Causal discovery: constraint-based methods

Charles K. Assaad, Emilie Devijver, Eric Gaussier

charles.assaad@ens-lyon.fr

Table of content

Preliminaries

Causal discovery with causal sufficiency

Tests

Conclusion

Table of content

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Conclusion

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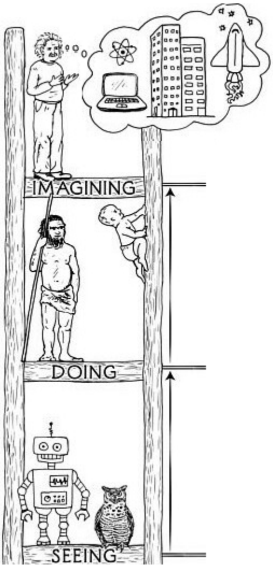

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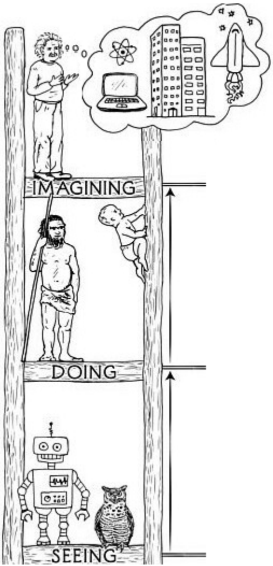

Where does a causal graph come from?

- Theory
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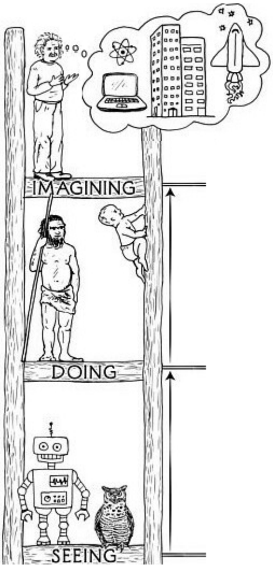
  - Costly
- Observations
  - Correlation does not imply causation!



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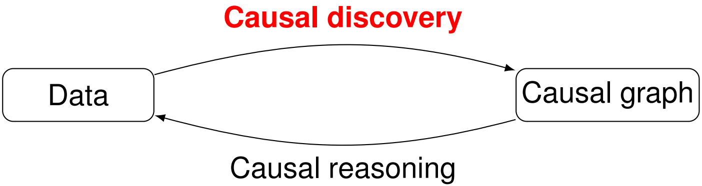

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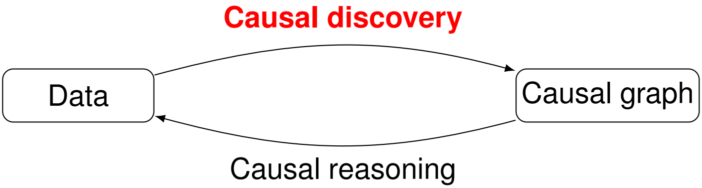

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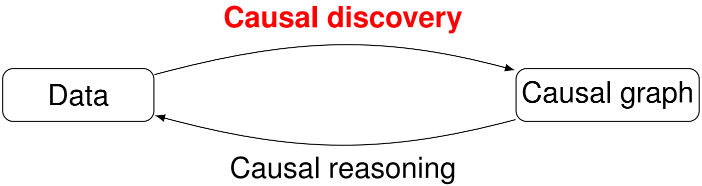

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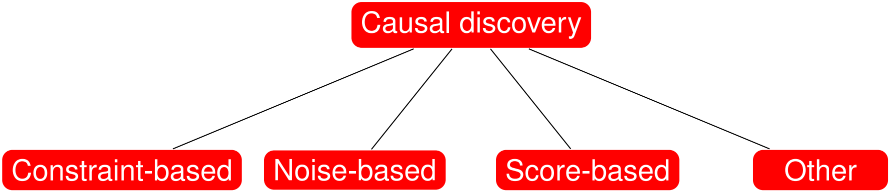
But it is possible under **additional assumptions**.

