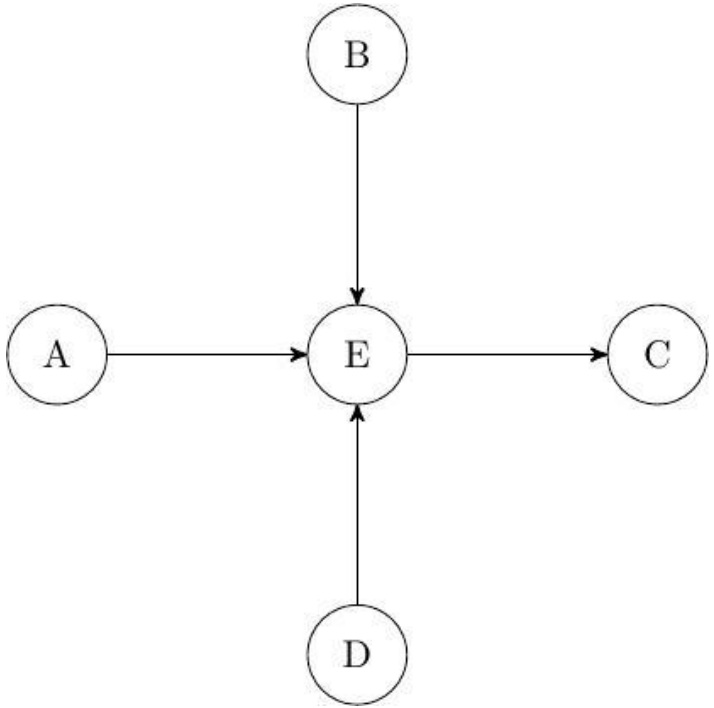

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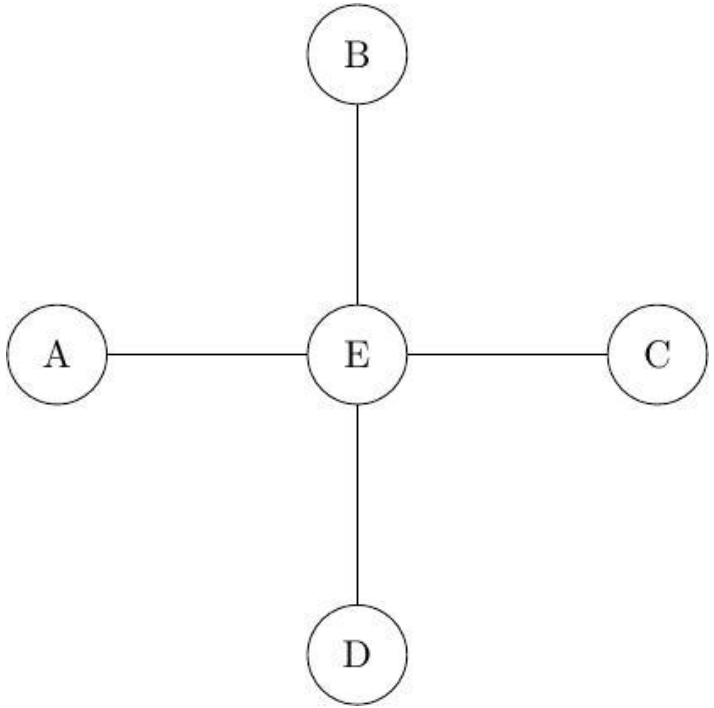

d-Separation

Let $A, B \in \mathcal{N}$, $A \neq B$, and $\boldsymbol{S} \subseteq \mathcal{N}$ a set of nodes not containing A and B.

A and B are **d-separated** given $\boldsymbol{S}$ if and only if there exists no undirected path p between A and B such that

- every collider on p has a descendant in $\boldsymbol{S}$ or is in $\boldsymbol{S}$ itself, and
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Otherwise A and B are called **d-connected**.

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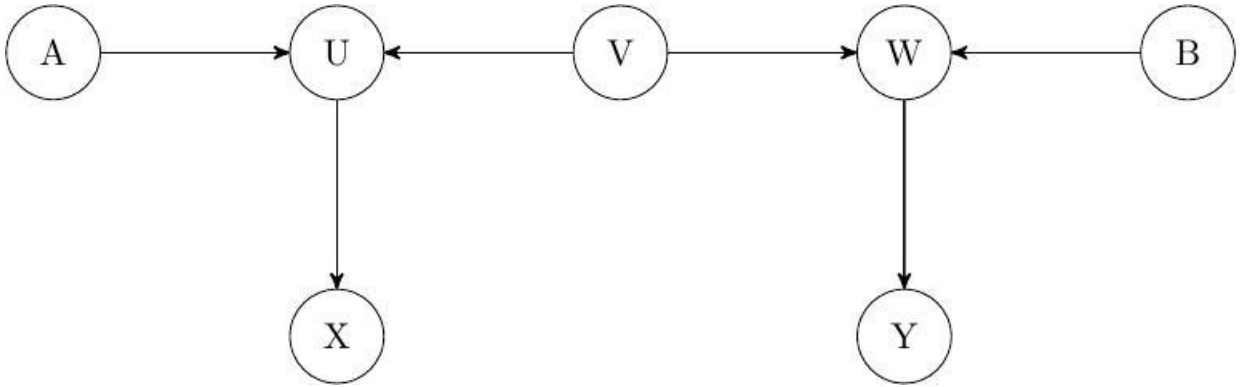

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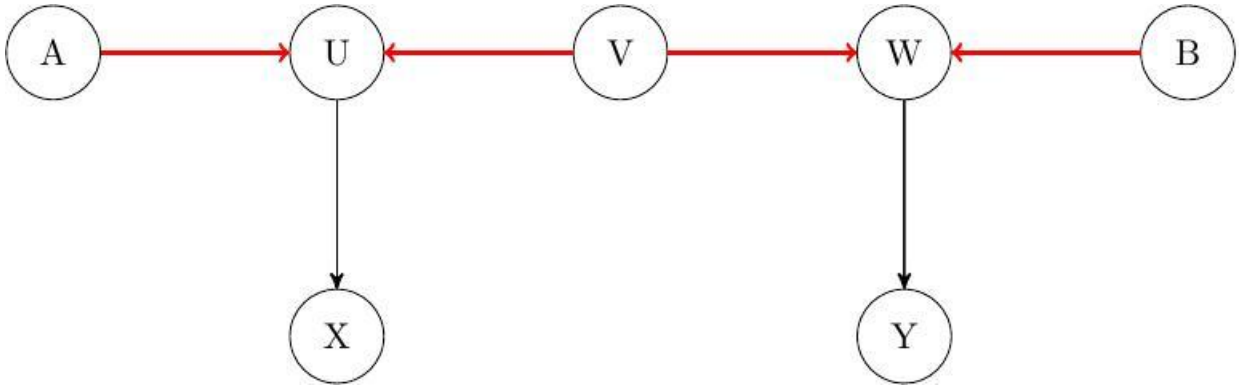

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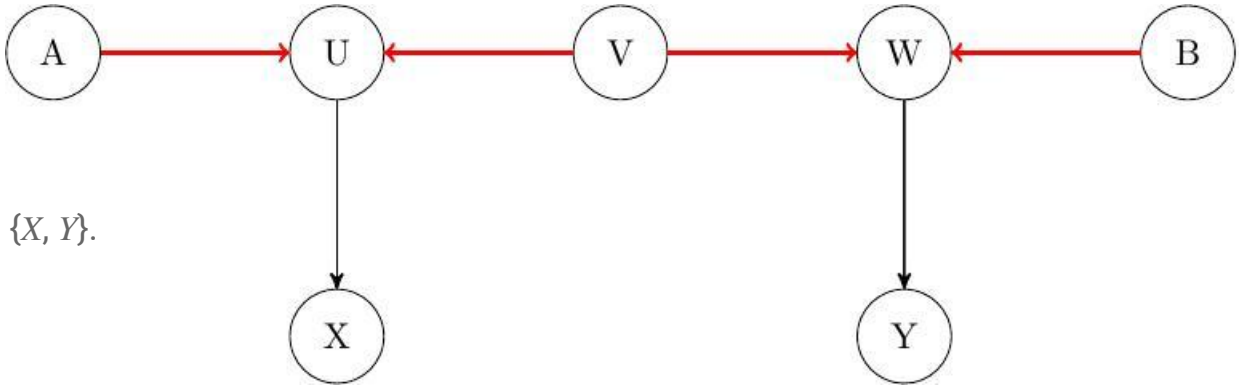

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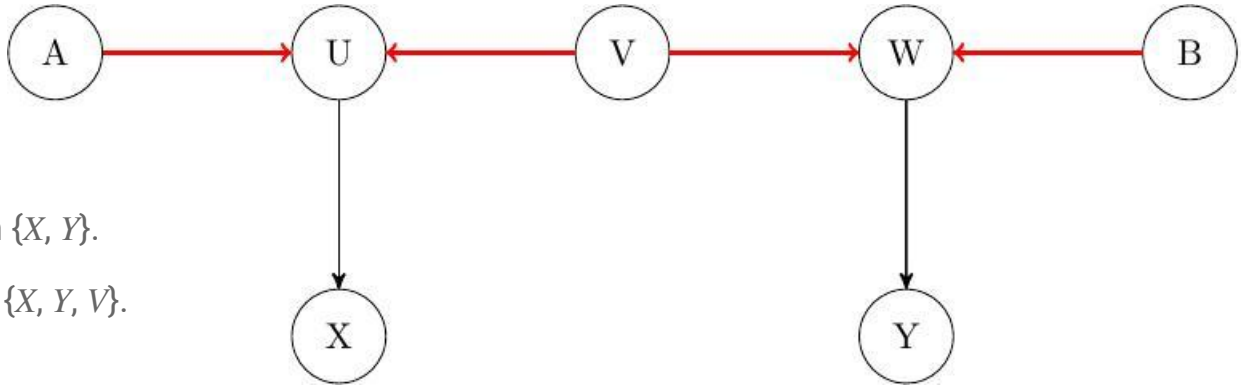


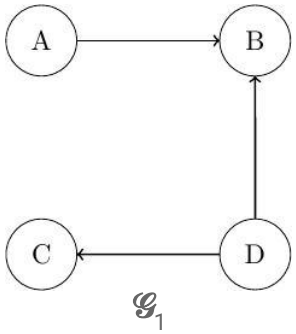
A and B are **d-connected** given $\{X, Y\}$.

A and B are **d-separated** given $\{X, Y, V\}$.

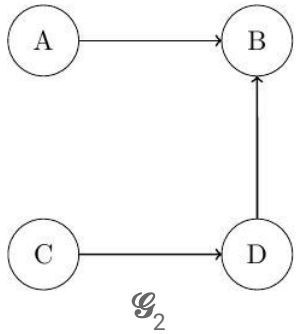
Markov equivalence class

Two DAGs with the same node set $\mathcal{N}$ are called **Markov equivalent** if and only if both share the same skeleton and the same colliders.

→ partitions space of DAGs into **equivalence classes** where all members of an equivalence class encode the same statistical model, i. e. contain the same conditional independence information and the same d-separation relations



$\mathcal{G}_1$



$\mathcal{G}_2$

Completed partially directed acyclic graph (CPDAG)

Let $[\mathcal{G}]$ be the Markov equivalence class of DAG $\mathcal{G} = (\mathcal{N}, \mathcal{E})$ and define the edge set

$$[\mathcal{E}] = \cup_{\mathcal{H} \in [\mathcal{G}]} \mathcal{E}(\mathcal{H}),$$

where $\mathcal{E}(\mathcal{H})$ denotes the set of edges of a DAG $\mathcal{H}$. That is, $(A, B) \in [\mathcal{E}]$ if there exists a DAG $\mathcal{H} \in [\mathcal{G}]$ with the edge $A \rightarrow B$ in its edge set.

The graph $\mathcal{C}(\mathcal{G}) = (\mathcal{N}, [\mathcal{E}])$ is called the **completed partially directed acyclic graph (CPDAG)** and consists of both directed and undirected edges.

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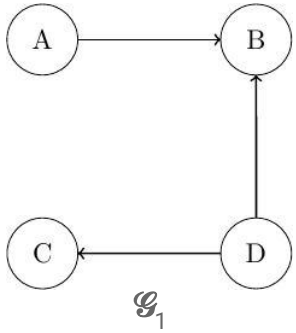

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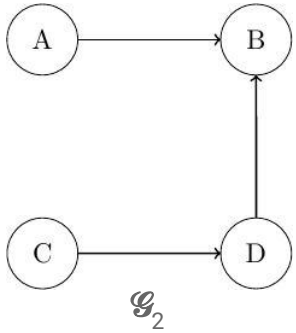

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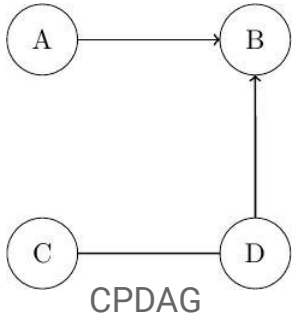

CPDAG

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History

- Invented by **P**eter Spirtes and **C**lark Glymour in 1991 as a more efficient alternative to the SGS algorithm
- Many improvements available (stable PC, parallel PC etc.)
- Implementations in R:
  - package *pcalg* by Markus Kalisch
  - package *ParallelPC* by Thuc Duy Le, Tao Hoang, Shu Hu, and Liang Zhang

Image sources:
https://www.cmu.edu/dietrich/philosophy/people/faculty/spirtes.html (left),
https://www.cmu.edu/dietrich/philosophy/people/emeritus/glymour.html (right)

Theoretical foundation

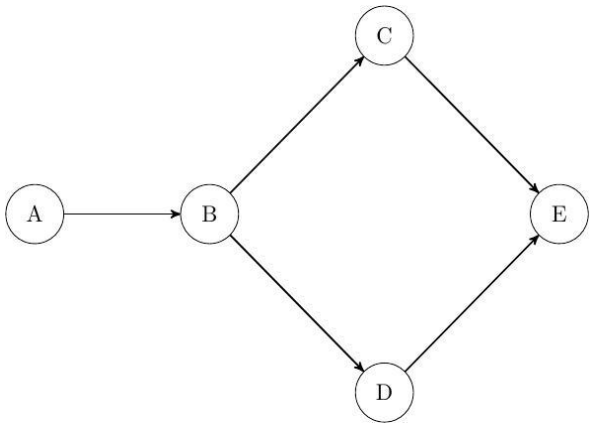
Theorem 1 (Sprites et al., 2000)

If nodes $\boldsymbol{A}$ and $\boldsymbol{B}$ are not adjacent in a DAG $\mathcal{G}$, then there is a set of nodes $\boldsymbol{S}$ which is either a subset of

$$adj(\boldsymbol{A}, \mathcal{G}) \qquad \text{or of} \qquad adj(\boldsymbol{B}, \mathcal{G})$$

such that $\boldsymbol{S}$ *d-separates* $\boldsymbol{A}$ and $\boldsymbol{B}$ in $\mathcal{G}$.

$\rightarrow \boldsymbol{S}$ disconnects $\boldsymbol{A}$ and $\boldsymbol{B}$



Proof: Sprites et al., 2000, Theorem 6.2 (page 417)

Theoretical foundation

Theorem 2 (Sprites et al., 2000)

Let the nodes $\mathcal{N}$ represent random variables $X = (X_N)_{N \in \mathcal{N}}$ which are multivariate Gaussian distributed $\mathcal{P}$ and let $\mathcal{P}$ be *faithful* to a DAG $\mathcal{G} = (\mathcal{N}, \mathcal{E})$. Assume that the perfect conditional independence information about all pairs of variables (A, B) in $\mathcal{N}$ given subsets S is given.

Then, the output of the PC-algorithm is the *CPDAG* that represents $\mathcal{G}$.

→ Even given infinite amount of data, the PC-algorithm is not able to identify the true DAG, only its equivalence class

Proof: Sprites et al., 2000, Theorem 5.1 (page 410)

Two-Step Computation

Step 1: Learning the Skeleton

Input: Complete undirected graph

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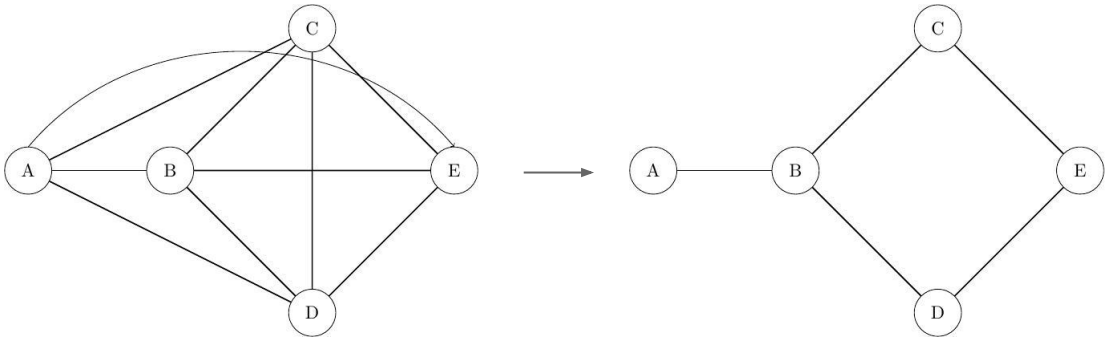

Example: Sprites, Glymour and Scheines, 2000

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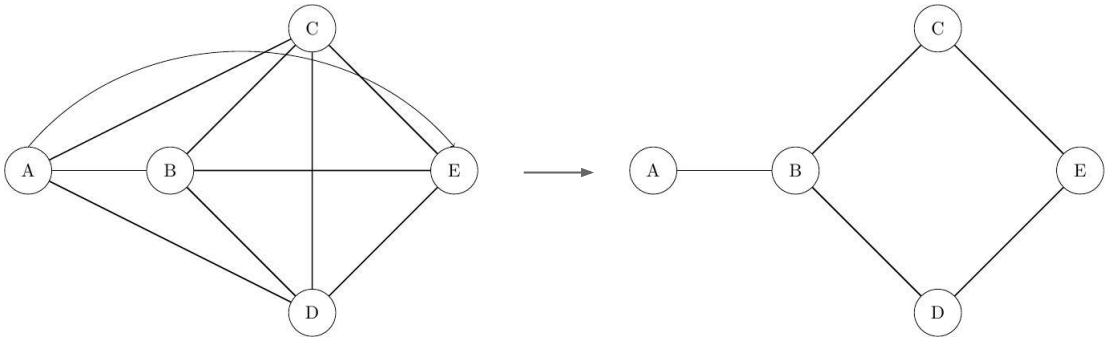
Output: Approximated CPDAG



