

# Path Constraints for Causal Discovery

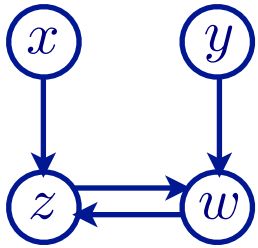
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Frederick Eberhardt

This is joint work with Antti Hyttinen, Patrik Hoyer & Matti Järvisalo

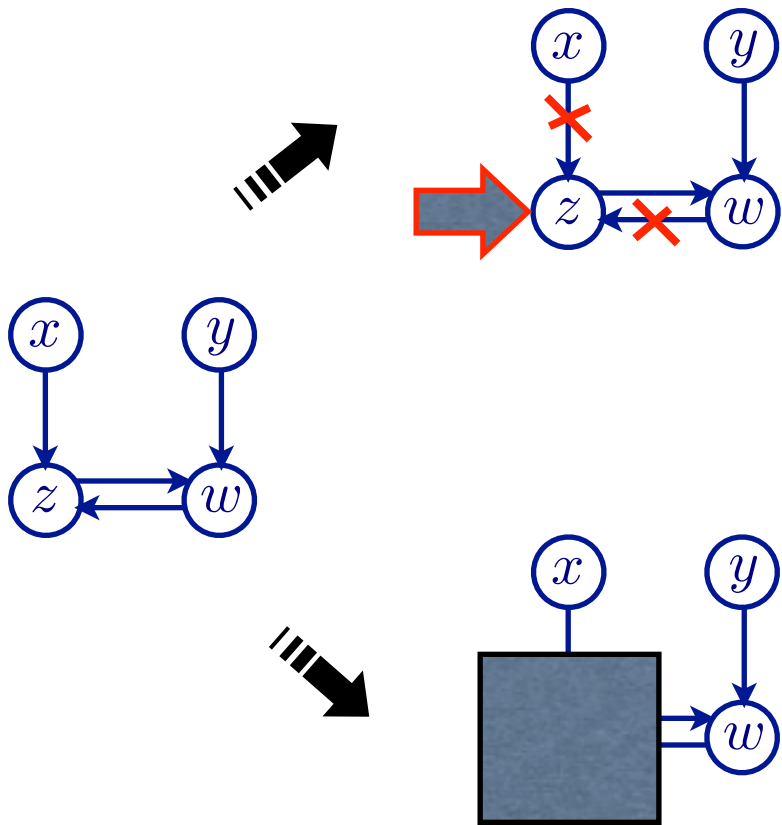
# Causal Structure Search

true  
model



# Causal Structure Search

true model  $\Rightarrow$  experimental conditions



# Causal Structure Search

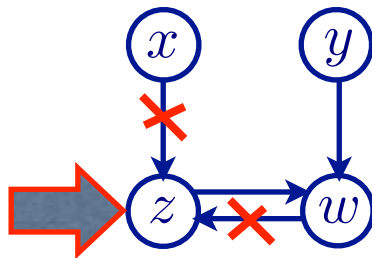
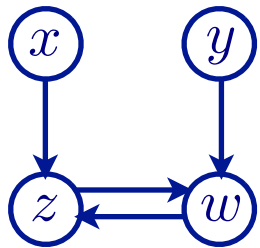
true model



experimental conditions

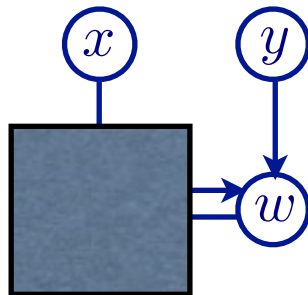


data sample



samples

	$w$	$x$	$y$	$z$



samples

	$w$	$x$	$y$

# Causal Structure Search

true model



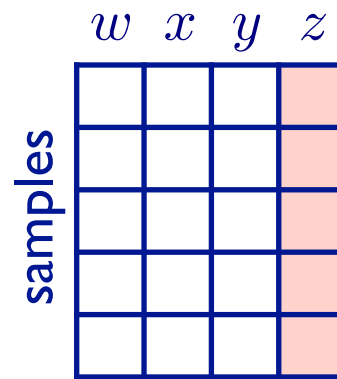
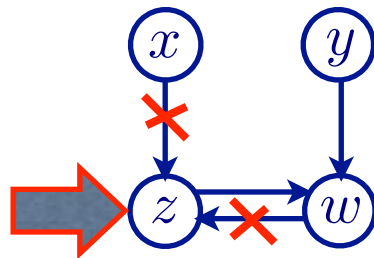
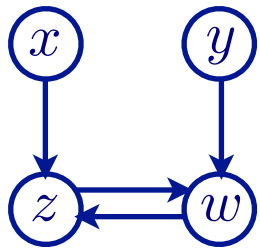
experimental conditions