Causal discovery (2/2)



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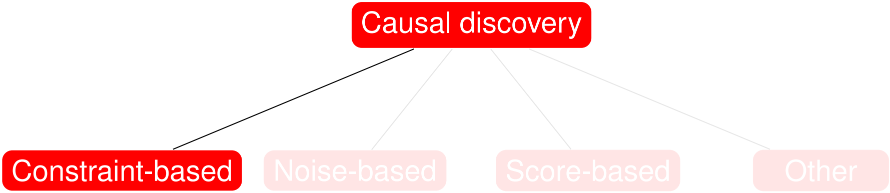

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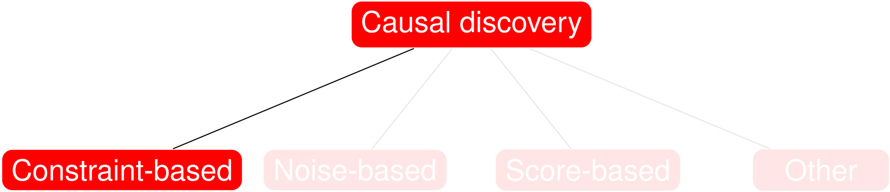

Constraint-based: run local tests of independence to create constraints on space of possible graphs.

Recap about causal graphical models (1/2)

Parental Markov Condition Given $\mathcal{G} = (\mathcal{V}, \mathcal{E})$,

$$\forall X \in \mathcal{V}, X \perp\!\!\!\perp_P \mathcal{V} \backslash \{Parents(X), Descendants(X)\} \mid Parents(X).$$

Causal sufficiency

$$\forall X \leftarrow Z \rightarrow Y, \text{ if } X, Y \in \mathcal{V} \text{ then } Z \in \mathcal{V}.$$

Skeleton the skeleton of a DAG $\mathcal{G}$ is an undirected graph with same adjacencies as $\mathcal{G}$.

Collider $X \rightarrow Z \leftarrow Y$.

V-structure (or unsheilded colliders, or immorality) If the two parent vertices are not adjacent, the collider is a v-structure.

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Theorem (probabilistic implications of d-separation) Given a DAG $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, a distribution $P(\mathcal{V})$ compatible with $\mathcal{G}$ and disjoint sets $\mathcal{X}, \mathcal{Y}, \mathcal{Z} \subset \mathcal{V}$:

(i) $\mathcal{X} \perp\!\!\!\perp_G \mathcal{Y} | \mathcal{Z} \Rightarrow \mathcal{X} \perp\!\!\!\perp_P \mathcal{Y} | \mathcal{Z}$ in every distribution P compatible with $\mathcal{G}$ (Also known as the global Markov property);

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A characterization of Markov equivalence classes for DAGs (1/2)

Completed partially directed acyclic graph (CPDAG) Let $[\mathcal{G}]$ be the Markov equivalence class of a DAG $\mathcal{G}$. The CPDAG $\mathcal{G}^*$ of $\mathcal{G}$ is the graph:

- With the same skeleton as $\mathcal{G}$;
- Where an edge is directed in $\mathcal{G}^*$ iff it occurs as a directed edge with the same orientation in every graph in $[\mathcal{G}]$;
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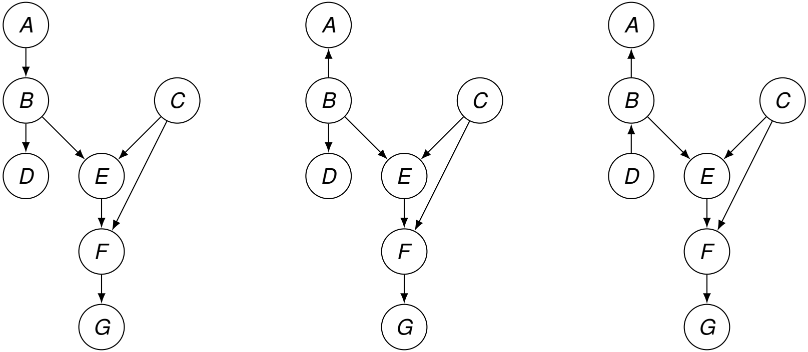

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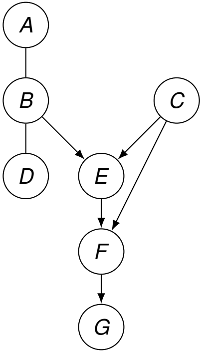

Constraint based question

Main question: Given $P(\mathcal{V})$ a compatible probability distribution of $\mathcal{G}$, can we discover $\mathcal{G}^*$ the CPDAG of $\mathcal{G}$?