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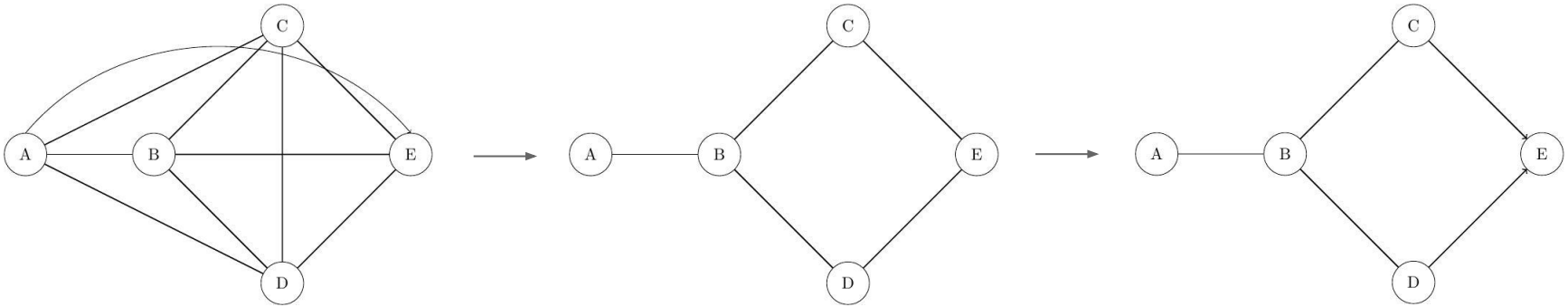

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Pseudocode

Algorithm 1: Step 1: Learning the skeleton

Data: Data set D with nodes $\mathcal{N}$, significance level α
Result: Skeleton $\mathcal{G}_{Skel}$, seperating sets S
$d \leftarrow 0$
repeat
  for *each ordered pair of adjacent nodes* X *and* Y **do**
    if $|adj(X, \mathcal{G}) \setminus \{Y\}| \geq d$ **then**
      for *each subset* $S \subseteq adj(X, \mathcal{G}) \setminus \{Y\}$ *and* $|S| = d$ **do**
        Test $CI(X, Y|S)$ on significance level α
        if $CI(X, Y|S)$ **then**
          Remove edge between X and Y
          Save S as separating set of (X, Y)
          Update $\mathcal{G}$ and $\mathcal{E}$
          break
        end
      end
    end
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  $d \leftarrow d + 1$
until $|adj(X, \mathcal{G}) \setminus \{Y\}| < d$ *for every pair of adjacent nodes*;

Kalisch and Bühlmann, 2007

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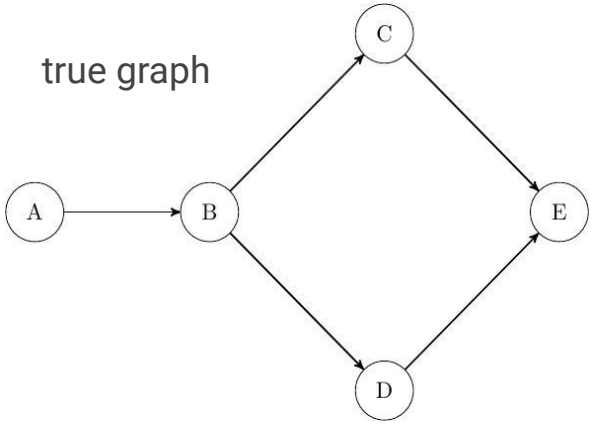

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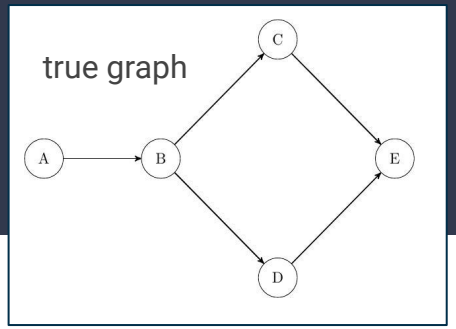

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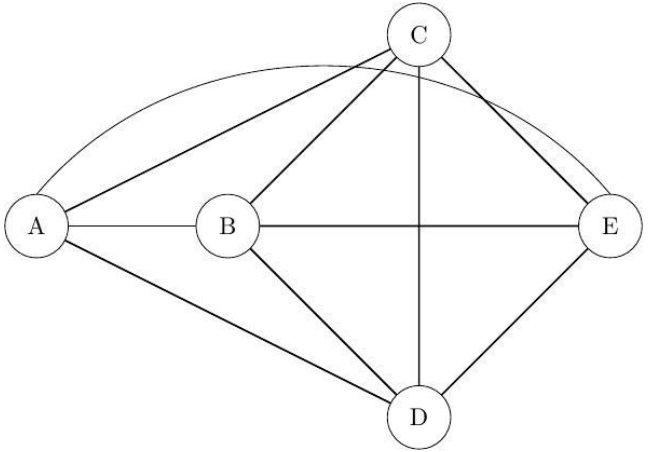
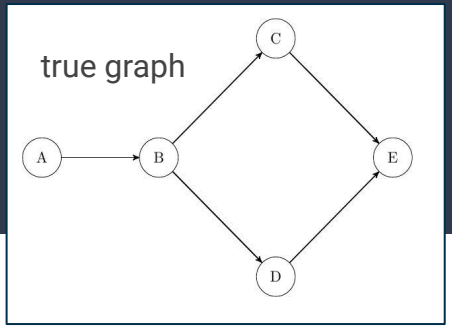


complete undirected graph

Pseudocode



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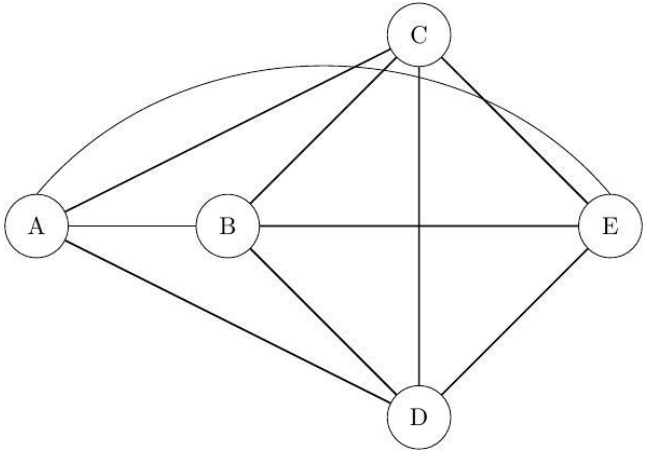

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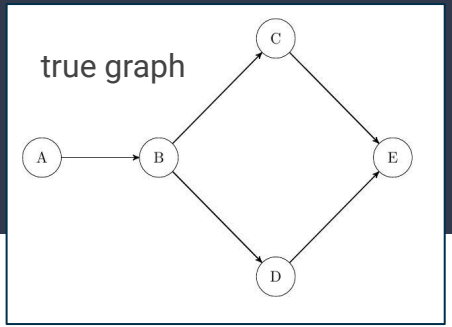

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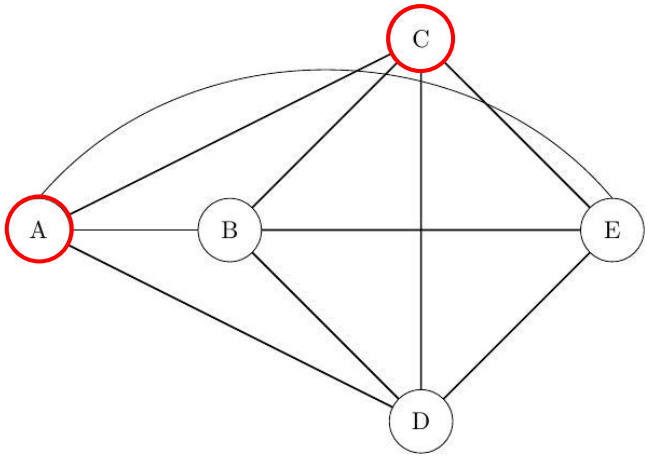

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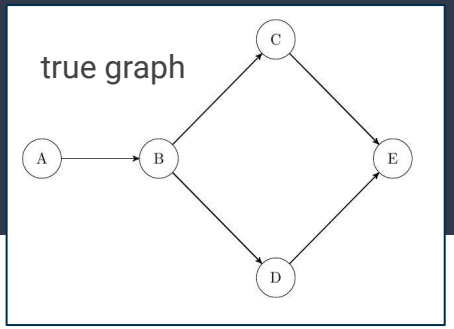

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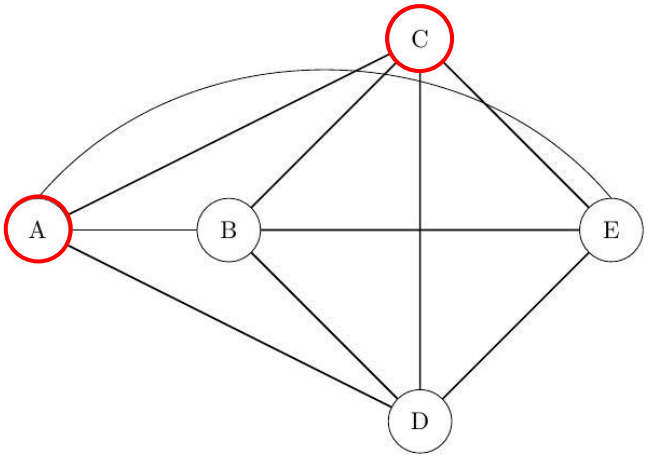

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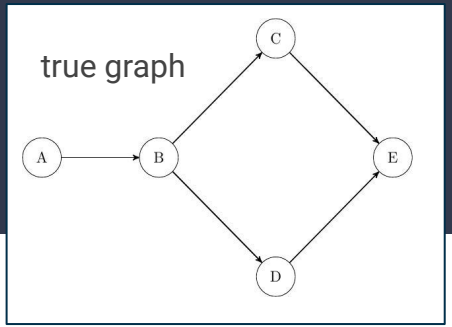

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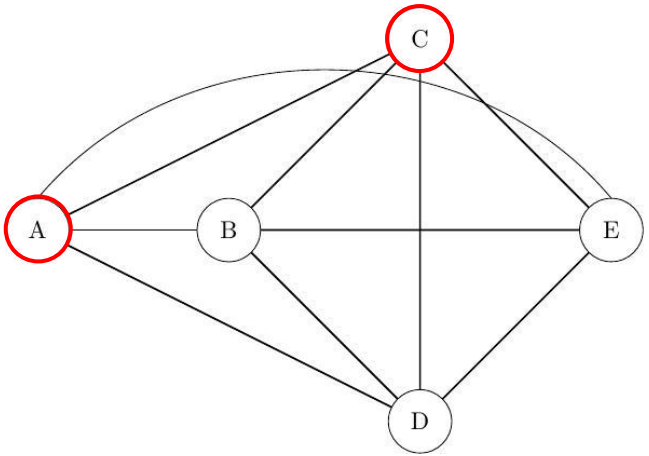

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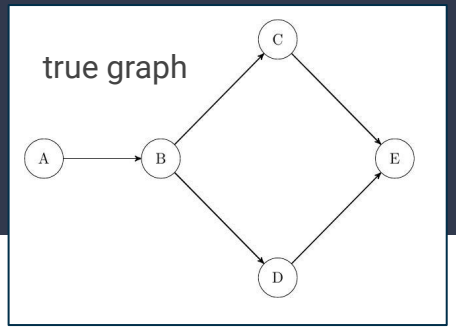

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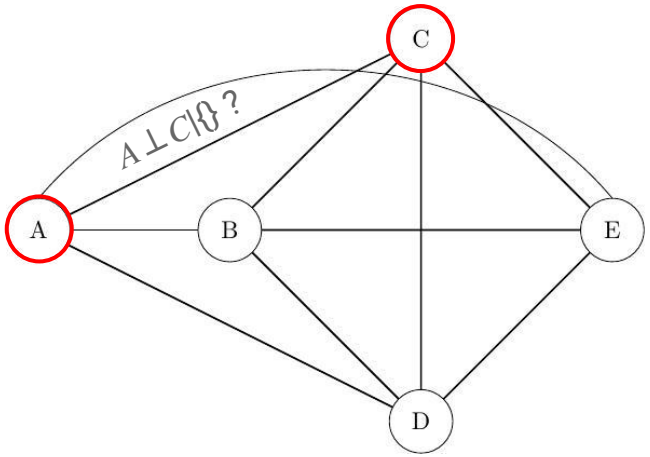

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The CI test in detail

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In practice: perfect CI information is unknown

→ How to estimate conditional independence from the data?

The CI test in detail

Recall: Property of the multivariate normal distribution:

For a multivariate normal distributed random vector $\boldsymbol{X} \in \mathbb{R}^p$ denote its partial correlation between components $\boldsymbol{X}^{(i)}$ and $\boldsymbol{X}^{(j)}$ $(i \neq j)$ given set $\{\boldsymbol{X}^{(r)}, r \in \boldsymbol{R} \subseteq \{1, \dots, p\} \setminus \{i, j\}\}$ by $\rho_{i,j \mid \boldsymbol{R}}$.

Then it holds:

$\rho_{i,j \mid \boldsymbol{R}} = 0$ if and only if $\boldsymbol{X}^{(i)}$ and $\boldsymbol{X}^{(j)}$ are *conditionally independent* given $\{\boldsymbol{X}^{(r)}, r \in R\}$.

→ **Idea:** Estimate partial correlation $\rho_{i,j \mid \boldsymbol{R}}$ and test whether it is close to zero

The CI test in detail

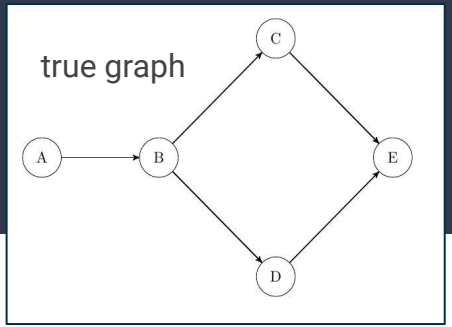
Testing of $\rho_{i,j \mid r}$ via Fisher's z-transform (Kalisch and Bühlmann, 2007):

- **Test statistic:** $Z(i,j \mid R) = 0.5 \log \left(\frac{1 + \rho_{i,j \mid \boldsymbol{R} \setminus t}}{1 - \rho_{i,j \mid \boldsymbol{R} \setminus t}} \right) \overset{H_0}{\sim} \mathcal{N}(0,1)$
- **Test:** Reject H_0: $\rho_{i,j \mid \boldsymbol{R}} = 0$ against H_1: $\rho_{i,j \mid \boldsymbol{R}} \neq 0$ if

$$(n - |R| - 3)^{0.5} \, |Z(i,j \mid R)| > \Phi^{-1}(1 - \alpha/2) \, ,$$

where Φ denotes the cumulative distribution function of a standard normal distribution

Pseudocode



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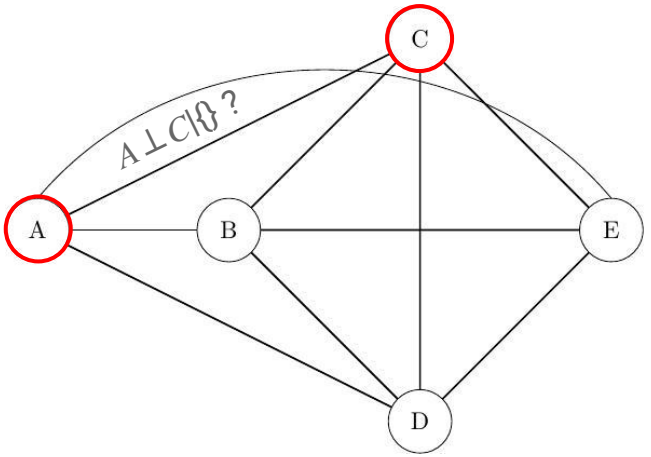

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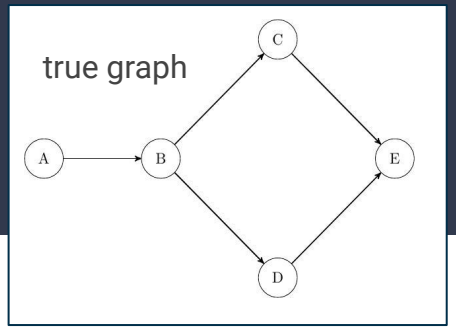

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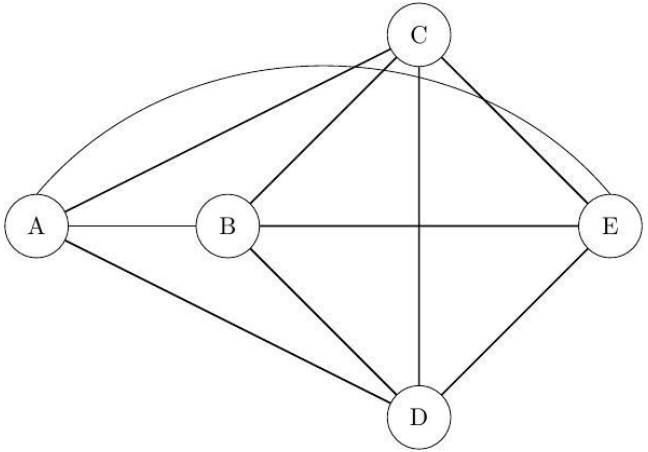

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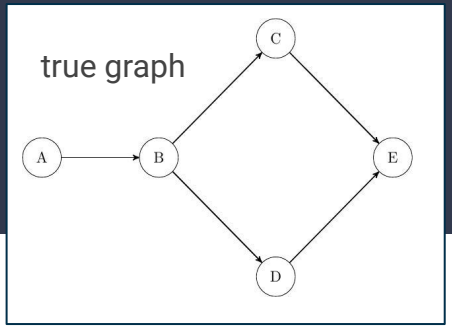

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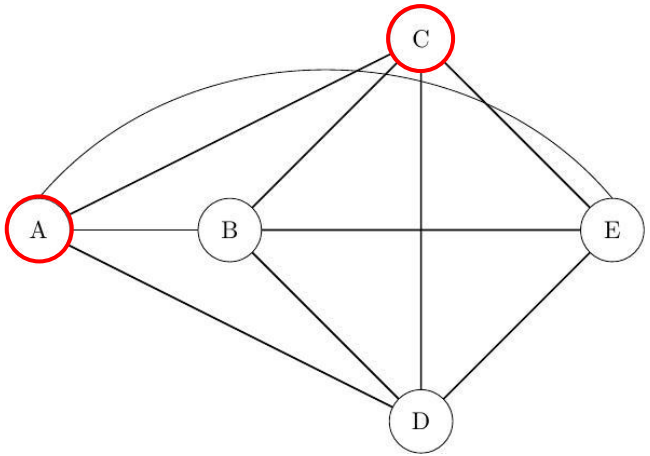

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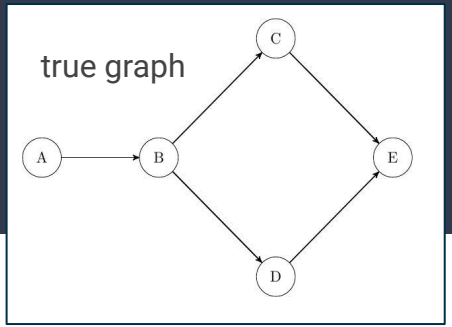