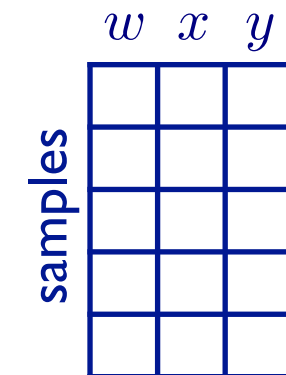
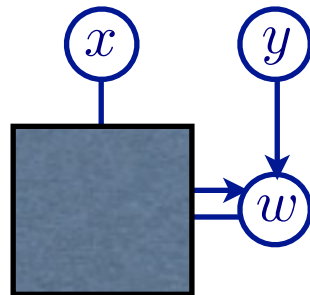
data sample



statistics



$x \perp y \parallel \{z\}$   
 $z \not\perp y \mid \{w\} \parallel \{z\}$   
 $cov(x, y \parallel \{z\})$   
 ...



$x \perp y$   
 $x \not\perp w$   
 $cov(x, y \mid \{w\})$   
 $\hat{\theta}$   
 ...

# Output

## statistics

$$x \perp y \parallel \{z\}$$

$$z \not\perp y \mid \{w\} \parallel \{z\}$$

$$\text{cov}(x, y \parallel \{z\})$$

...

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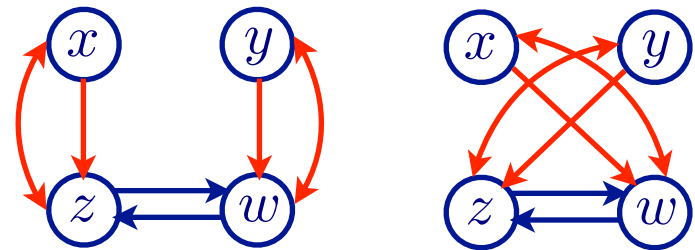
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equivalence classes



# Output

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$$x \perp y \mid \{z\}$$

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$$\text{cov}(x, y \mid \{z\})$$

...

$$x \perp y$$

$$x \not\perp w$$

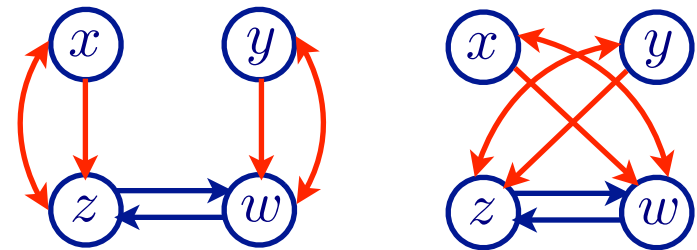
$$\text{cov}(x, y \mid \{w\})$$

$$\hat{\theta}$$

...



## equivalence classes



## model specifications

	w	x	y	z
w	0	0	?	a
x	0	0	0	0
y	0	0	0	0
z	b	?	?	0

direct edges

	w	x	y	z
w	0	0	?	?
x	0	0	0	?
y	?	0	0	0
z	?	?	0	0

confounders



# Search Space Assumptions

- Causal Markov
- Causal Faithfulness

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- Causal Markov
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- overlapping data sets
- set of variables is jointly causally insufficient
- cyclic or acyclic causal structure
- experimental and observational data sets
- d-separation oracle
  - in the cyclic case we can consider a linear Gaussian parameterization (see Spirtes, 1995)
  - known problems for the discrete case (see Pearl & Dechter, 1996, and Neal, 2000)

# SAT-based causal discovery

graphical constraints

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- $x$  is a cause of  $y$



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- $x$  and  $y$  are correlated conditional on  $\mathbf{C}$  in an experiment where  $x$  was subject to intervention

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## propositional constraints (in CNF) on true graph

$$(A \vee B \vee C) \wedge (D \vee E)$$

$A$

$B \wedge E$

...