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Because $X \perp\!\!\!\perp_P Y \mid Z \not\Longrightarrow X \perp\!\!\!\perp_G Y \mid Z$.

Faithfulness

Faithfulness We say that a graph $\mathcal{G}$ and a compatible probability distribution P are faithful to one another if all and only the conditional independence relations true in P are entailed by the Markov condition applied to $\mathcal{G}$.

faithfulness and d-sep

Theorem (implication of faithfulness on d-sep) $P(\mathcal{V})$ is faithful to directed acyclic graph $\mathcal{G}$ with vertex set $\mathcal{V}$ iff for all disjoint sets of vertices $\mathcal{X}, \mathcal{Y}, \mathcal{Z} \subset \mathcal{V}$, $\mathcal{X} \perp\!\!\!\perp_P \mathcal{Y} \mid \mathcal{Z}$ iff $\mathcal{X} \perp\!\!\!\perp_G \mathcal{Y} \mid \mathcal{Z}$.

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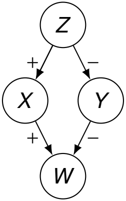
Violation of faithfulness (1/2)

Example 1: Canceling out

Consider



where

- $Z = \epsilon_z$
- $X = a_{zx} \times Z + \epsilon_x$
- $Y = a_{zy} \times Z + \epsilon_y$
- $W = a_{xw} \times X - \frac{a_{zx} a_{xw}}{a_{zy}} \times Y + \epsilon_w$

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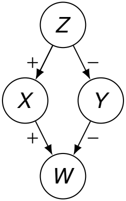

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By canceling out

- $Z \perp\!\!\!\perp_P W$

Violation of faithfulness (2/2)

Example 2: Determinism

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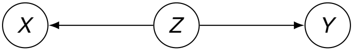

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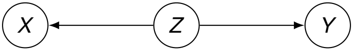

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By determinism

- $X \perp\!\!\!\perp_P Z \mid Y$

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Finding skeleton and v-structures

Theorem (faithfulness, adjacencies and v-structures) If $P(\mathcal{V})$ is faithful to some directed acyclic graph, then $P(\mathcal{V})$ is faithful to directed acyclic graph $\mathcal{G}$ with vertex $\mathcal{V}$ iff:

- For $X, Y \in \mathcal{V}$, X and Y are adjacent iff $\forall \mathcal{S} \subseteq \mathcal{V} \backslash \{X, Y\}$, $X \not\perp\!\!\!\perp_P Y \mid \mathcal{S}$;
- For $X, Y, Z \in \mathcal{V}$ such that X is adjacent to Z and Z is adjacent to Y and X and Y are not adjacent, $X \rightarrow Z \leftarrow Y$ in $\mathcal{G}$ iff $\forall \mathcal{S} \in \mathcal{V} \backslash \{X, Y\}$ such that $Z \in \mathcal{S}$, $X \not\perp\!\!\!\perp_P Y \mid \mathcal{S}$.

(proof in (Verma and Pearl, 1992))

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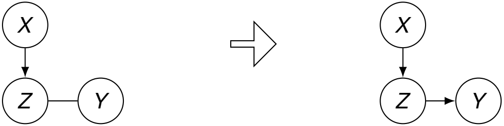
- Point 1 can be used to discover the skeleton of $\mathcal{G}$ from $P(\mathcal{V})$;
- Given the skeleton of $\mathcal{G}$, point 2 can be used to find all v-structures.

Orientation rules

R1:



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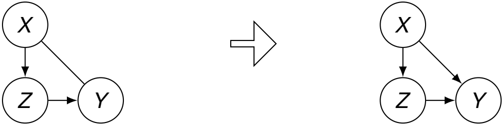
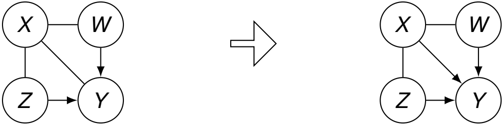


R3:



Orientation rules correctness

Pattern A pattern of a DAG $\mathcal{G}$ is a graph with the same skeleton as $\mathcal{G}$ but where only v-structures are oriented.