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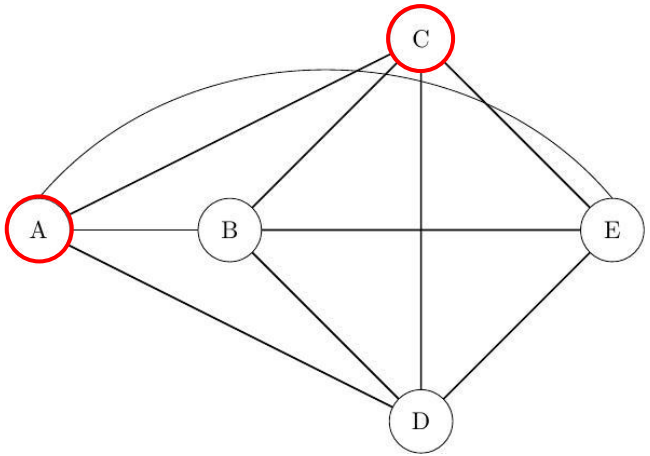

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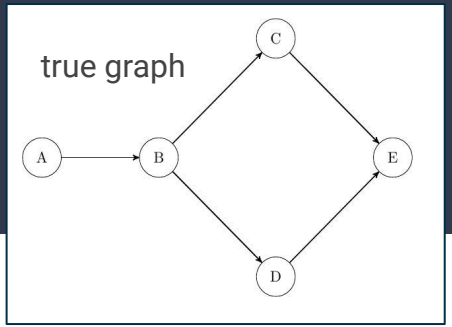

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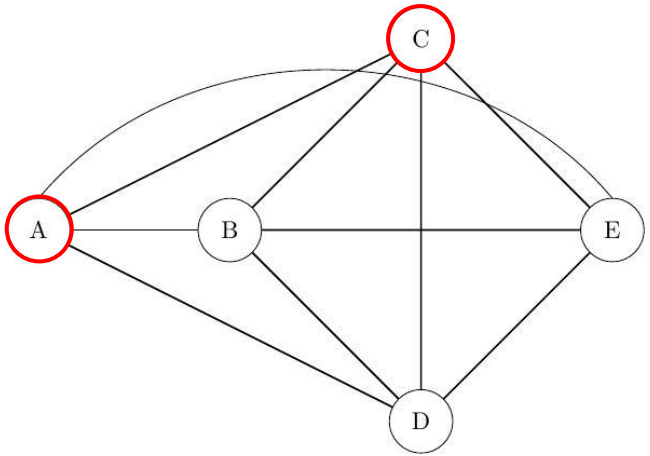

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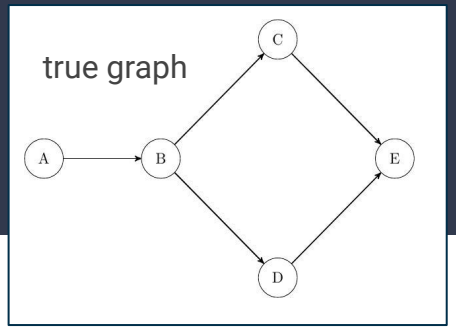

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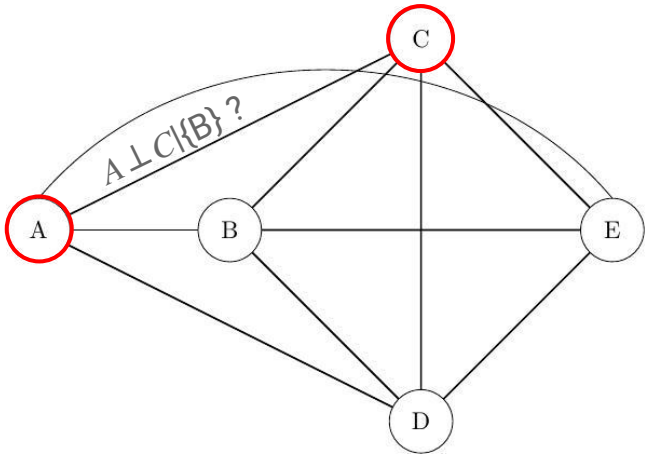

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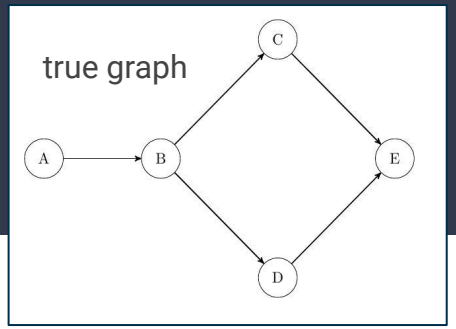

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      for *each subset* $S \subseteq adj(X, \mathcal{G}) \setminus \{Y\}$ *and* $|S| = d$ **do**
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        if $CI(X, Y|S)$ **then**
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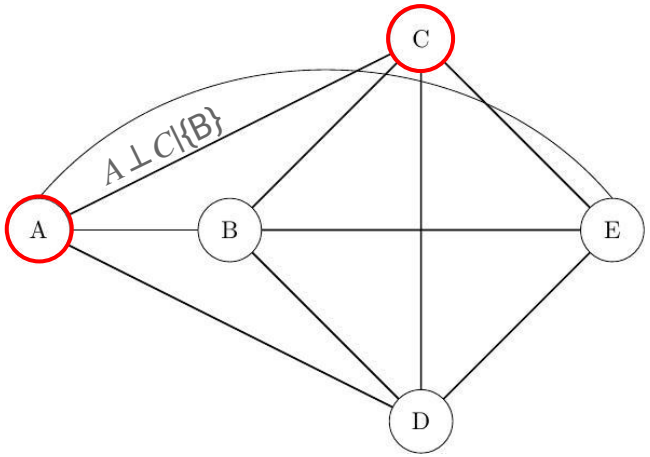
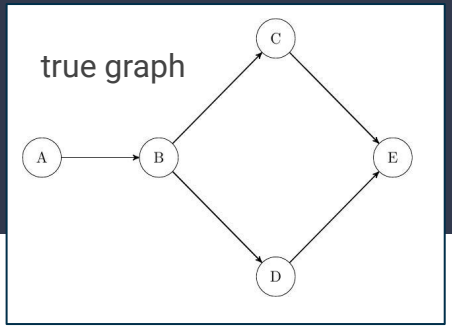
          Save S as separating set of (X, Y)
          Update $\mathcal{G}$ and $\mathcal{E}$
          break
        end
      end
    end
  end
  $d \leftarrow d + 1$
until $|adj(X, \mathcal{G}) \setminus \{Y\}| < d$ *for every pair of adjacent nodes*;

$d = 1$



$adj(A, \mathcal{G}) \setminus \{C\} = \{B, D, E\}$
$|S| = 1 \rightarrow S = \{B\}$

Pseudocode



Algorithm 1: Step 1: Learning the skeleton

Data: Data set D with nodes $\mathcal{N}$, significance level α
Result: Skeleton $\mathcal{G}_{Skel}$, seperating sets S

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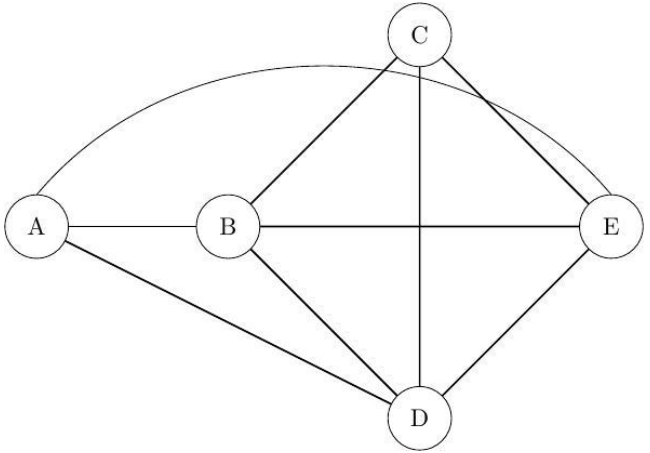

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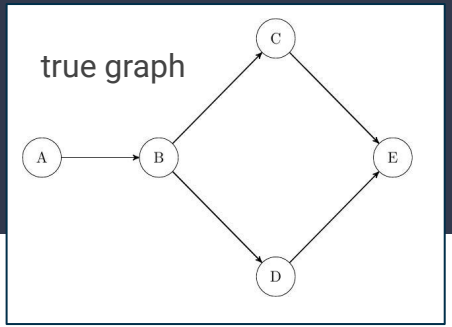

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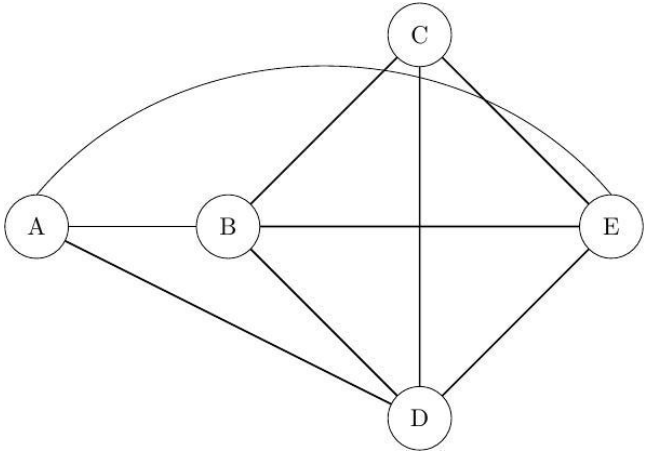

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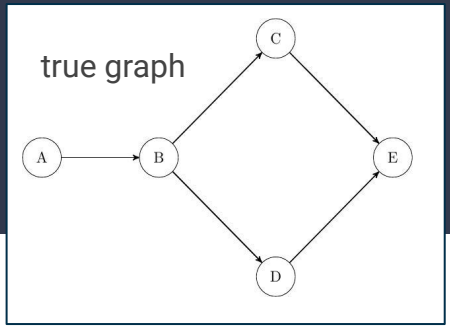
Pseudocode



Algorithm 1: Step 1: Learning the skeleton

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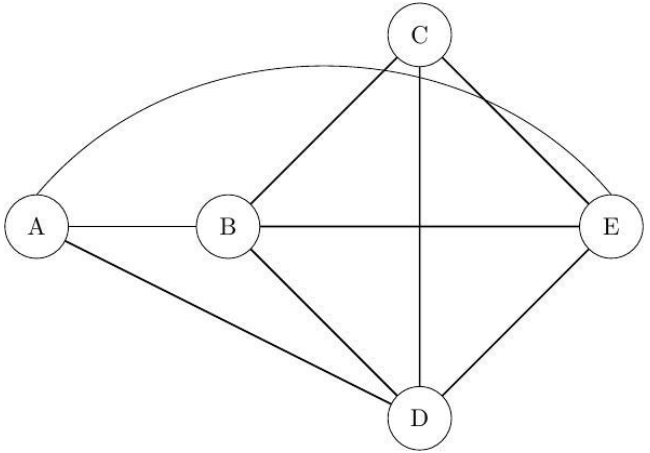
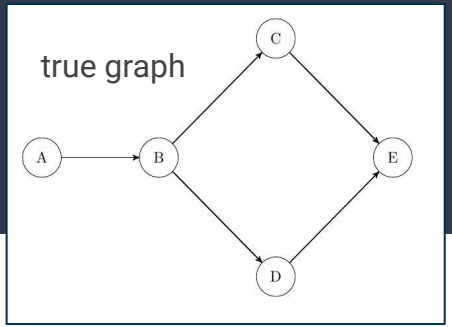
d = 1



$\mathcal{E}_{new} = \mathcal{E} \setminus \{(A, C)\}$

$\mathcal{G}_{new} = (\mathcal{N}, \mathcal{E}_{new})$

Pseudocode



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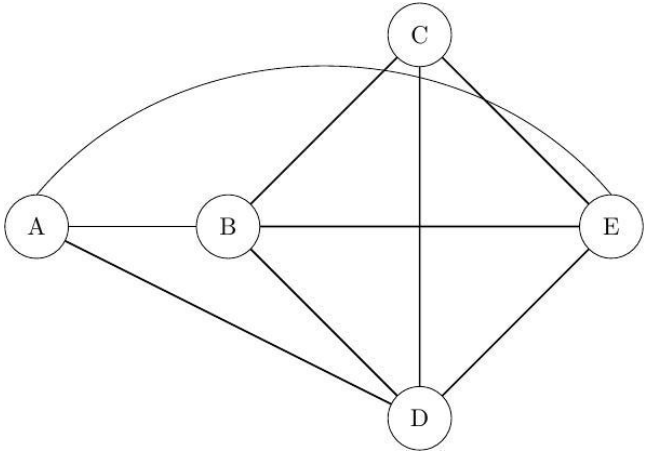
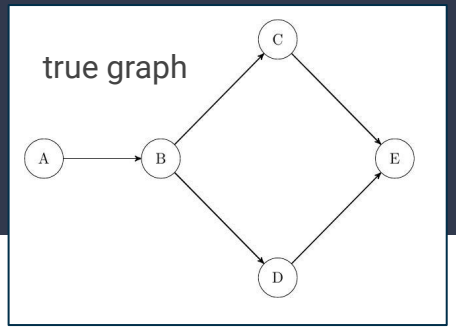
          break
        end
      end
    end
  end
  $d \leftarrow d + 1$
until $|adj(X, \mathcal{G}) \setminus \{Y\}| < d$ *for every pair of adjacent nodes*;

d = 1



Pseudocode



Algorithm 1: Step 1: Learning the skeleton

Data: Data set D with nodes $\mathcal{N}$, significance level α
Result: Skeleton $\mathcal{G}_{Skel}$, seperating sets S
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          Update $\mathcal{G}$ and $\mathcal{E}$
          break
        end
      end
    end
  end
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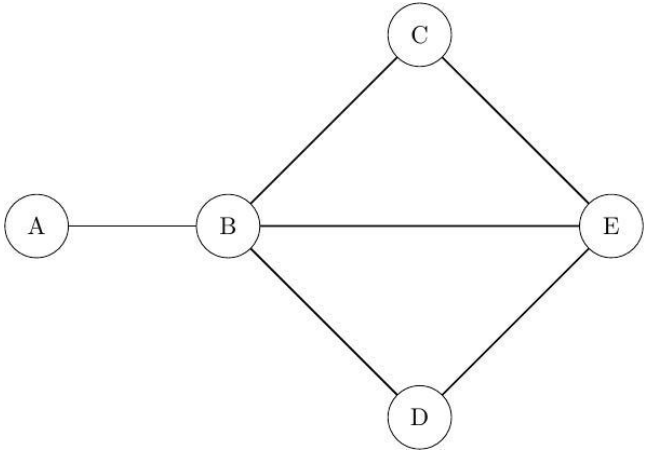
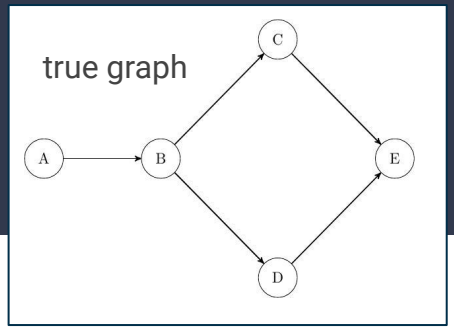
until $|adj(X, \mathcal{G}) \setminus \{Y\}| < d$ *for every pair of adjacent nodes*;

d = 2



Pseudocode



Algorithm 1: Step 1: Learning the skeleton

Data: Data set D with nodes $\mathcal{N}$, significance level α
Result: Skeleton $\mathcal{G}_{Skel}$, seperating sets S
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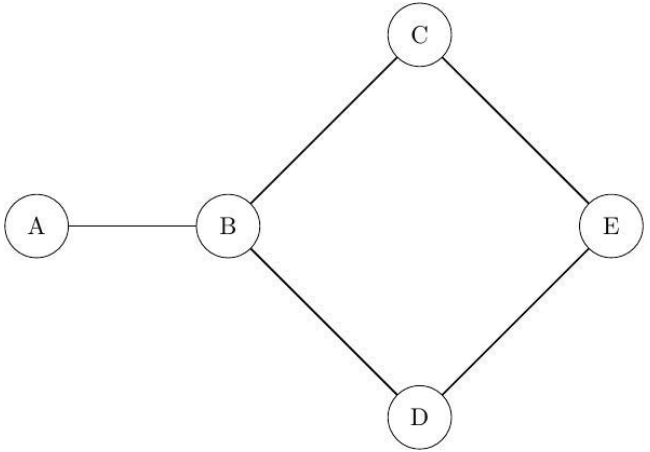
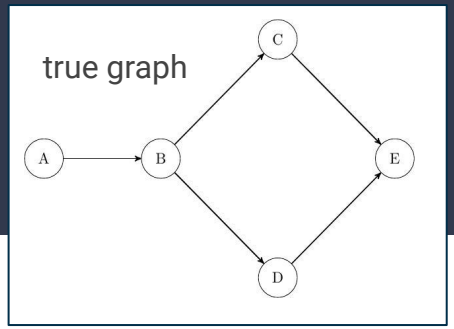
        Test $CI(X, Y|S)$ on significance level α
        if $CI(X, Y|S)$ **then**
          Remove edge between X and Y
          Save S as separating set of (X, Y)
          Update $\mathcal{G}$ and $\mathcal{E}$
          break
        end
      end
    end
  end
  $d \leftarrow d + 1$
until $|adj(X, \mathcal{G}) \setminus \{Y\}| < d$ *for every pair of adjacent nodes*;

d = 3



Pseudocode



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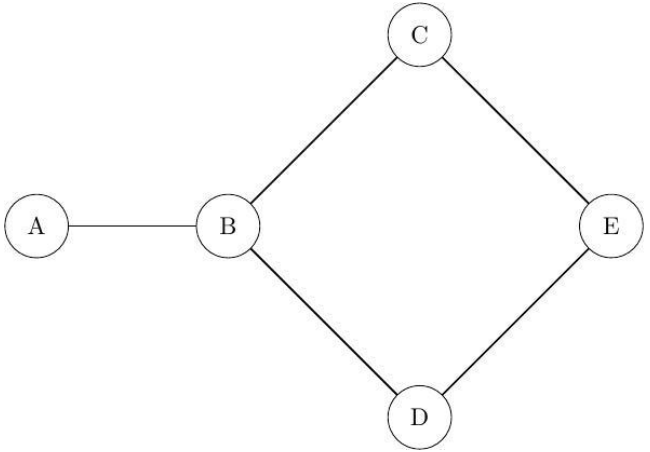

Pseudocode

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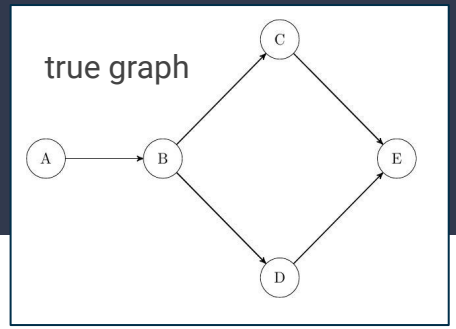
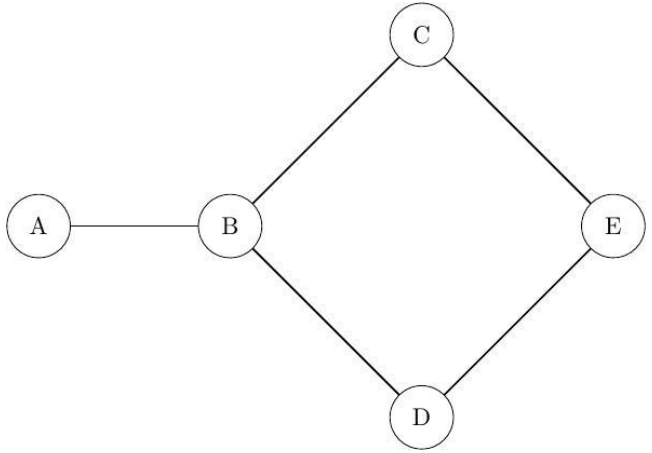
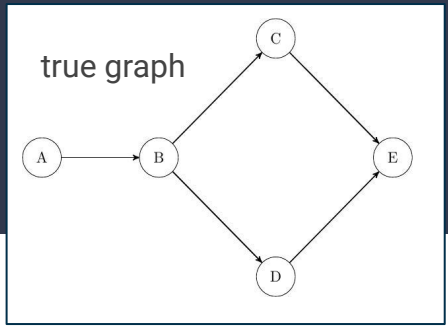