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$w$	0	0	?	1
$x$	0	0	0	0
$y$	0	0	0	0
$z$	?	?	?	0

direct edges

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confounders

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direct edges

	$w$	$x$	$y$	$z$
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$x$	0	0	0	?
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confounders

# SATisfiability solver

- finds a truth value assignment for a Boolean formula in Conjunctive Normal Form (CNF)



# SATisfiability solver

- finds a truth value assignment for a Boolean formula in Conjunctive Normal Form (CNF)
- a Boolean term  $X$  is a **backbone variable** if  $X$  takes the same value (T or F) in all satisfying truth value assignments of a given formula

Encoding: track the endpoints of paths

$$[x \neq y \mid \mathbf{C} \parallel \mathbf{J}]$$



# Encoding: track the endpoints of paths

$$[x \not\sim y \mid \mathbf{C} \parallel \mathbf{J}]$$



# Encoding: track the endpoints of paths

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$$\bigvee_{l=1}^{l_{\max}} \left( \begin{array}{c} x \xrightarrow{l} y \\ \vee \\ x \xleftarrow{l} y \\ \vee \\ x \xleftrightarrow{l} y \\ \vee \\ x \overset{l}{\dashrightarrow} y \end{array} \right)$$

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$$\bigvee_{l=1}^{l_{\max}} \left( \begin{array}{c} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \end{array} \right)$$

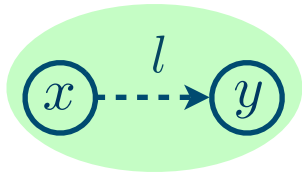
The diagram shows a disjunction of four path configurations between nodes  $x$  and  $y$ , each enclosed in a colored oval. The first configuration (green) shows a path from  $x$  to  $y$  with a dashed arrow labeled  $l$ . The second configuration (green) shows a path from  $y$  to  $x$  with a dashed arrow labeled  $l$ . The third configuration (red) shows a bidirectional path between  $x$  and  $y$  with dashed arrows labeled  $l$ . The fourth configuration (yellow) shows a path from  $x$  to  $y$  with a dashed arrow labeled  $l$ .

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$$[x \neq y \mid \mathbf{C} \parallel \mathbf{J}]$$



$$\bigvee_{l=1}^{l_{\max}} \left( \begin{array}{c} \text{---} \\ x \text{---} \overset{l}{\rightarrow} y \text{---} \\ \text{---} \end{array} \vee \begin{array}{c} \text{---} \\ x \text{---} \overset{l}{\leftarrow} y \text{---} \\ \text{---} \end{array} \vee \begin{array}{c} \text{---} \\ x \text{---} \overset{l}{\leftrightarrow} y \text{---} \\ \text{---} \end{array} \vee \begin{array}{c} \text{---} \\ x \text{---} \text{---} y \text{---} \\ \text{---} \end{array} \right)$$



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$$[x \not\sim y \mid \mathbf{C} \parallel \mathbf{J}]$$



$$\bigvee_{l=1}^{l_{\max}} \left( \begin{array}{cccc} \text{---} & & \text{---} & \text{---} \\ \text{---} & & \text{---} & \text{---} \\ \text{---} & & \text{---} & \text{---} \\ \text{---} & & \text{---} & \text{---} \end{array} \right)$$

$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \Leftrightarrow \bigvee_{z \notin \mathbf{C}} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \vee \bigvee_{z \in \mathbf{C}} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array}$$