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Theorem (orientation soundness) Given a pattern of some DAG, the three orientation rules $R1$, $R2$, $R3$ are sound.
(proof on board)

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Theorem (orientation completeness) The result of recursively applying rules $R1$, $R2$, $R3$ to a pattern of some DAG is a CPDAG.
(proof in (Meek, 1995))

The SGS algorithm

Algorithm 1 SGS

Input: $P(\mathcal{V})$
Output: CPDAG $\mathcal{G}^*$

Form the complete undirected graph $\mathcal{G}^*$ on vertex set $\mathcal{V}$
for all $X - Y$ in $\mathcal{G}^*$
and subsets $\mathcal{S} \subseteq \mathcal{V} \backslash \{X, Y\}$ **do**
  if $\exists \mathcal{S} \subseteq \mathcal{V} \backslash \{X, Y\}$ such that $X \perp\!\!\!\perp_P Y \mid \mathcal{S}$ **then**
    Delete edge $X - Y$ from $\mathcal{G}^*$
  end if
end for
for all $X - Z - Y$ in $\mathcal{G}^*$ such that $X \notin Adj(Y, \mathcal{G})$ **do**
  if $\nexists\, \mathcal{S} \subseteq \mathcal{V} \backslash \{X, Y\}$ such that $Z \in \mathcal{S}$ and $X \perp\!\!\!\perp_P Y \mid \mathcal{S}$ **then**
    Orient $X \rightarrow Z \leftarrow Y$ in $\mathcal{G}^*$
  end if
end for
Recursively apply rules R1-R3 until no more edges can be oriented
Return $\mathcal{G}^*$

$Adj(Y, \mathcal{G})$: Adjacencies of Y in $\mathcal{G}$

Correctness of SGS

Theorem (correctness) Assume the distribution $P(\mathcal{V})$ is Markov and faithful to some DAG $\mathcal{G}$ and assume that we are given perfect conditional independence information about all pairs of variables. Let $\mathcal{G}^*$ be the CPDAG of $\mathcal{G}$. The SGS algorithm returns $\mathcal{G}^*$.

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Proof: By Theorem (faithfulness, adjacencies and v-structures), Theorem (orientation soundness) and Theorem (orientation completness).

Computational complexity of SGS

Running time of SGS depends *exponentially* on the *number of vertices* in the graph:

- For all pairs check all subsets;
- For all triples check all subsets.

A better approach?

Optimizing the procedure for skeleton construction

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By the Parental Markov condition:

$X \notin Adj(Y, \mathcal{G})$ iff $X \perp\!\!\!\perp_P Y \mid Parents(X, \mathcal{G})$ or $X \perp\!\!\!\perp_P Y \mid Parents(Y, \mathcal{G})$

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Since the graph $\mathcal{G}$ is unknown:

- The parent set is unknown ahead of time;
- We look at $\mathcal{S} \subseteq Adj(X, \mathcal{G}')$ and $\mathcal{S}' \subseteq Adj(Y, \mathcal{G}')$ for some G' which is a supergraph of the true unknown skeleton;
- We can pursue an iterative strategy such that we increase the size of $\mathcal{S}$ iteratively.

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Lemma (either d-sep or d-connect) Given the distribution $P(V)$ that is Markov and faithful to some DAG $\mathcal{G}$, if $Z \in Adj(X, \mathcal{G})$, $Z \in Adj(Y, \mathcal{G})$ and $Y \notin Adj(X, \mathcal{G})$, then either Z is in every set of variables that d-separates X and Y or it is in no set of variables that d-separates X and Y.
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(proof on board)

$sepset(X, Y)$: subset that permitted the separation of X and Y during the skeleton construction.

A better approach?

Optimizing the procedure for finding v-structures

Lemma (either d-sep or d-connect) Given the distribution $P(V)$ that is Markov and faithful to some DAG $\mathcal{G}$, if $Z \in Adj(X, \mathcal{G})$, $Z \in Adj(Y, \mathcal{G})$ and $Y \notin Adj(X, \mathcal{G})$, then either Z is in every set of variables that d-separates X and Y or it is in no set of variables that d-separates X and Y.
(proof on board)

$sepset(X, Y)$: subset that permitted the separation of X and Y during the skeleton construction.

R0: For all triples $X - Z - Y \in \mathcal{G}^*$ such that $Y \notin Adj(X, \mathcal{G}^*)$, if $Z \notin sepset(X, Y)$ then orient $X \rightarrow Z \leftarrow Y$ in $\mathcal{G}^*$.