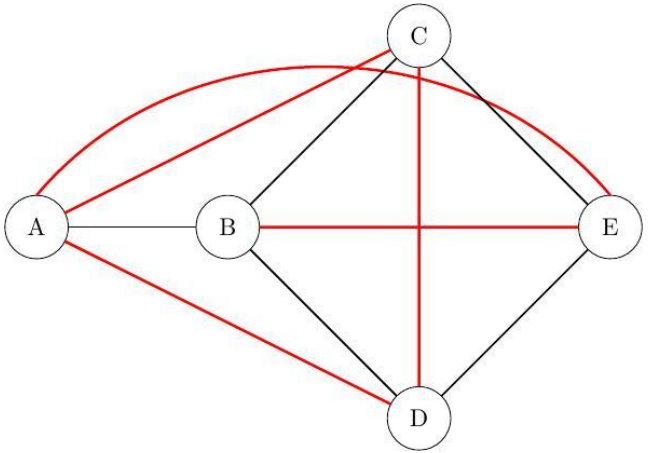
skeleton

Pseudocode



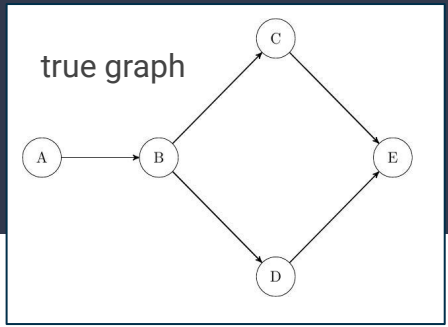
Interim results of step 1:

	Seperating set	Removed edge
$A \perp C \mid \{B\}$	{B}	$A - C$
$A \perp D \mid \{B\}$	{B}	$A - D$
$A \perp E \mid \{B\}$	{B}	$A - E$
$C \perp D \mid \{B\}$	{B}	$C - D$
$B \perp E \mid \{C, D\}$	$\{C, D\}$	$B - E$



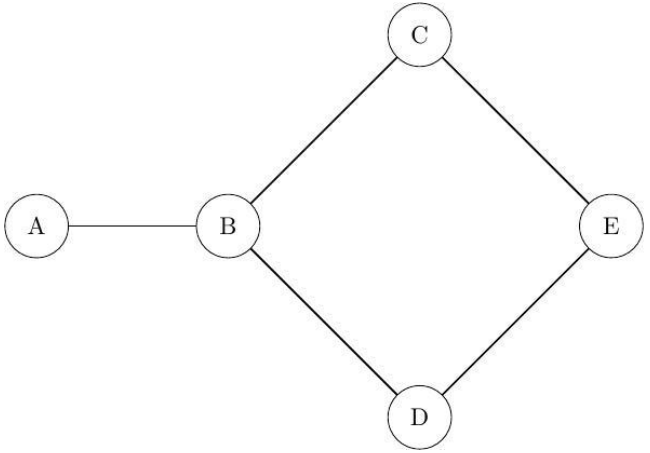
skeleton

Pseudocode

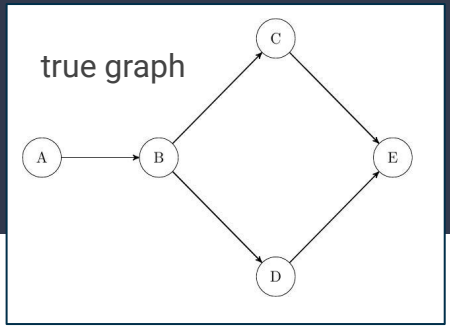


Algorithm 2: Step 2: Learning the CPDAG

Data: Skeleton $\mathcal{G}_{Skel}$, separating sets S
Result: CPDAG
for *all pairs of non-adjacent nodes* X *and* Y *with common neighbor* U **do**
  if $U \notin S(X, Y)$ **then**
    Orient $X - U - Y$ as $X \rightarrow U \leftarrow Y$
  end
end
Orient as many undirected edges as possible by applying the following rules:
repeat
  Rule 1 Orient $Y - U$ into $Y \rightarrow U$ when there is edge $X \rightarrow Y$ s.t. X and U are non-adjacent.
  Rule 2 Orient $X - Y$ into $X \rightarrow Y$ when there is $X \rightarrow U \rightarrow Y$.
  Rule 3 Orient $X - Y$ into $X \rightarrow Y$ when there is $X \rightarrow U \rightarrow Y$ and $X \rightarrow V \rightarrow Y$ s.t. U and V are non-adjacent.
  Rule 4 Orient $X - Y$ into $X \rightarrow Y$ when there is $X \rightarrow U \rightarrow V$ and $U \rightarrow V \rightarrow Y$ s.t. U and Y are non-adjacent.
until *no more edges can be oriented*;



Pseudocode



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Data: Skeleton $\mathcal{G}_{Skel}$, separating sets S
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  Rule 3 Orient $X - Y$ into $X \rightarrow Y$ when there is $X \rightarrow U \rightarrow Y$ and $X \rightarrow V \rightarrow Y$ s.t. U and V are non-adjacent.
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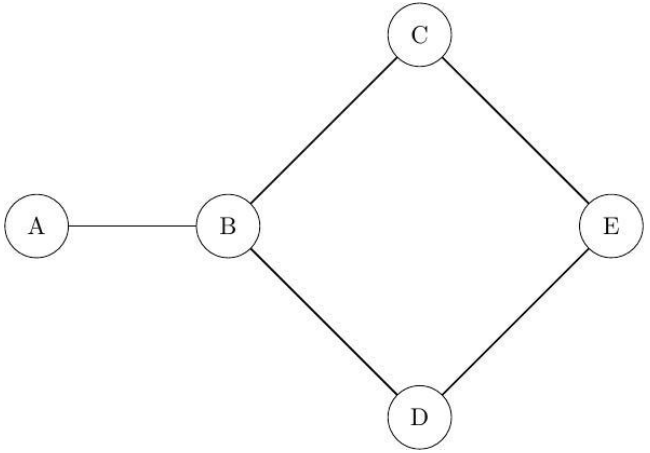
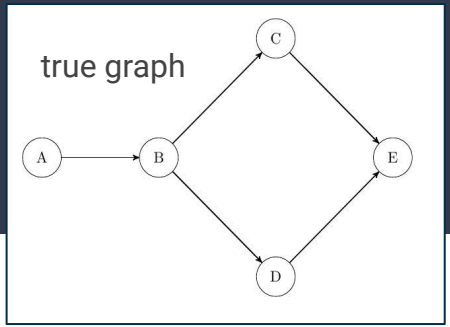


Pseudocode



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Data: Skeleton $\mathcal{G}_{Skel}$, separating sets S

Result: CPDAG

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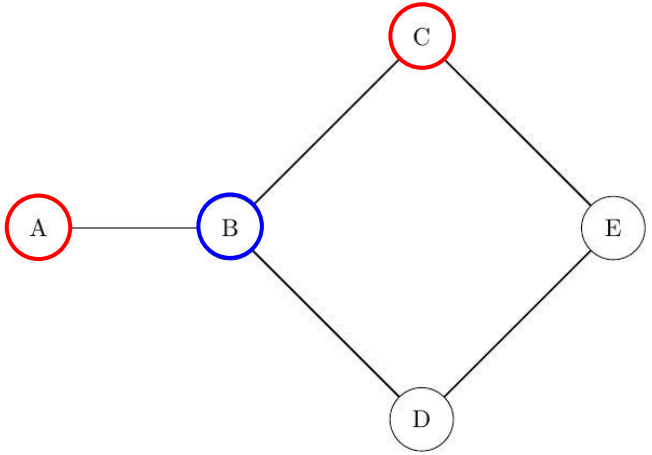
until *no more edges can be oriented*;



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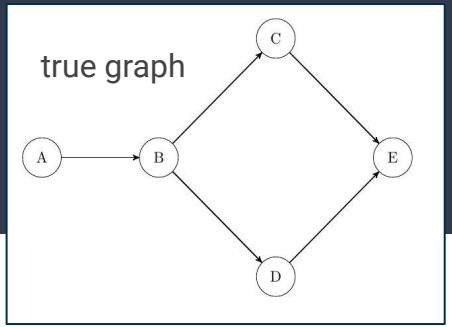

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Result: CPDAG

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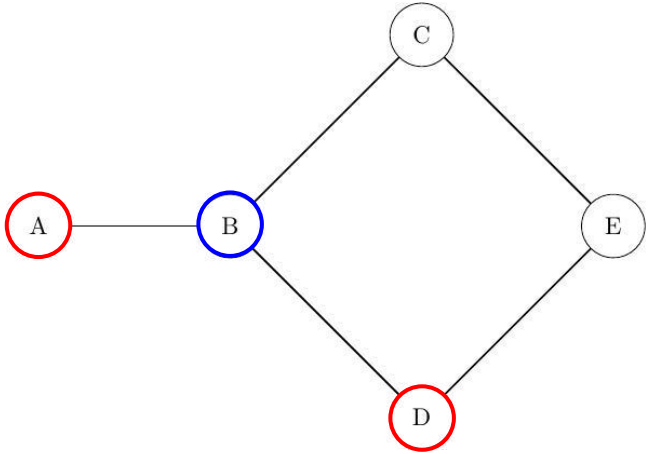
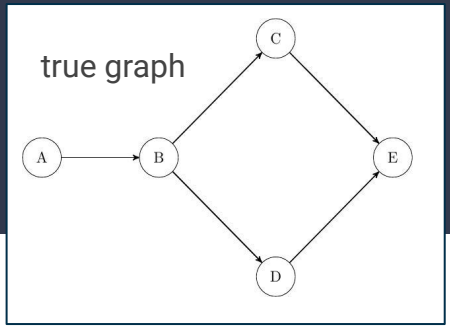
until *no more edges can be oriented*;



Pseudocode



Algorithm 2: Step 2: Learning the CPDAG

Data: Skeleton $\mathcal{G}_{Skel}$, separating sets S

Result: CPDAG

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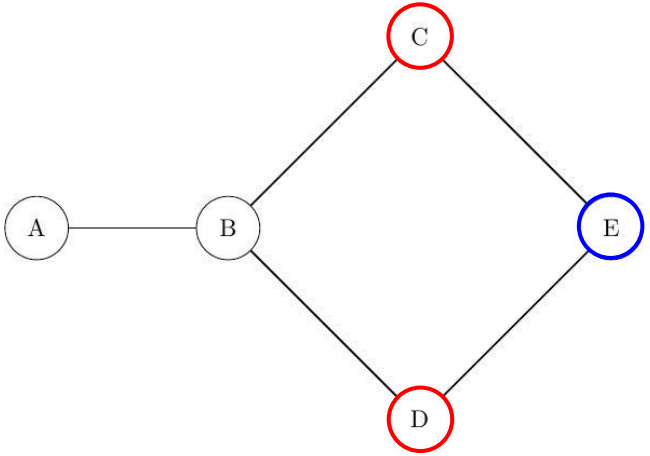

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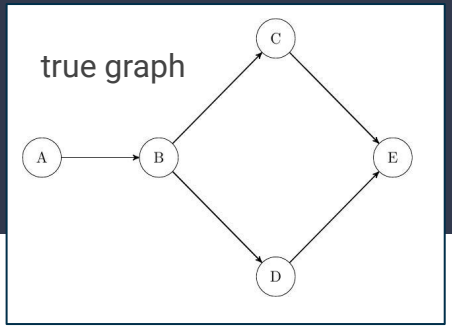

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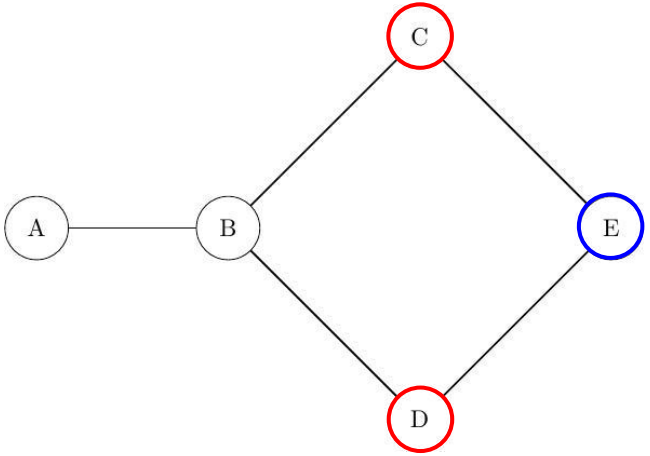
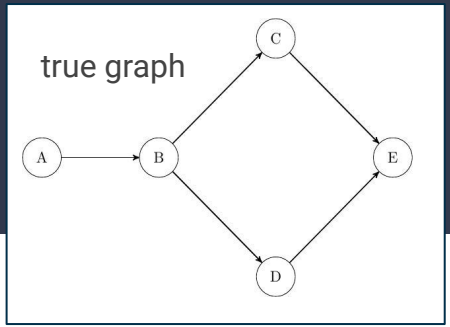


$S(C, D) = \{B\} \ni E$

Pseudocode



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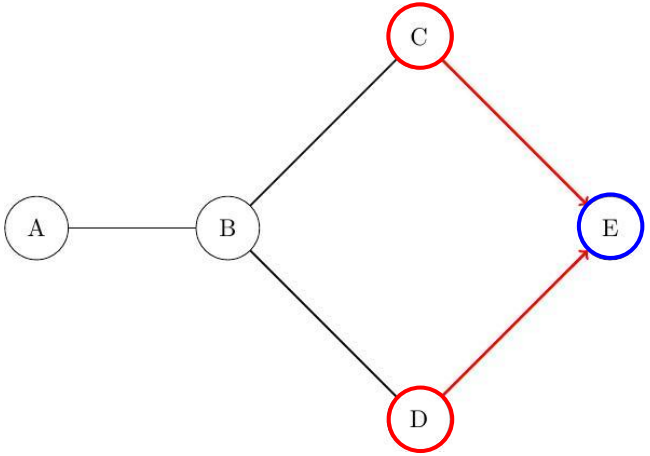

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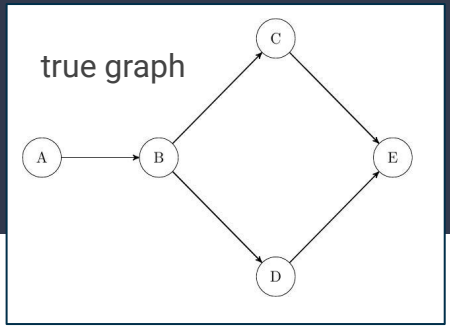

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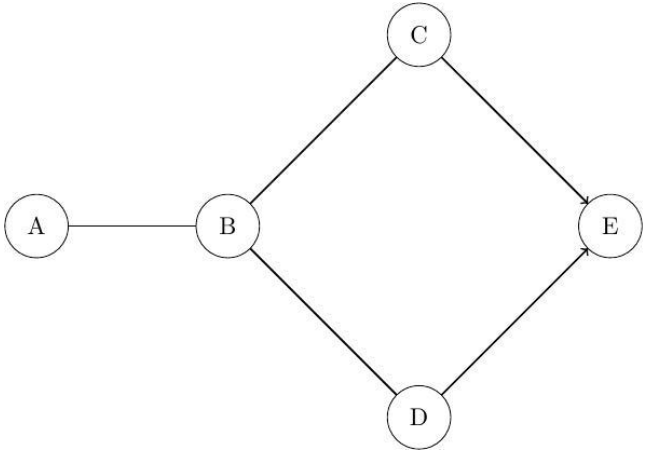
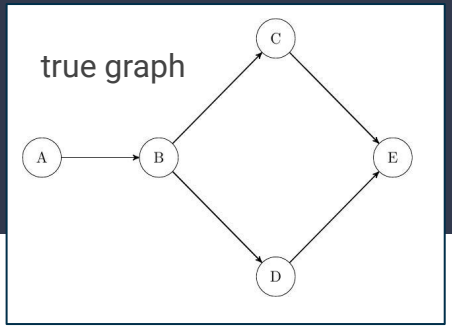


Pseudocode



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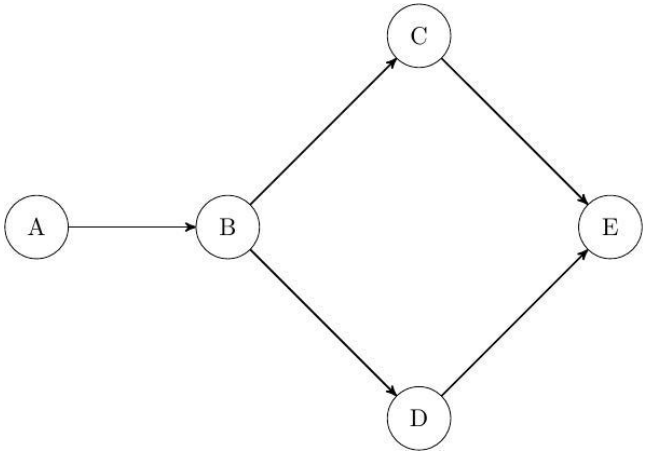
until *no more edges can be oriented*;

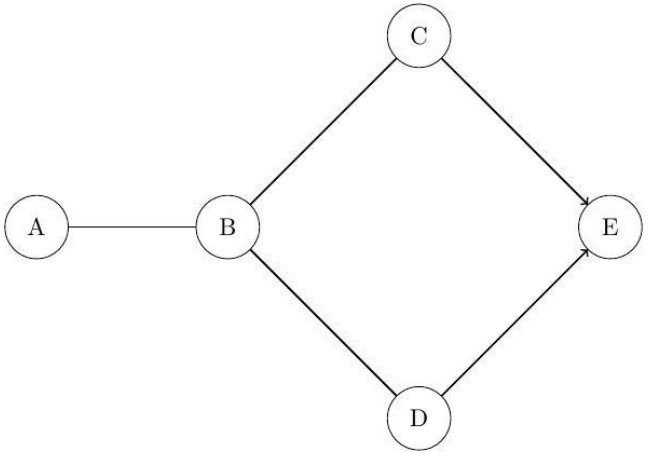
oriented based on invalid edges inducing new colliders or directed edges

Pseudocode

Final result of PC:



true graph



approximated CPDAG

Agenda

1) Basic Definitions
2) Introduction to the PC-Algorithm
3) **Limitations of the PC-Algorithm**
4) The stable PC-Algorithm
5) The parallel PC-Algorithm
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Limitations of the original PC-Algorithm

Ordering

Problem:

Output graph is dependent on the order in which CI tests are performed

Solution: Stable PC-algorithm

(Colombo and Maathuis, 2012)

Runtime

Problem:

Many CI tests necessary

→ high runtime

Solution: Parallel PC-algorithm

(Le et al., 2014)

Gaussian Distribution

Problem:

Consistency only holds for Gaussian distribution

→ what if it is non-Gaussian?