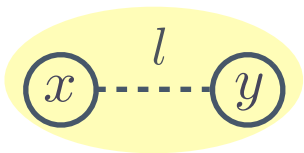
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$$\bigvee_{l=1}^{l_{\max}} \left( \begin{array}{c} \text{green oval} \\ x \xrightarrow{l} y \\ \text{green oval} \end{array} \vee \begin{array}{c} \text{green oval} \\ x \xleftarrow{l} y \\ \text{green oval} \end{array} \vee \begin{array}{c} \text{red oval} \\ x \xleftrightarrow{l} y \\ \text{red oval} \end{array} \vee \begin{array}{c} \text{yellow oval} \\ x \xrightarrow{l} y \\ \text{yellow oval} \end{array} \right)$$

$$\begin{array}{c} \text{green oval} \\ x \xrightarrow{l} y \\ \text{green oval} \end{array} \Leftrightarrow \bigvee_{z \notin \mathbf{C}} \begin{array}{c} x \xrightarrow{1} z \xrightarrow{l-1} y \end{array} \vee \bigvee_{z \in \mathbf{C}} \begin{array}{c} x \xrightarrow{1} z \xleftarrow{l-1} y \end{array}$$





# Encoding: track the endpoints of paths

$$[x \not\sim y \mid \mathbf{C} \parallel \mathbf{J}]$$

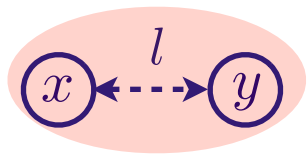


$$\bigvee_{l=1}^{l_{\max}} \left( \begin{array}{c} \text{---} \\ x \text{---} \overset{l}{\text{---}} \text{---} y \\ \text{---} \end{array} \vee \begin{array}{c} \text{---} \\ x \text{---} \overset{l}{\text{---}} \text{---} y \\ \text{---} \end{array} \vee \begin{array}{c} \text{---} \\ x \text{---} \overset{l}{\text{---}} \text{---} y \\ \text{---} \end{array} \vee \begin{array}{c} \text{---} \\ x \text{---} \overset{l}{\text{---}} \text{---} y \\ \text{---} \end{array} \right)$$

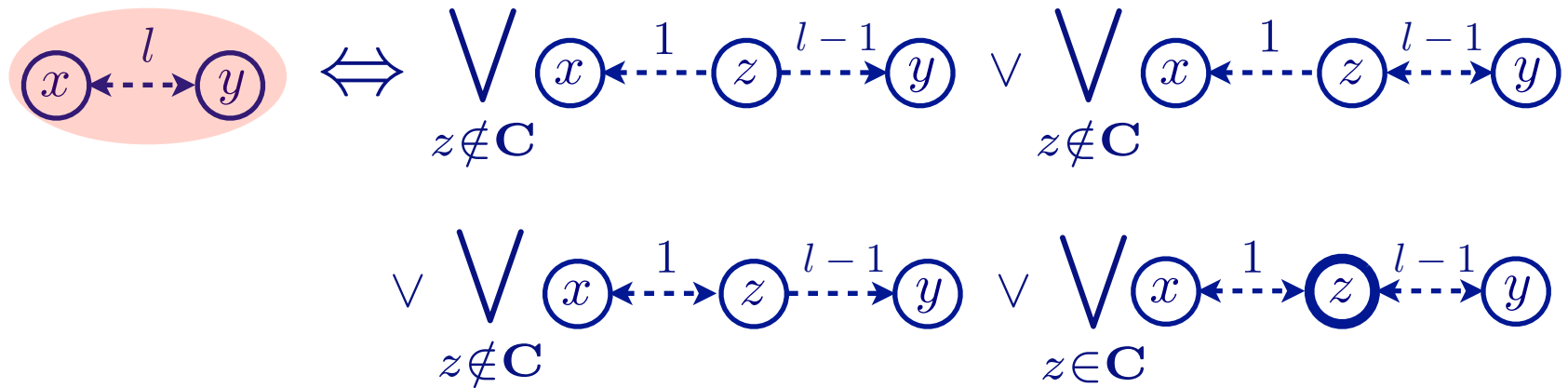
$$\begin{array}{c} \text{---} \\ x \text{---} \overset{l}{\text{---}} \text{---} y \\ \text{---} \end{array} \iff \bigvee_{z \notin \mathbf{C}} \begin{array}{c} \text{---} \\ x \text{---} \overset{1}{\text{---}} z \text{---} \overset{l-1}{\text{---}} y \\ \text{---} \end{array} \vee \bigvee_{z \in \mathbf{C}} \begin{array}{c} \text{---} \\ x \text{---} \overset{1}{\text{---}} z \text{---} \overset{l-1}{\text{---}} y \\ \text{---} \end{array}$$