The PC algorithm

Algorithm 2 PC

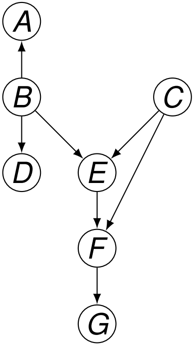
Input: $P(\mathcal{V})$

Output: CPDAG $\mathcal{G}^*$

Form the complete undirected graph $\mathcal{G}^*$ on vertex set $\mathcal{V}$
Let $n = 0$
repeat
    for all $X - Y$ in $\mathcal{G}^*$ such that $|Adj(X, \mathcal{G}^*)| \geq n$
    and subsets $\mathcal{S} \subseteq Adj(X, \mathcal{G}^*) \setminus \{Y\}$ such that $|\mathcal{S}| = n$ **do**
        if $X \perp\!\!\!\perp_P Y \mid \mathcal{S}$ **then**
            Delete edge $X - Y$ from $\mathcal{G}^*$
            Let $sepset(X, Y) = sepset(Y, X) = \mathcal{S}$
        end if
    end for
    Let $n = n + 1$
until for each pair of adjacent vertices (X, Y), $|Adj(X, \mathcal{G}^*) \setminus \{Y\}| \leq n$
Apply R0
Recursively apply rules R1-R3 until no more edges can be oriented
Return $\mathcal{G}^*$

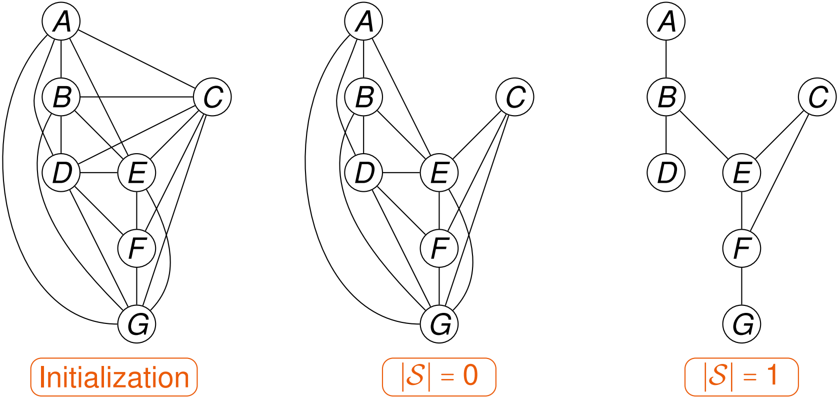
PC in action (1/3)

- Suppose the true graph on right;
- Assumptions: CMC, faithfulness, causal sufficiency.



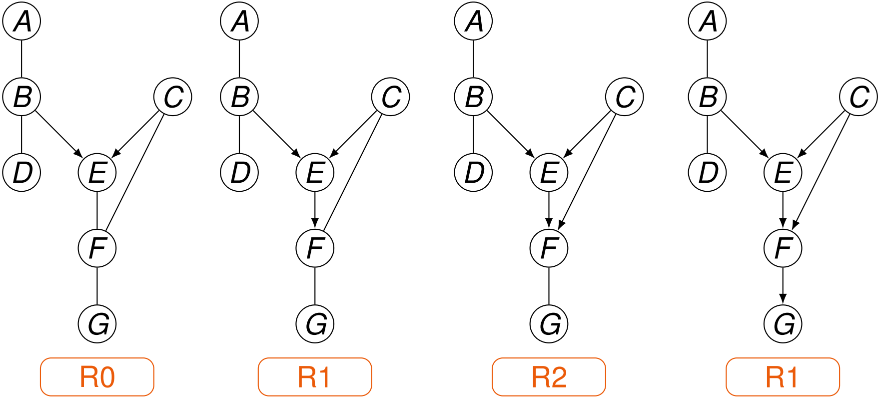
PC in action (2/3)

Skeleton construction:



PC in action (3/3)

Orientation:



Correctness of PC

Theorem (correctness) Assume the distribution $P(\mathcal{V})$ is Markov and faithful to some DAG $\mathcal{G}$ and assume that we are given perfect conditional independence information about all pairs of variables. Let $\mathcal{G}^*$ be the CPDAG of $\mathcal{G}$. The PC algorithm returns $\mathcal{G}^*$.
(proof in (Spirtes and Glymour, 1991))

Computational complexity of PC

Running time of PC depends *exponentially* on the *maximal degree* of the graph **but** for a fixed maximal degree running time over the *number of vertices* is *polynomial*.