Solution: Rank PC-algorithm

(Harris and Drton, 2013)

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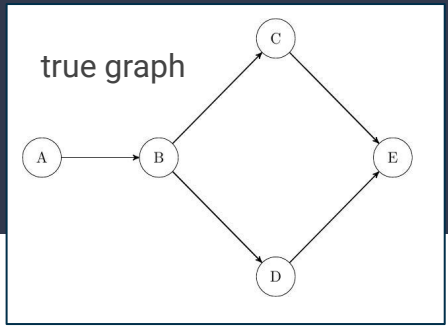
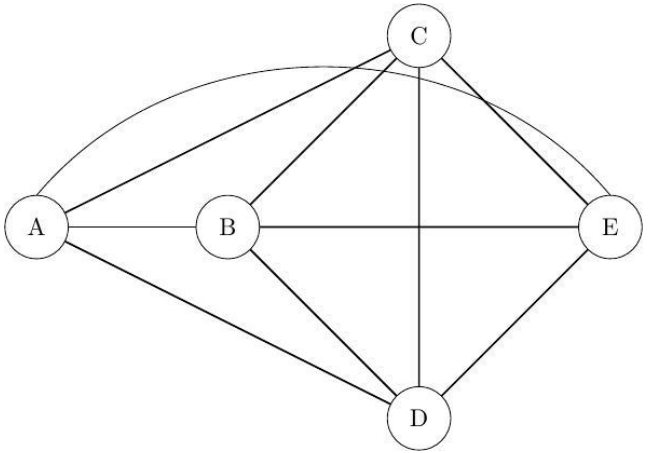
The stable PC-Algorithm

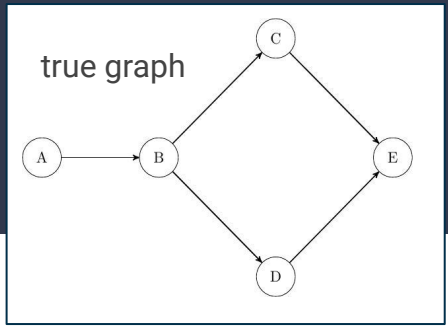


Problem:

Incorrectly removing/retaining edge results in changes of set S



The stable PC-Algorithm



Problem:

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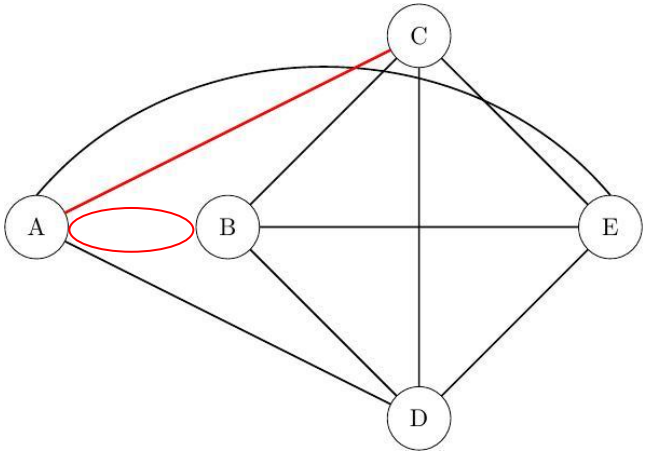
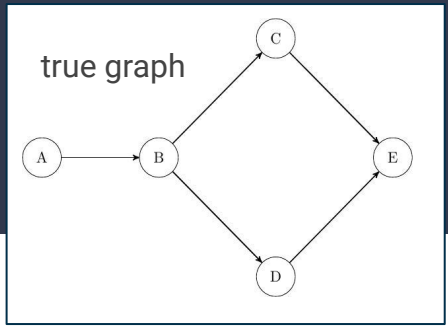
→ output graph depends on order in which CI tests are performed



$adj(A, \mathcal{G}) \setminus \{C\} = \{D, E\}$

$S \nexists B$ for all possible sets S

The stable PC-Algorithm



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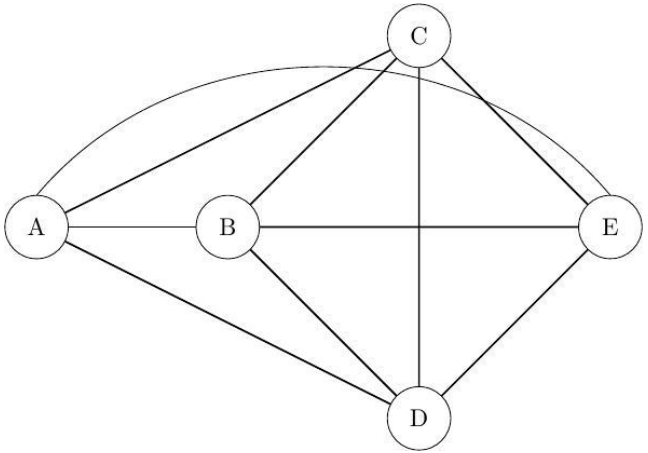

Idea:

Keep adjacency sets of nodes unchanged in each level d

Idea

Algorithm 1: Step 1: Learning the skeleton

Data: Data set D with nodes $\mathcal{N}$, significance level α
Result: Skeleton $\mathcal{G}_{Skel}$, seperating sets S
$d \leftarrow 0$
repeat
  for *each ordered pair of adjacent nodes* X *and* Y **do**
    if $|adj(X, \mathcal{G}) \setminus \{Y\}| \geq d$ **then**
      for *each subset* $S \subseteq adj(X, \mathcal{G}) \setminus \{Y\}$ *and* $|S| = d$ **do**
        Test $CI(X, Y|S)$ on significance level α
        if $CI(X, Y|S)$ **then**
          Remove edge between X and Y
          Save S as separating set of (X, Y)
          Update $\mathcal{G}$ and $\mathcal{E}$
          break
        end
      end
    end
  end
  $d \leftarrow d + 1$
until $|adj(X, \mathcal{G}) \setminus \{Y\}| < d$ *for every pair of adjacent nodes*;

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now: update $\mathcal{G}$ and $\mathcal{E}$ at the end of level d and store the adjaceny sets of all nodes for the search of the right S

Limitation

Disadvantages:

- Adjacency sets and set S are possibly larger than in the original PC

  → more CI tests necessary

- Even more increased runtime than for the original PC

Possible Solution: Parallel PC-algorithm

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Idea

Parallelism:

- Break down big task into several different smaller subtasks
- Distribute them over different cores of the computer’s CPU

Idea

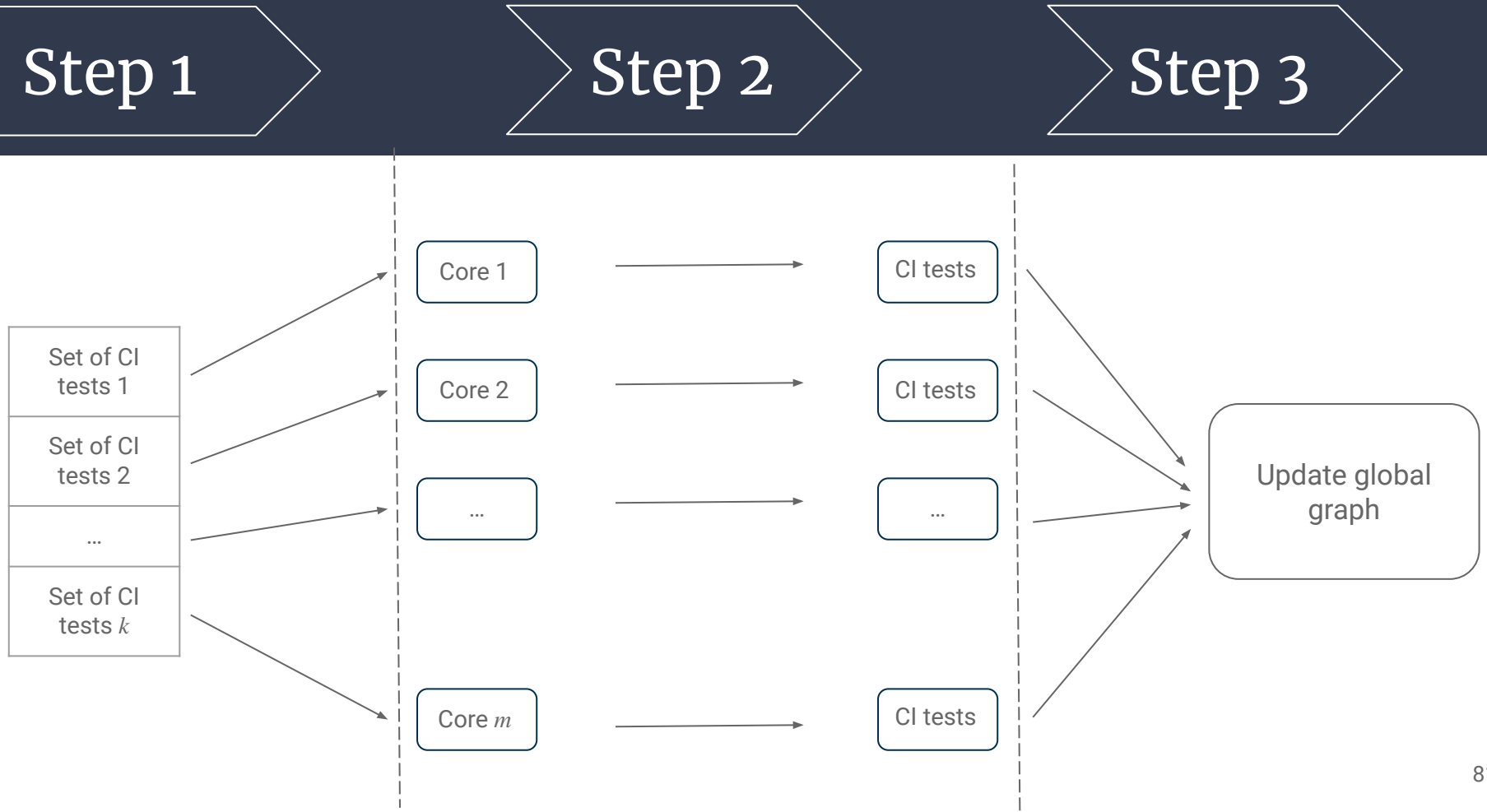
Parallelism:

- Break down big task into several different smaller subtasks
- Distribute them over different cores of the computer's CPU

Prerequisite: subtasks need to be independent

→ But: CI test results of particular level d influence CI test results of following level d + 1

→ Idea: parallelize CI tests within each level


Step 1
Step 2
Step 3
Set of CI tests 1
Set of CI tests 2
...
Set of CI tests k
Core 1
Core 2
...
Core m
CI tests
CI tests
...
CI tests
Update global graph

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Comparison of all previously discussed algorithms

Data simulation → CPDAG construction → Evaluation

Repeat the following steps:

1. Simulate random DAG $\mathscr{G}$
   - dimension p
   - sparsity s
2. Draw random samples from $\mathscr{G}$
   - sample size n
   - distribution

Run original/stable/parallel PC-algorithm with different settings for α = 0.01 and 10 simulations:

- dimension p
- sample size n
- ordering

Comparison of:

- Run time in s
- Structural Hamming Distance
- True Positive Rate
- False Positive Rate
- True Discovery Rate

Reference: Kalisch et al., 2012

Evaluation measures

Structural Hamming Distance (SHD)	Number of edge insertions, deletions or flips in order to transform **estimated** CPDAG to **true** CPDAG (or vice versa)
True Positive Rate (TPR)	Number of correctly found edges in **estimated** CPDAG divided by number of true edges in **true** CPDAG
False Positive Rate (FPR)	Number of incorrectly found edges in **estimated** CPDAG divided by number of true gaps in **true** CPDAG
True Discovery Rate (TDR)	Number of correctly found edges divided by number of found edges both in **estimated** CPDAG

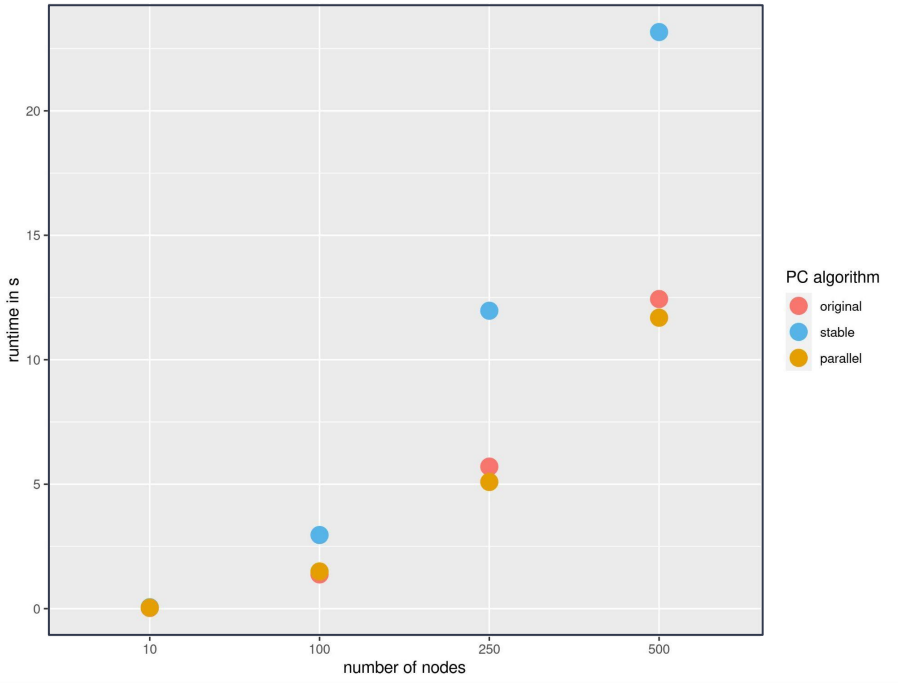
Reference: CRAN-documentation of *pcalg* package, 2022

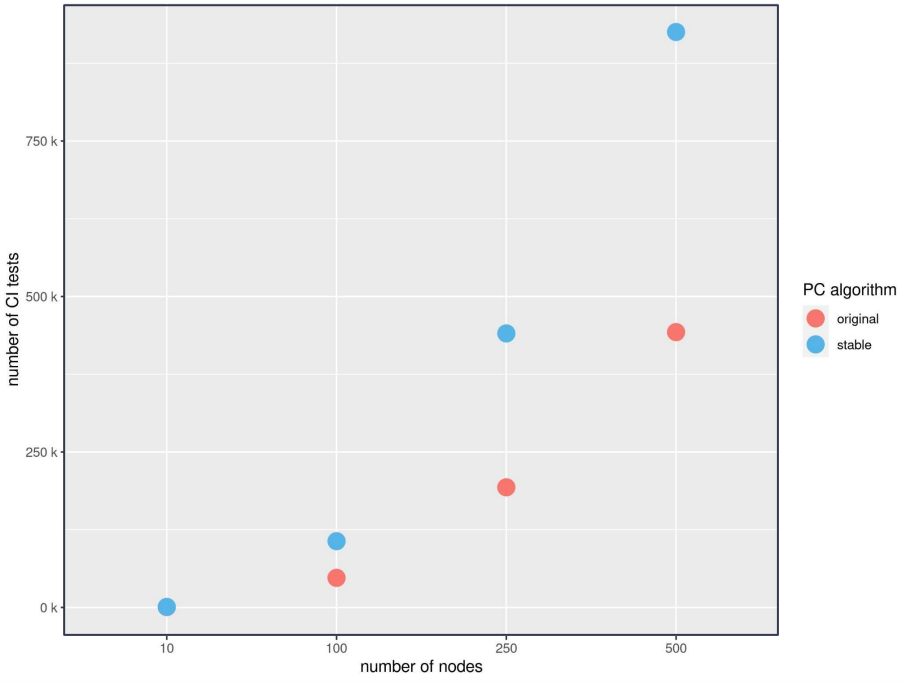
Setting 1: different dimensions

n = 1000

$p \in \{10, 100, 250, 500\}$

expected neighborhood size: 5





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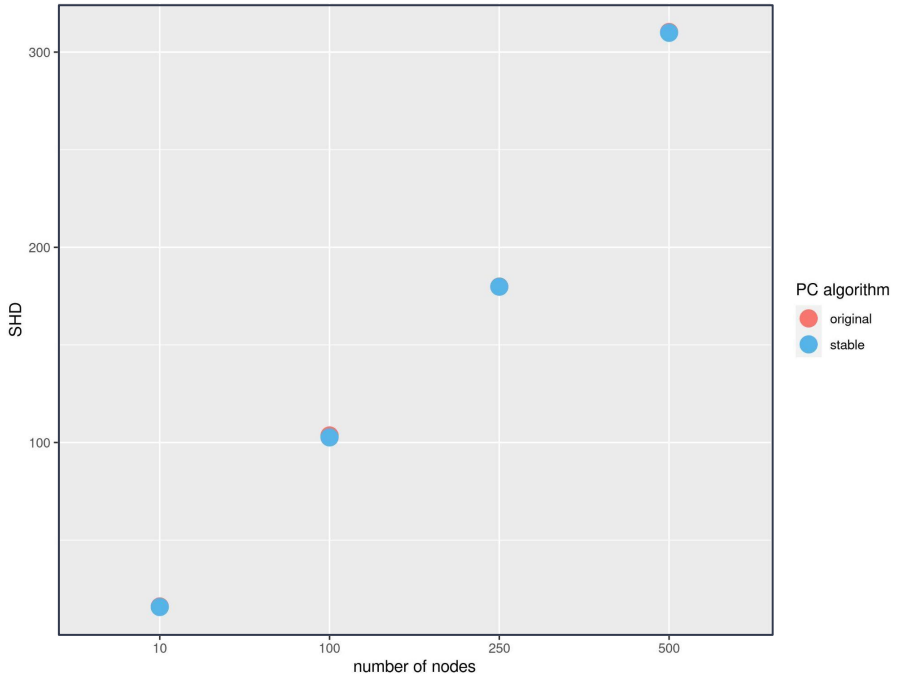