Exercise 1

Consider data that are generated from a chain $X \rightarrow Y \rightarrow Z$. Assuming that all assumptions are satisfied, which CPDAG would a constraint based causal discovery algorithm report?

If you could supply prior knowledge to the algorithm on only one arc that is required to be present, what arc (if any) would allow the entire structure to be learned? Explain briefly.

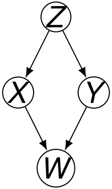
Exercise 2

Consider data that truly come from a fork $X \leftarrow Y \rightarrow Z$.
Assuming that all assumptions are satisfied, which CPDAG would a constraint based causal discovery algorithm report?

If you could supply prior knowledge to the algorithm on only one arc that is required to be present, what arc (if any) would allow the entire structure to be learned? Explain briefly.

Exercise 3

- Suppose the true graph on right;
- Assumptions: CMC, causal sufficiency, no deterministic relations;
- Generative process:

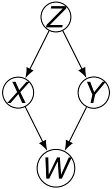


$$Z = \xi_z \qquad \xi_z \sim N(0,1);$$
$$X = a * Z + \xi_x \qquad \xi_x \sim N(0,1);$$
$$Y = b * Z + \xi_y \qquad \xi_y \sim N(0,1);$$
$$W = c * X - \frac{a * c}{b} * Y + \xi_w \qquad \xi_w \sim N(0,1).$$

- Given a compatible distribution what would be the output of the PC algorithm?

Exercise 4

- Suppose the true graph on right;
- Assumptions: CMC, causal sufficiency, deterministic relations, no canceling out paths;
- Given a compatible distribution what would be the output of the PC algorithm?



Exercise 5

- Suppose the true graph on right;
- Assumptions: CMC, faithfulness;
- Given a compatible distribution what would be the output of the PC algorithm if Z is unobserved?

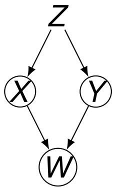


Table of content

Preliminaries

Causal discovery with causal sufficiency

Tests

Conclusion

Conditional independence tests

With finit data, SGS and PC needs a procedure for deciding whether $X \perp\!\!\!\perp_P Y \mid \mathcal{S}$.

In practice, test the null hypothesis:

$$H_0 : X \perp\!\!\!\perp_P Y \mid \mathcal{S}$$

and reject the null hypothesis if some test statistic $T(x) < \alpha$, where α is a user-specified significance threshold. That is, if we reject the null hypothesis, we keep the edge, and if we fail to reject, we remove the edge.

Examples of conditional independence tests

Tests	Assumptions
Fisher Z-transform	Linear, gaussian
χ^2 test	Multinomial discrete
Kernel-based CI test	-
Local permutation test	-

Consistency

Theorem (consistency) Assume the distribution $P(\mathcal{V})$ is Markov and faithful to some DAG $\mathcal{G}$. Let $\mathcal{G}^*$ be the CPDAG of $\mathcal{G}$ and let $\hat{\mathcal{G}}^*$ be the output of SGS, PC with some consistent conditional independence test and significative level α. Then there is a sequence of $\alpha_n \to 0 (n \to \infty)$ such that $\lim_{n\to\infty} \Pr(\hat{\mathcal{G}}^* = \mathcal{G}^*) = 1$.
(proof in (Spirtes et al, 2000))

Exercise 7

As the significance level is lowered to 0, what would you expect to happen to the graph skeleton learned by constraint based causal discovery algorithms? As the significance level is increased to 1? Explain.

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Conclusion

- Under faithfulness and causal sufficiency constraint-based methods can discover a CPDAG (SGS, PC).
- Advantages:
  - Nonparametric (in principle);
  - PC is relatively scalable;
  - Lots of work on improvements.
- Drawbacks:
  - Cannot discover the entire true graph;
  - Faithfulness is not testable;
  - Cannot parallelize;
  - No confidence intervals;
  - Individual errors may propagate.

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Some extensions

- Causal discovery without causal sufficiency;
- Incorporating background knowledge;
- Order independent;
- Time series.

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References (1/2)

Direct inspirations for part 1

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Additional readings

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