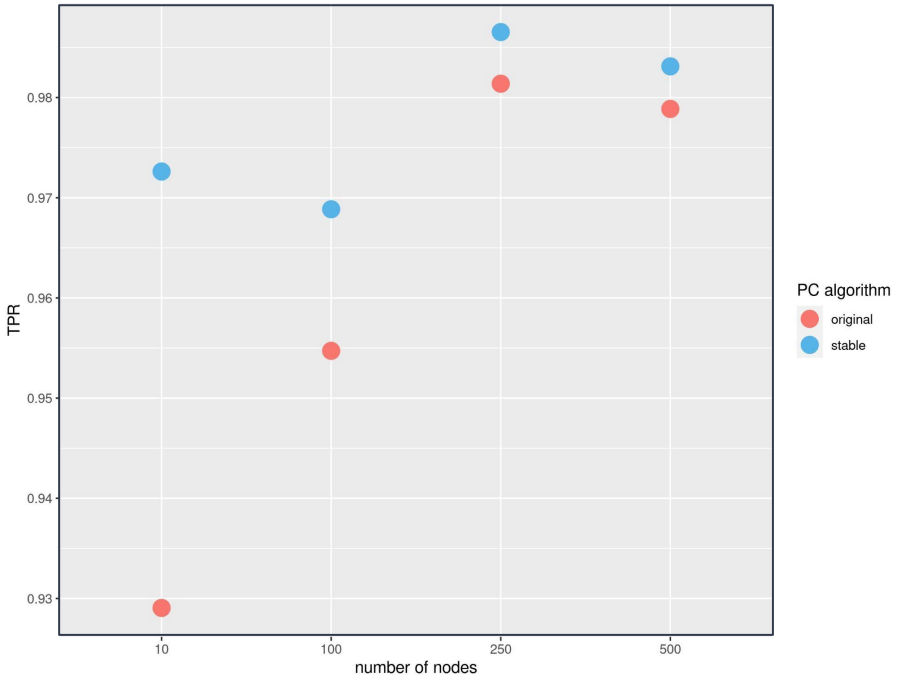

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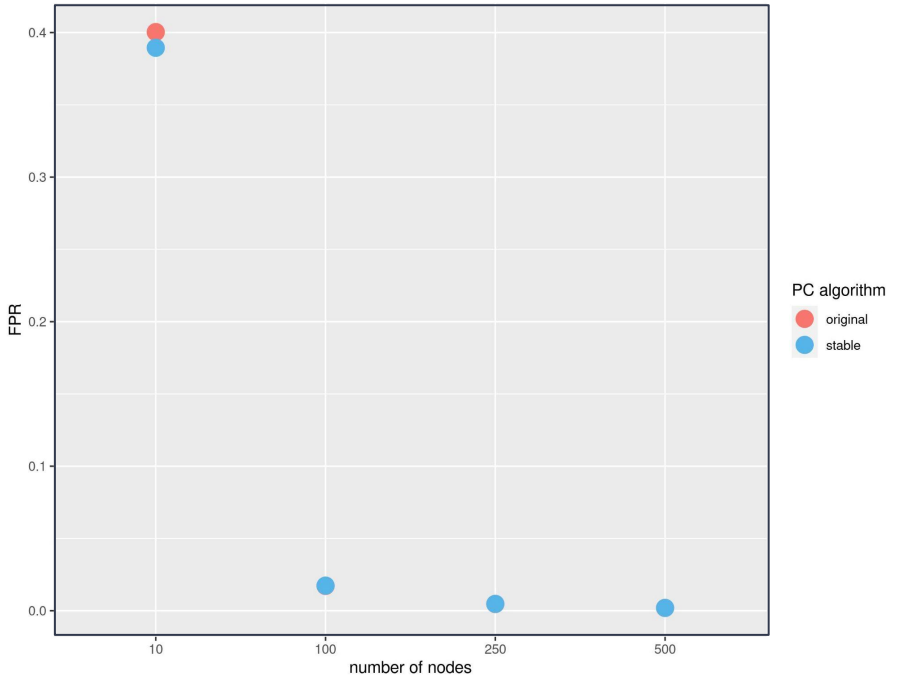
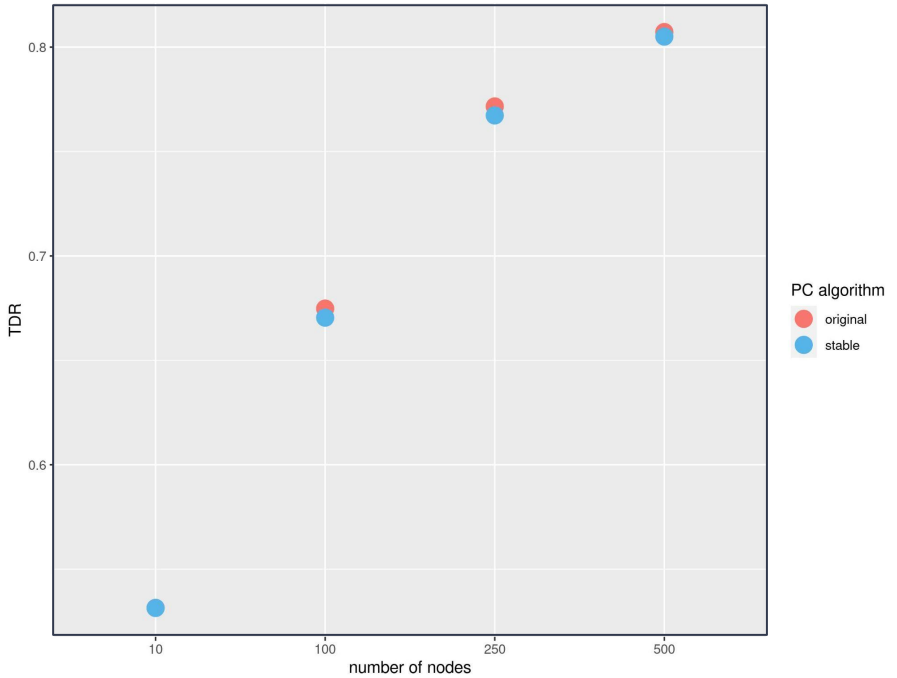


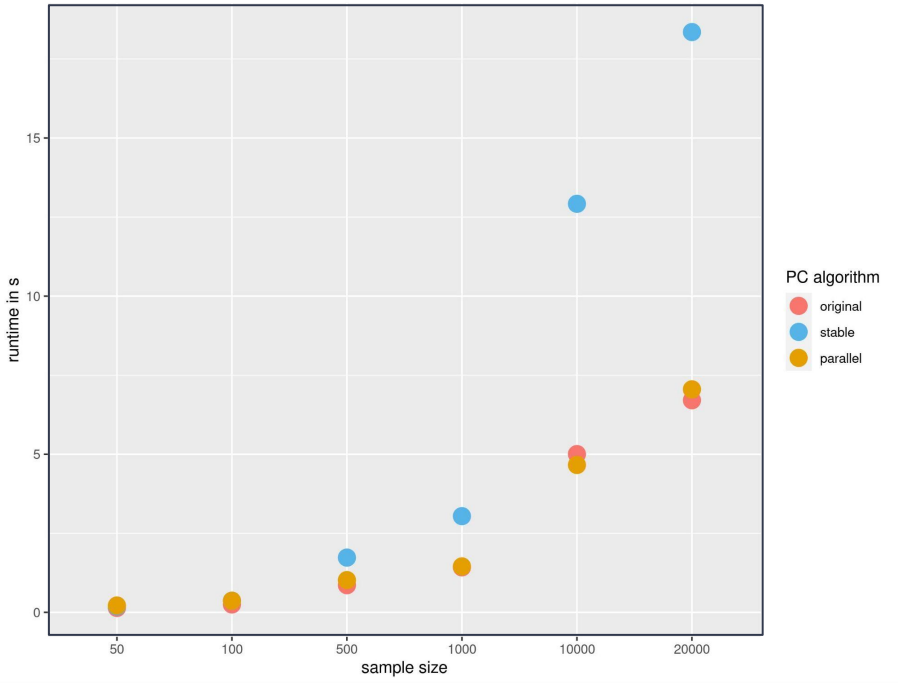


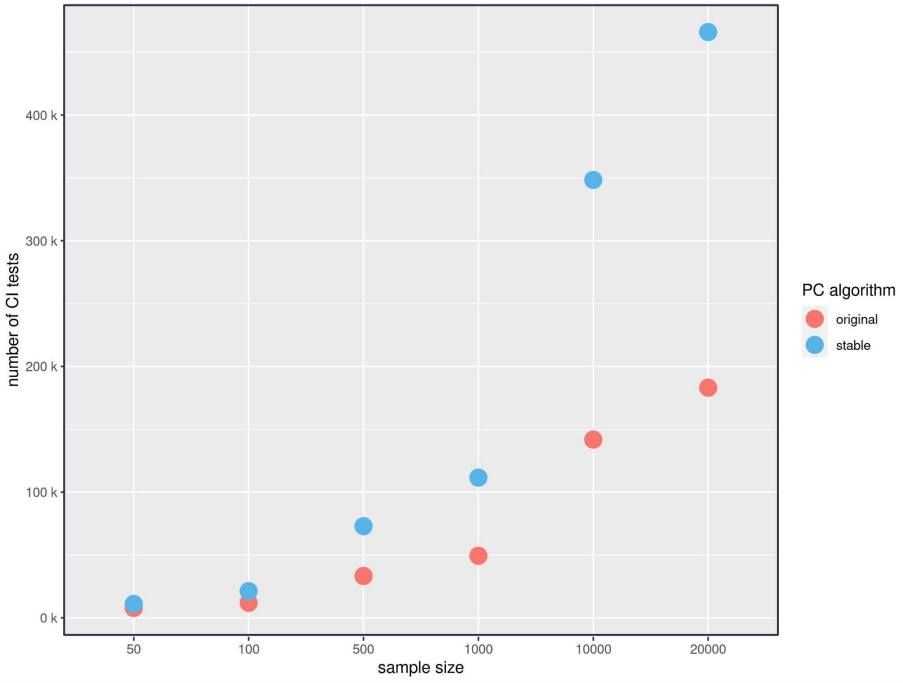
Setting 2: different sample sizes

$n \in \{50, 100, 500, 1k, 10k, 20k\}$

$p = 100$

expected neighborhood size: 5



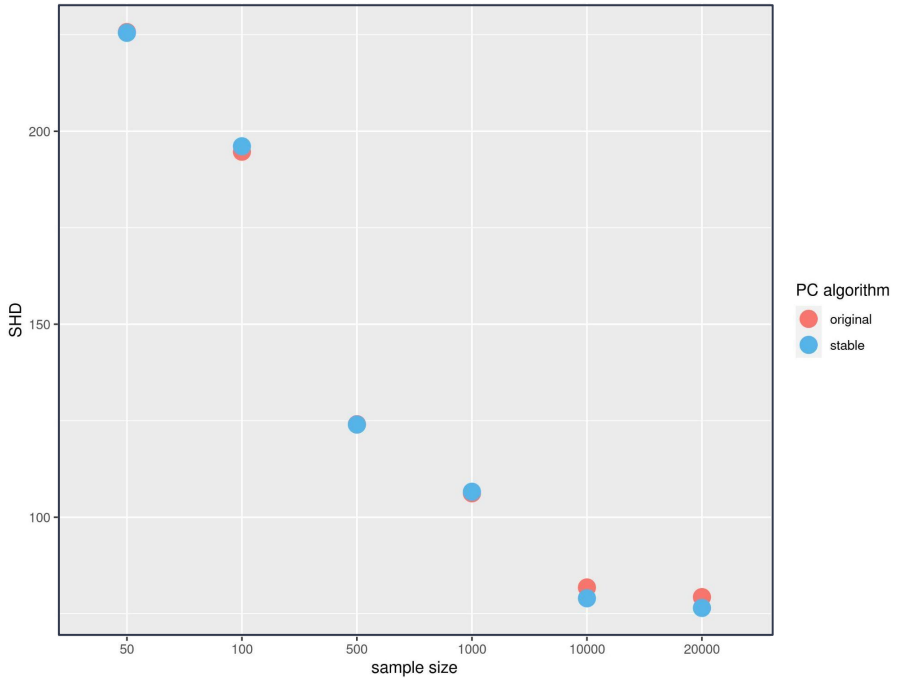


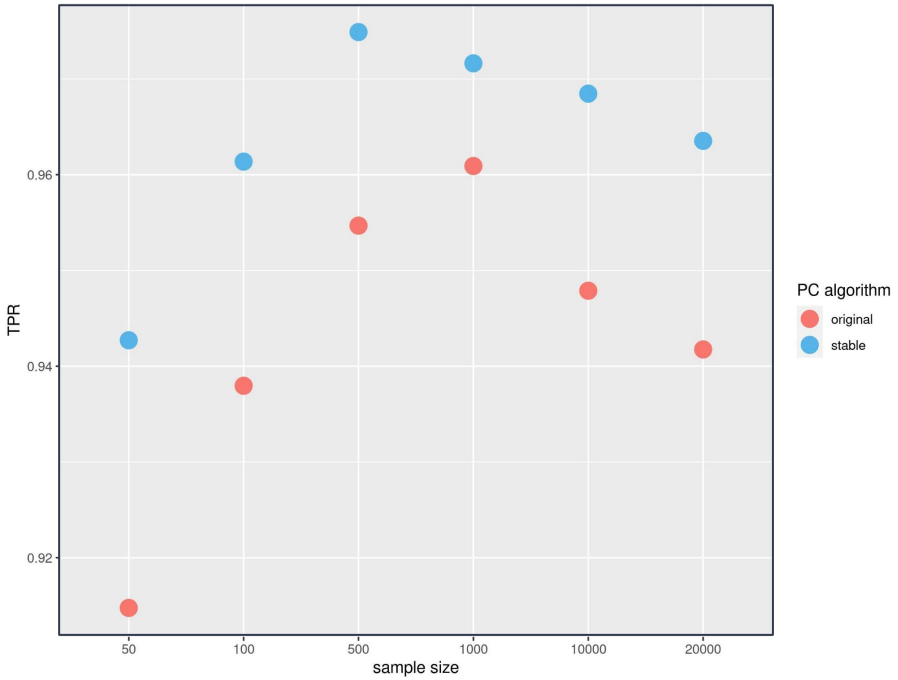
Setting 2: different sample sizes

$n \in \{50, 100, 500, 1k, 10k, 20k\}$

$p = 100$

expected neighborhood size: 5



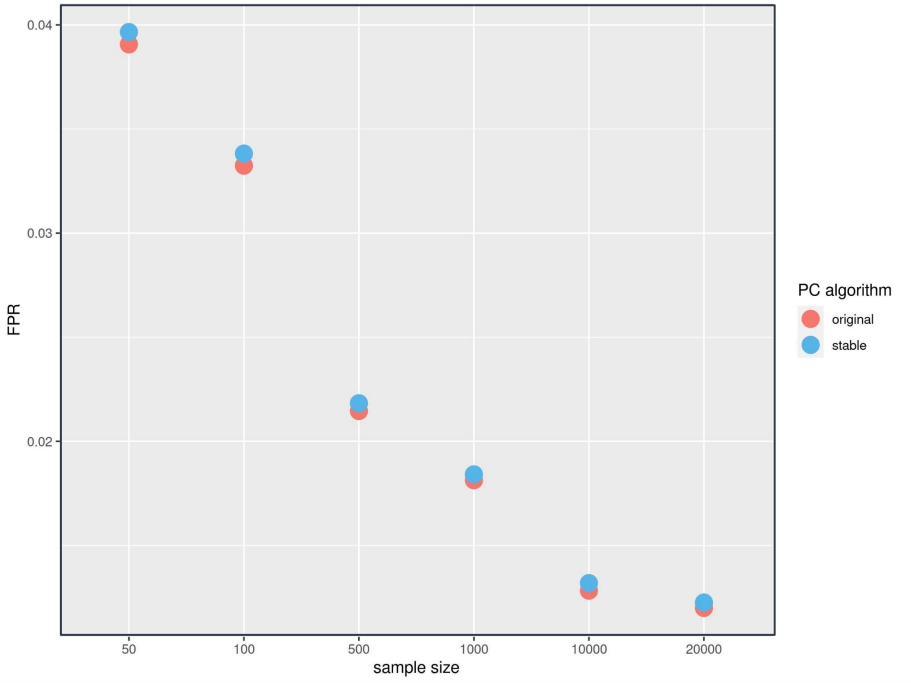


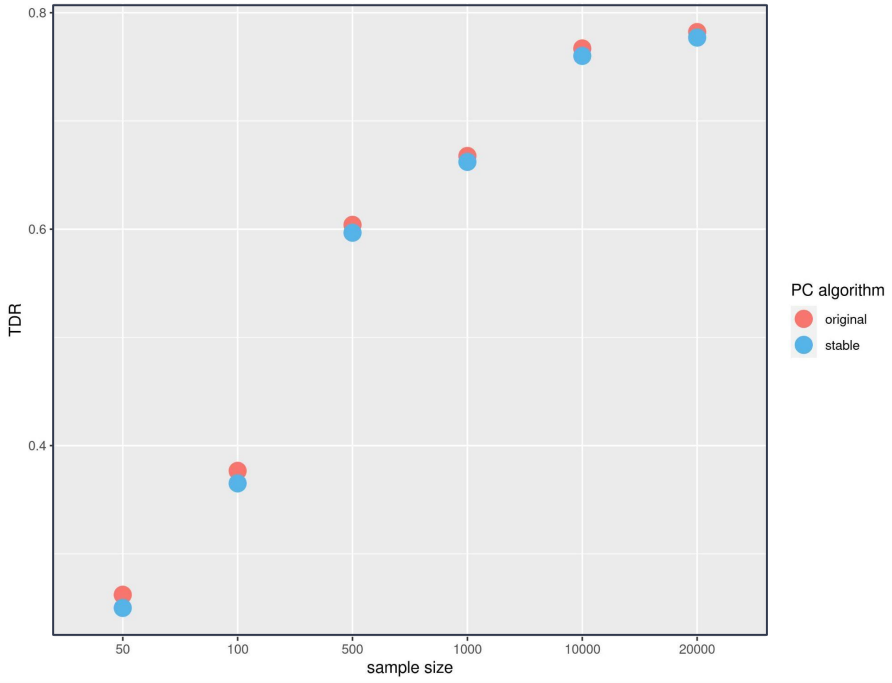
Setting 2: different sample sizes

$n \in \{50, 100, 500, 1k, 10k, 20k\}$

$p = 100$

expected neighborhood size: 5



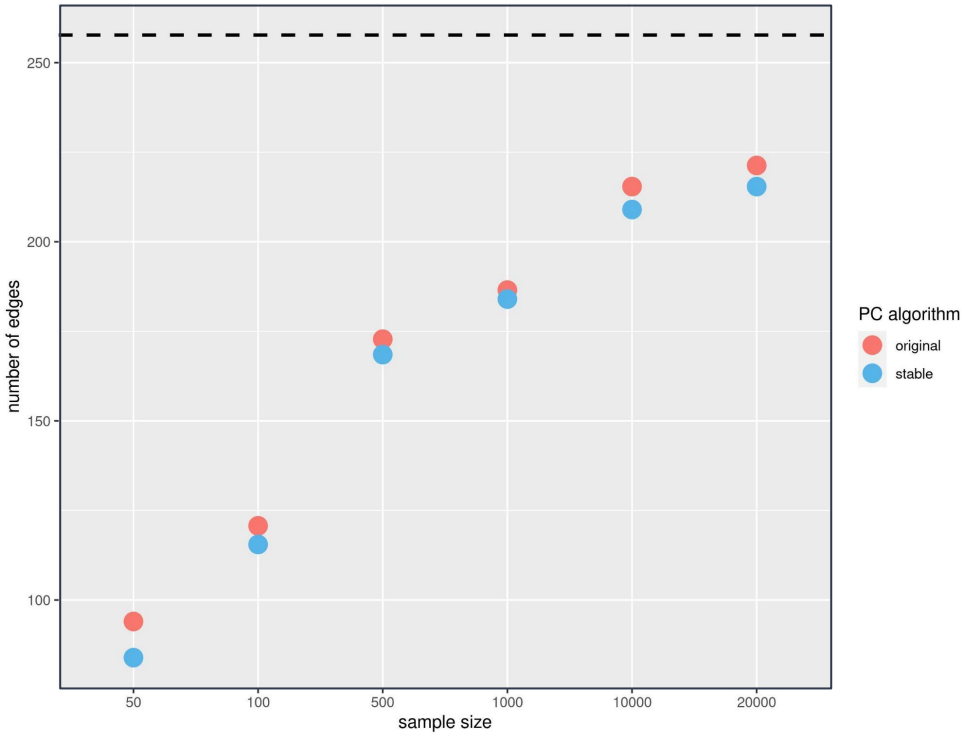


Setting 2: different sample sizes

$n \in \{50, 100, 500, 1k, 10k, 20k\}$

$p = 100$

number of simulations: 10

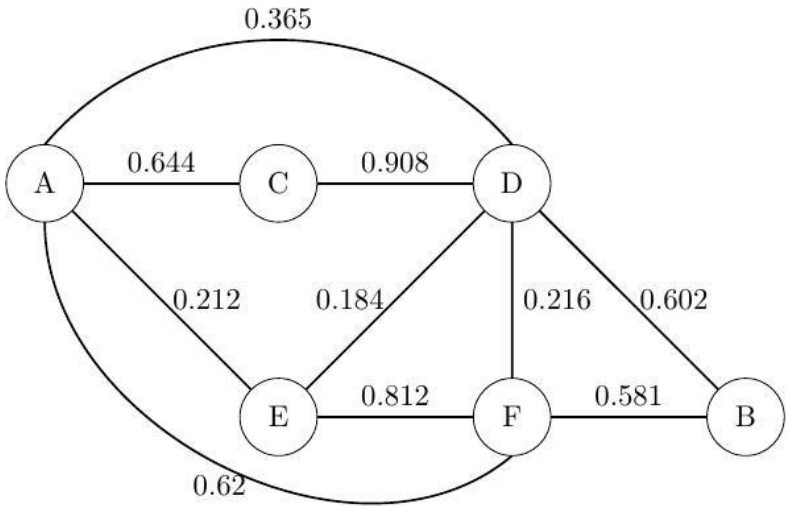


Setting 3: different ordering

Parameter settings:

- sample size: n = 20
- number of nodes: p = 6
- expected neighborhood size: 3
- significance level: α = 0.05
- 4 different orderings of variables

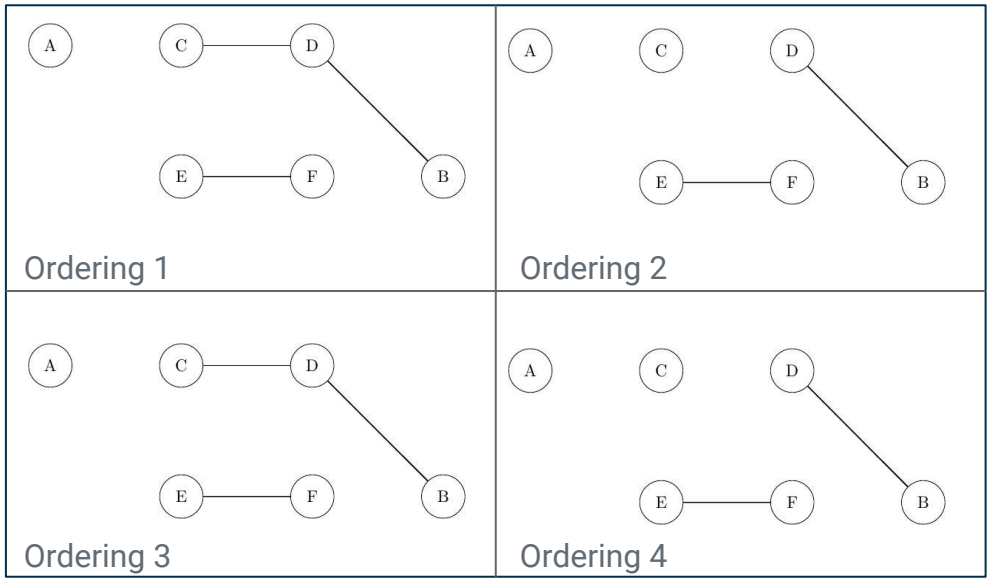
→ Compare different outcomes of original and stable PC-algorithm

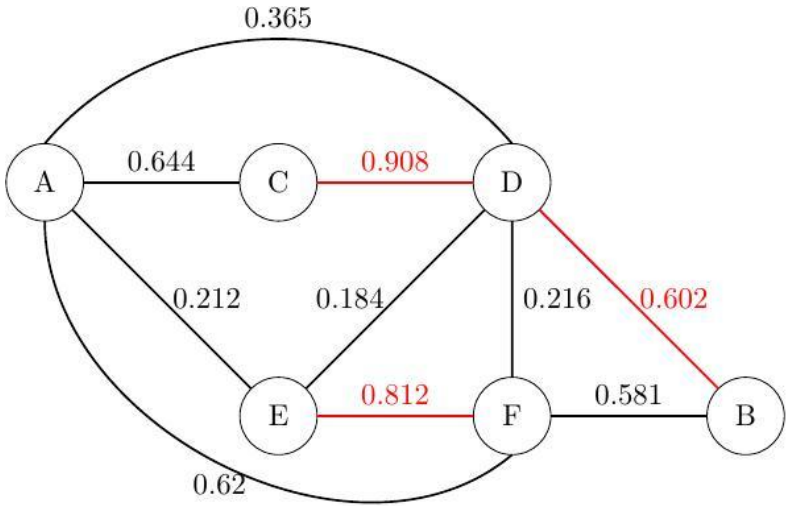


true weighted skeleton

Setting 3: different ordering

Results of original PC-algorithm

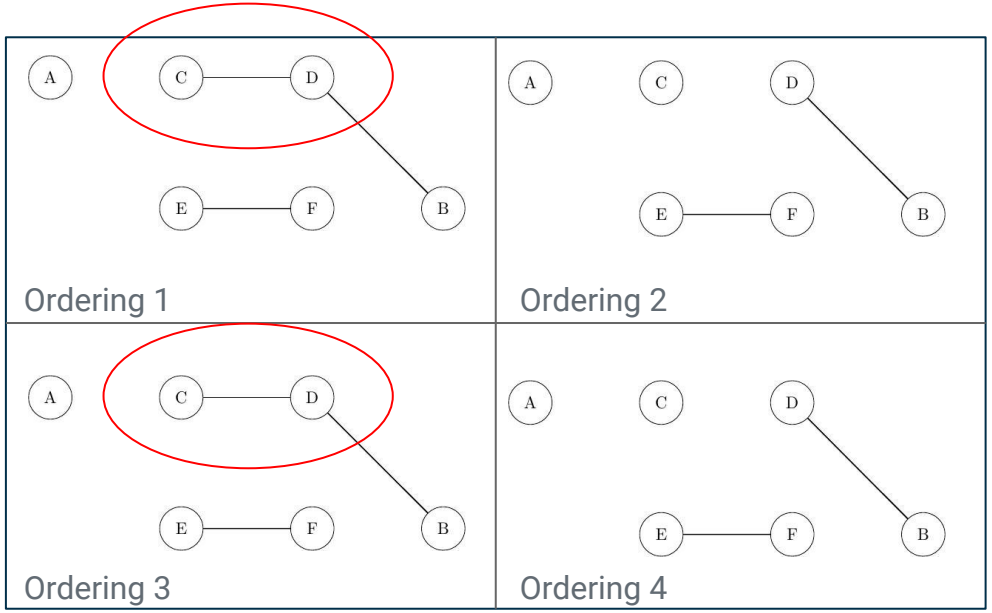


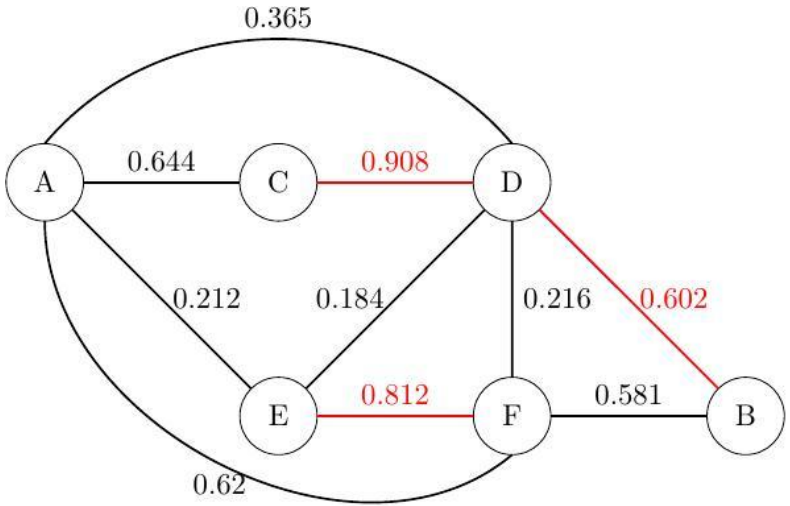


true weighted skeleton

Setting 3: different ordering

Results of original PC-algorithm

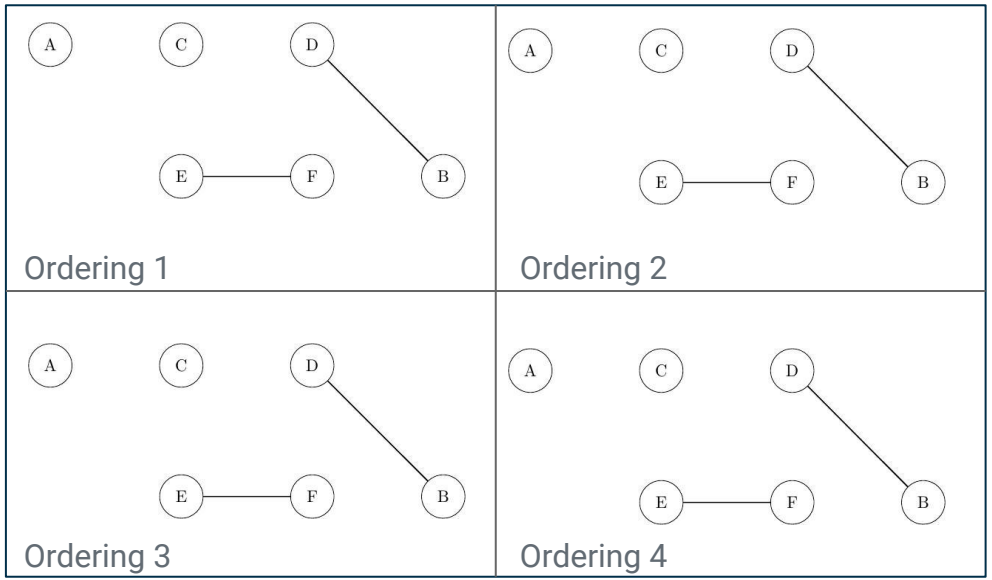


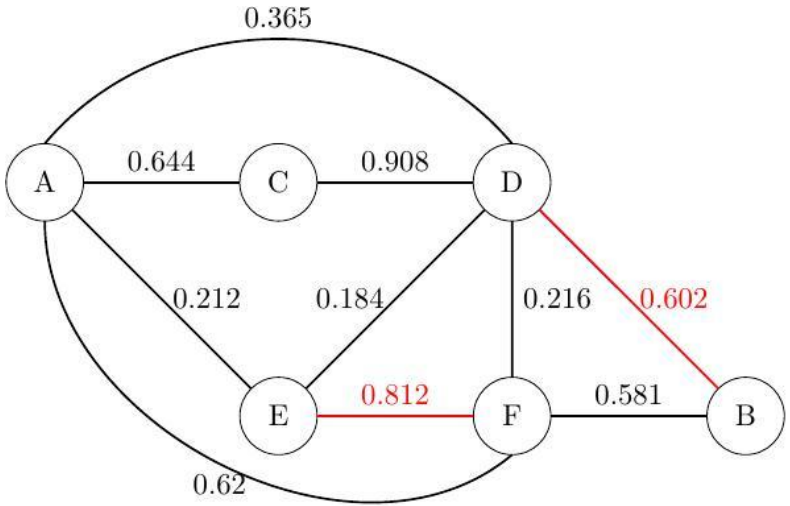


true weighted skeleton

Setting 3: different ordering

Results of stable PC-algorithm





true weighted skeleton

Setting 3: different ordering

Results for higher dimensions:

- sample size: n = 100
- number of nodes: p = 50
- significance level: α = 0.05
- sparsity: s = 0.06
- expected neighborhood size: 3
- 10 different orderings

ordering	1	2	3	4	5	6	7	8	9	10
original	106	108	110	110	110	108	110	110	110	106
stable	102	102	102	102	102	102	102	102	102	102

Table 1: Number of edges in the estimated skeleton for 10 different orderings estimated by original and stable PC-algorithm.

Results of the simulation study

- **Runtime:**
  - increasing the dimensionality and increasing the sample size increases the runtime
  - parallel PC is a lot faster than stable PC (especially with high number of cores)
  - original PC: similar to parallel because of less CI tests
- **Dimension:** increasing the dimensionality improves TPR, FPR and TDR, but SHD increases, too
- **Sample size:** increasing the sample size increases the goodness of fit except for TPR

Agenda

1) Basic Definitions
2) Introduction to the PC-Algorithm
3) Limitations of the PC-Algorithm
4) The stable PC-Algorithm
5) The parallel-PC-Algorithm
6) Simulation Study in R
7) **Final Notes and Discussion**

Conclusion

Goal of PC-algorithm: detecting conditional independence relationships between nodes in a DAG whose underlying data-generating distribution is faithful and multivariate normal and outputs the corresponding CPDAG

Ordering

Problem:

Output graph is dependent on the order in which CI tests are performed

Solution: Stable PC-algorithm

Runtime

Problem:

Many CI tests necessary

→ high runtime

Solution: Parallel PC-algorithm

Gaussian Distribution

Problem:

Consistency only holds for Gaussian distribution

→ what if it is non-Gaussian?

Solution: Rank PC-algorithm

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Harris N., Drton M. (2013). *PC Algorithm for Nonparanormal Graphical Models,* Journal of Machine Learning Research, 14, p. 3365-3383.

Le T.D., Hoang T., Li J., Liu L., Liu H., Hu S. (2014). *A fast PC algorithm for high dimensional causal discovery with multi-core PCs,* Journal of LaTeX class files, Vol. 13, No. 9.

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Kalisch M., Bühlmann P. (2007). *Estimating High-Dimensional Directed Acyclic Graphs with the PC-Algorithm,* Journal of Machine Learning Research, 8, p. 613-636.

Colombo D., Maathuis, M.H. (2012). *A modification of the PC algorithm yielding order-independant skeletons,* ArXiv e-prints.

Kalisch M., Mächler M., Colombo D., Maathuis, M.H., Bühlmann P. (2012). *Causal Inference Using Graphical Models with the R package pcalg,* Journal of Statistical Software, Vol. 47, Issue 11.

Backup

Faithfulness

Let the nodes $\mathcal{N}$ represent random variables $\boldsymbol{X} = (X_N)_{N \in \mathcal{N}}$.

The joint distribution $\mathcal{P}$ of $\boldsymbol{X}$ is **faithful** to DAG $\mathcal{G}$ if for any triple of pairwise disjoint subsets $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{S} \subseteq \mathcal{N}$, we have that $\boldsymbol{S}$ d-separates $\boldsymbol{A}$ and $\boldsymbol{B}$ if and only if $X_{\boldsymbol{A}}$ and $X_{\boldsymbol{B}}$ are conditionally independent given $X_{\boldsymbol{S}}$, i.e. $X_{\boldsymbol{A}} \perp X_{\boldsymbol{B}} \mid X_{\boldsymbol{S}}$.

→ not a strict assumption in practice as the majority of distributions is faithful

→ non-faithful distributions of the multivariate Gaussian family form a Lebesgue null-set in the space of distributions associated with a DAG

→ under faithfulness, statistical tests of conditional independence can be used to determine d-separation relations in a DAG

Assumptions

- Data-generating distribution is *faithful*

  → conditional independence relations can be read off the graph

- All nodes $\mathcal{N}$ correspond to multivariate *gaussian* distributed random variables

  → conditional independence can be inferred from partial correlations:

For a multivariate normal distributed random vector $\boldsymbol{X} \in \mathbb{R}^p$ denote its partial correlation between components $\boldsymbol{X}^{(i)}$ and $\boldsymbol{X}^{(j)}$ $(i \neq j)$ given set $\{\boldsymbol{X}^{(r)}, r \in \boldsymbol{R} \subseteq \{1, \dots, p\} \setminus \{i, j\}\}$ by $\rho_{i,j \mid \boldsymbol{R}}$.

Then it holds:

$\rho_{i,j \mid \boldsymbol{R}} = 0$ if and only if $\boldsymbol{X}^{(i)}$ and $\boldsymbol{X}^{(j)}$ are *conditionally independent* given $\{\boldsymbol{X}^{(r)}, r \in R\}$.

The CI test in detail

Recursive estimation of $\rho_{i,j \mid \boldsymbol{r}}$ (Kalisch and Bühlmann, 2007):

$\rho_{i,j \mid \varnothing}$: regular correlation coefficient

For some $t \in R$:

$$\rho_{i,j \mid \boldsymbol{R} \setminus t} = \frac{\rho_{i,j \mid \boldsymbol{R} \setminus t} - \rho_{i,t \mid \boldsymbol{R} \setminus t}\, \rho_{j,t \mid \boldsymbol{R} \setminus t}}{\sqrt{(1 - \rho^2_{i,t \mid \boldsymbol{R} \setminus t})\,(1 - \rho^2_{j,t \mid \boldsymbol{R} \setminus t})}}$$

(iteratively increase set R)

Idea of the rank PC-algorithm (RPC)

Replace the standard Pearson-type correlation by **rank-based** measures of correlation in the CI tests:

1) Estimate Spearman's ρ:

$$\hat{\rho}^S = \frac{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{\mathrm{rank}(X_i)}{n+1}-\frac{1}{2}\right)\left(\frac{\mathrm{rank}(Y_i)}{n+1}-\frac{1}{2}\right)}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{\mathrm{rank}(X_i)}{n+1}-\frac{1}{2}\right)^2}\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{\mathrm{rank}(Y_i)}{n+1}-\frac{1}{2}\right)^2}} = 1-\frac{6}{n\left(n^2-1\right)}\sum_{i=1}^{n}\left(\mathrm{rank}(X_i)-\mathrm{rank}(Y_i)\right)^2$$

2) Estimate the corresponding correlation matrix
3) Determine partial correlations
4) Test for conditional independence

} same procedure as in original PC-algorithm

Consistency for high-dimensional data

Theorem 3 (Kalisch and Bühlmann, 2007) :

Under the assumption that the data are realisations from independent *multivariate* Gaussian random vectors s.t. their distribution is *faithful* to a suitably *sparse* DAG $\mathcal{G}$ and an additional regularity assumption, both step 1 and step 2 of the PC-algorithm are consistent for high-dimensional data, i.e. there exists $\alpha_n \to 0$ $(n \to \infty)$ and $\beta_n \to 0$ $(n \to \infty)$ such that

$$\mathbb{P}(\mathcal{G}_{\text{skel},n,\text{ PC}}(\alpha_n) = \mathcal{G}_{\text{skel},n,\text{ true}}) = 1 - \mathcal{O}(\exp(-Cn^{1-2d})) \to 1 \quad (n \to \infty) \text{ for some } 0 < C < \infty \text{ and } 0 < d < 0.5$$

and

$$\mathbb{P}(\mathcal{G}_{\text{CPDAG, PC}}(\alpha_n) = \mathcal{G}_{\text{CPDAG, true}}) = 1 - \mathcal{O}(\exp(-Cn^{1-2d})) \to 1 \quad (n \to \infty) \text{ for some } 0 < C < \infty \text{ and } 0 < d < 0.5$$

This result holds for all three presented PC-algorithms.

In Theory: the “perfect” significance level α

Kalisch and Bühlmann, 2007, showed in their proof of the consistency of the PC-algorithm that in theory

$$\alpha = \alpha_n = 2\,(1 - \Phi(n^{0.5}\, c_n / 2))$$

which depends on the unknown lower bound c_n of partial correlations

$$\inf\{|\rho_{i,j\,|\,\boldsymbol{R}}|\colon i, j, R \text{ with } \rho_{i,j\,|\,\boldsymbol{R}} \neq 0\} \geq c_n.$$

That means that increasing the sample size we should ideally decrease the significance level.

Runtime of the different PC-algorithms

- original PC (Kalisch and Bühlmann, 2007):
  - worst case: exponential in number of nodes
  - but: if true underlying DAG is sparse, polynomial in number of nodes (often reasonable assumption in practice)
- stable PC:
  - especially for higher dimensions number of CI tests increases exponentially (see simulation study)

    → even higher runtime
- parallel PC:
  - simulation study shows that parallel PC has best runtime of all three for higher dimensions

Sketch: Proof of Theorem 1

Suppose that A and B are not adjacent, and A is not an ancestor of B. Let the total order *Ord* on the variables in $\mathcal{G}$ be such that all ancestors of A and all ancestors of B except for A are prior to A, and all other nodes are after A.

Then $S(\mathcal{G}, A)$ for order *Ord* is a subset of D-SEP(A, B). Hence one can show that if B is not in D-SEP(A, B) then D-SEP(A, B) d-separates A from B in G. B is in D-SEP(A, B) if and only if there is a path from A to B in which each node except the endpoints is a collider on the path, and each node on the path is an ancestor of A or B.

But then there is an inducing path between A and B, and one can show that A and B are adjacent, contrary to the assumption.

Reference: Sprites et al., 2000

Sketch: Proof of Theorem 2

- Faithfulness assumption → conditional independence in joint distribution of the nodes is equivalent to the d-separation relations
- Determination of the skeleton: two variables in a DAG are d-separated by a subset of the remaining variables if and only if they are d-separated by their parent nodes
- PC-algorithm is guaranteed to check these conditional interdependencies: at any point in the algorithm the current graph is a supergraph of the true CPDAG and the algorithm checks conditional independencies given all subsets of the adjacency sets (which include the parent sets)

Reference: Colombo and Maathuis, 2012

The parallel PC-Algorithm

Three-stage process within each level d :

Step 1: Distribute CI tests evenly among the cores by grouping CI tests of same edge together.

Step 2: Each core performs its set of CI tests in parallel with other cores.

Step 3: Integrate CI test results from all cores into global graph.

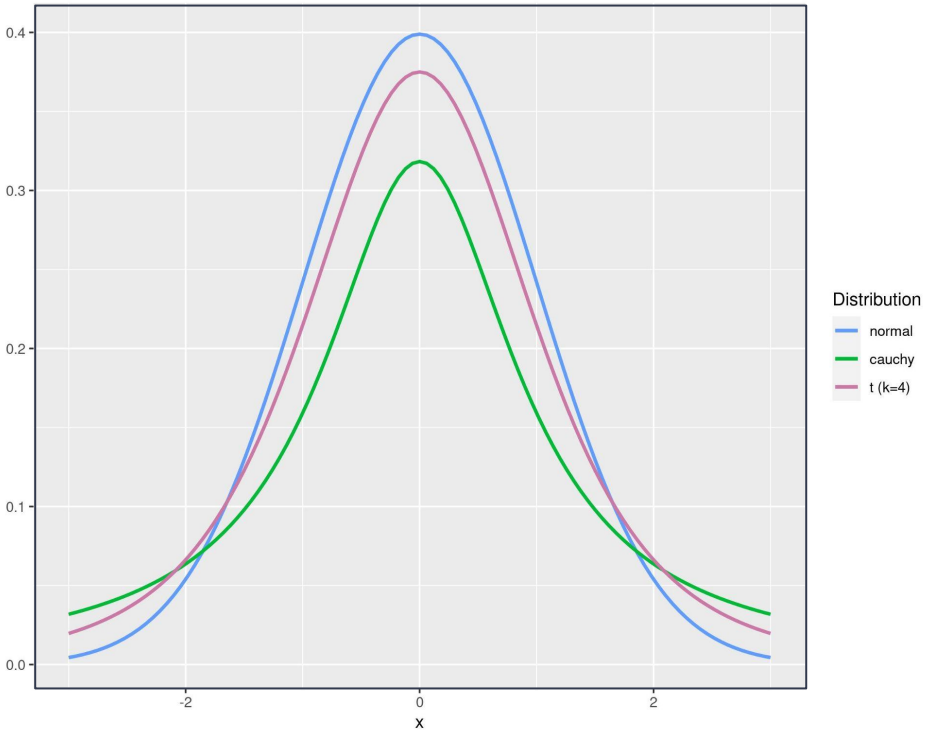
Possible extension for big data sets: additional memory-efficient indicator to detect free memory

Setting: different distributions

$n \in \{100, 1000\}$

$p \in \{10, 100\}$

expected neighborhood size: 3



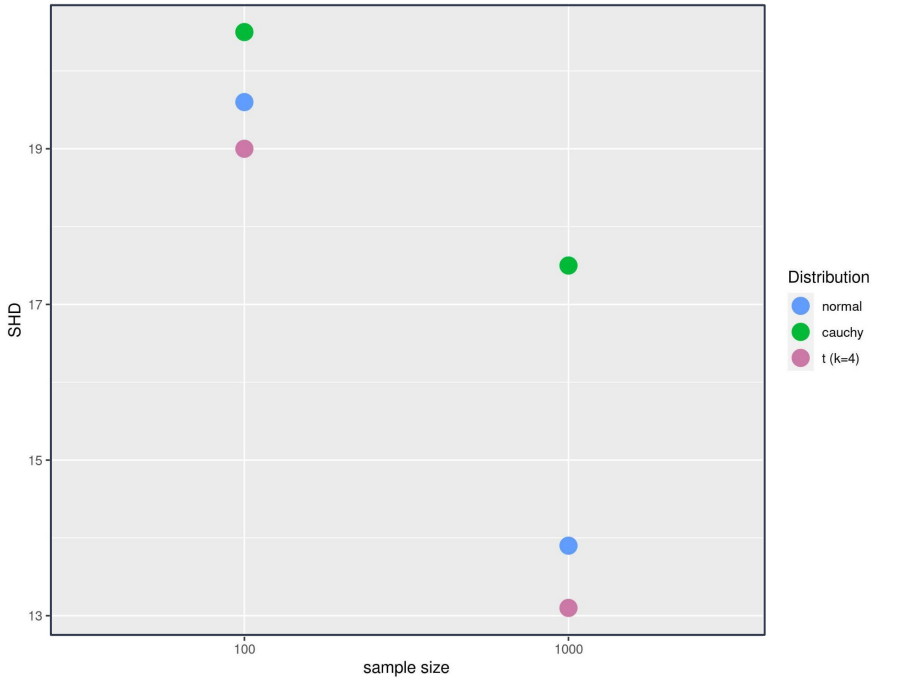
Setting: different distributions

$n \in \{100, 1000\}$

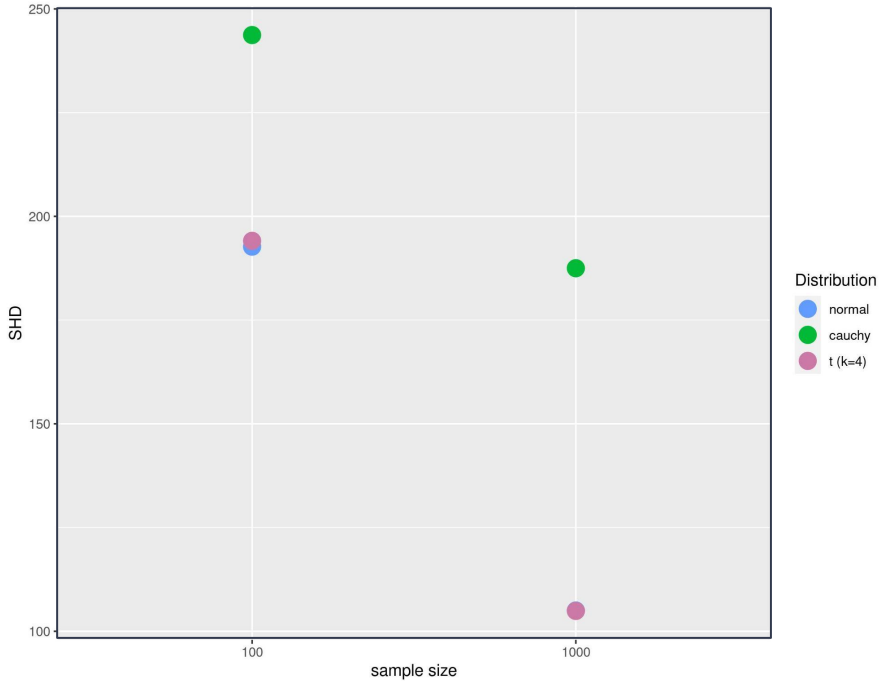
$p \in \{10, 100\}$

expected neighborhood size: 3

p = 10



p = 100

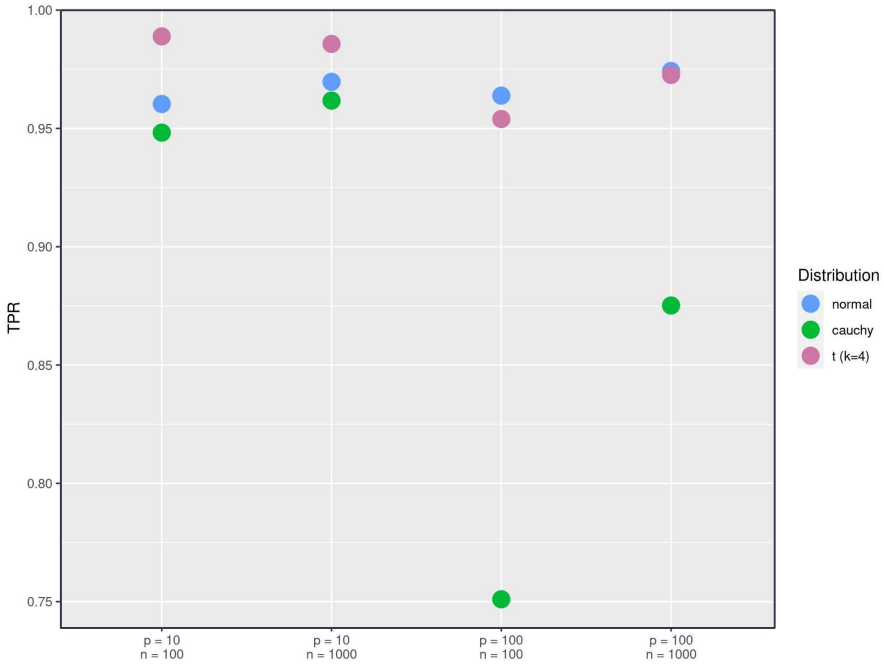


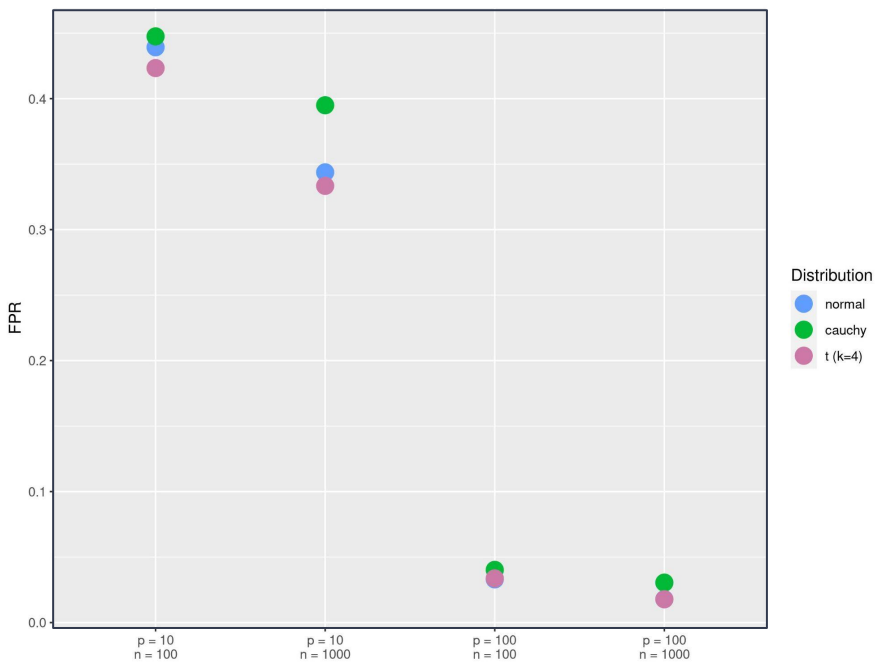
Setting: different distributions

$n \in \{100, 1000\}$

$p \in \{10, 100\}$

expected neighborhood size: 3



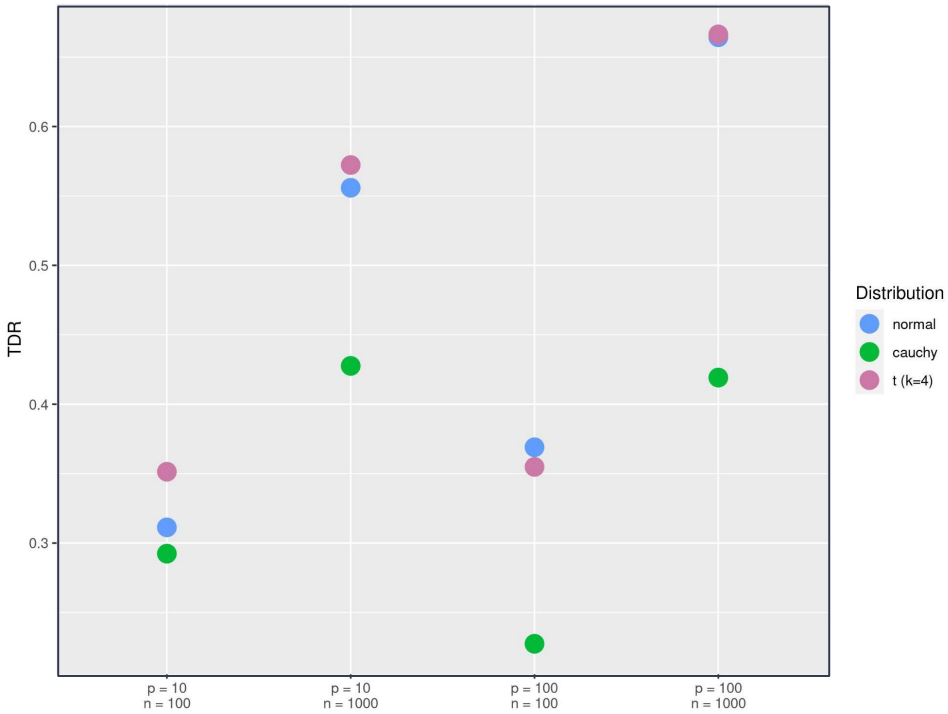


Setting: different distributions

$n \in \{100, 1000\}$

$p \in \{10, 100\}$

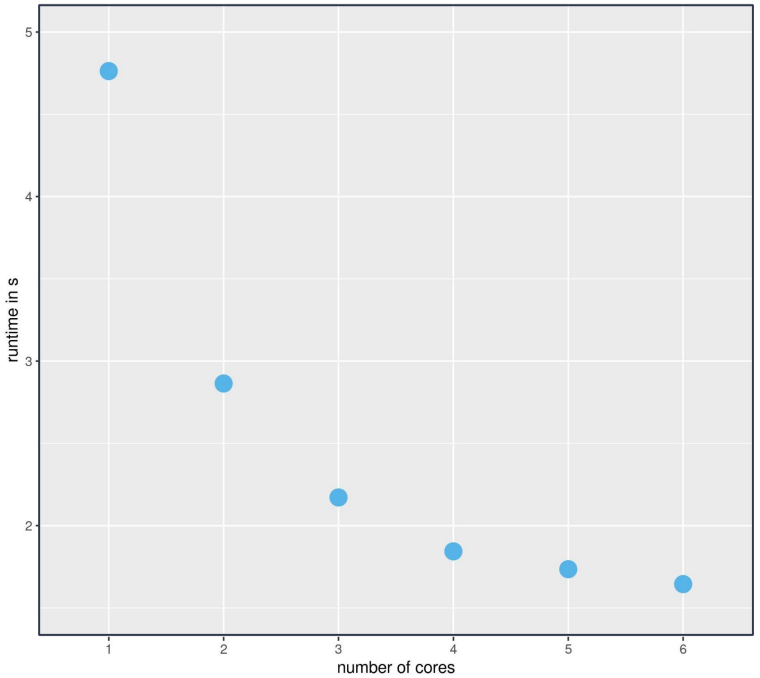
expected neighborhood size: 3



Setting: different number of cores

Parameter settings for parallel PC-algorithm:

- sample size: n = 1000
- number of nodes: p = 100
- expected neighborhood size: 30
- number of cores: 1 to 6



Conclusion

- The PC-algorithm detects conditional independence relationships between nodes in a DAG whose underlying data-generating distribution is faithful and multivariate normal.
- The output is the CPDAG, the representant of the Markov equivalence class of the true graph, if the conditional independence relationships are known.
- Two-Step-Computation via learning the skeleton and orienting edges
- Limitations of the original PC:
    - ordering → stable PC: update edge set and graph in the end of each level, not in between
    - runtime → parallel PC: run stable PC on multiple cores
    - normal distribution → rank PC: adapt CI test to be more robust

Possible extensions of the PC-algorithm

- **Conservative PC-algorithm** (CPC) by Ramsey et al. (1995): weaker form of faithfulness
- **Fast Causal Inference algorithm** (FCI) by Spirtes et al. (1999): Learn a Markov equivalence class of DAGs with latent and selection variables
- **Cyclic causal discovery** (CCD) by Richardson (1996): Learn Markov equivalence classes of directed (not necessarily acyclic) graphs under the assumption of causal sufficiency
- **Score-based** and **hybrid** methods

Reference: Causal Inference - Theory and Applications in Enterprise Computing by Dr. Matthias Uflacker, Johannes Huegle, Christopher Schmidt, 2019