$$\begin{array}{c} \text{---} \\ x \text{---} \overset{l}{\text{---}} \text{---} y \\ \text{---} \end{array} \iff \bigvee_{z \notin \mathbf{C}} \begin{array}{c} \text{---} \\ x \text{---} \overset{1}{\text{---}} z \text{---} \overset{l-1}{\text{---}} y \\ \text{---} \end{array} \vee \bigvee_{z \in \mathbf{C}} \begin{array}{c} \text{---} \\ x \text{---} \overset{1}{\text{---}} z \text{---} \overset{l-1}{\text{---}} y \\ \text{---} \end{array}$$

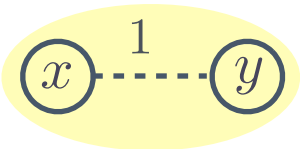
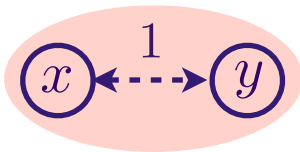
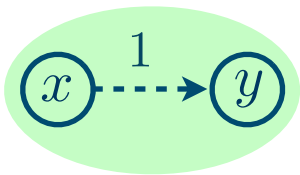
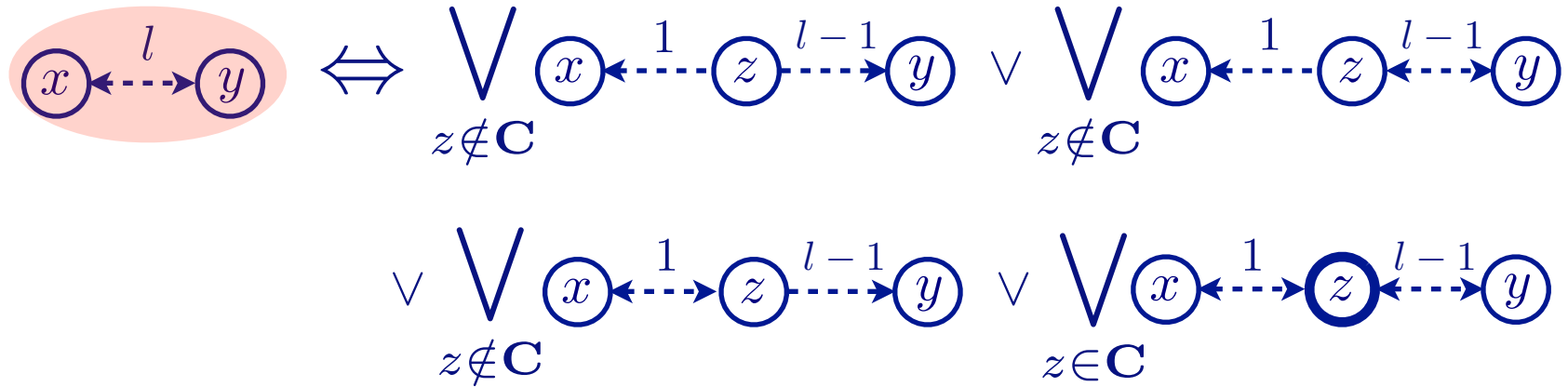
# Encoding continued



# Encoding continued



# Encoding continued



# Encoding continued

$$\begin{aligned}
 \textcircled{x} \overset{l}{\dashrightarrow} \textcircled{y} &\iff \bigvee_{z \notin \mathbf{C}} \textcircled{x} \overset{1}{\dashrightarrow} \textcircled{z} \overset{l-1}{\dashrightarrow} \textcircled{y} \vee \bigvee_{z \notin \mathbf{C}} \textcircled{x} \overset{1}{\dashrightarrow} \textcircled{z} \overset{l-1}{\dashleftarrow} \textcircled{y} \\
 &\vee \bigvee_{z \notin \mathbf{C}} \textcircled{x} \overset{1}{\dashrightarrow} \textcircled{z} \overset{l-1}{\dashrightarrow} \textcircled{y} \vee \bigvee_{z \in \mathbf{C}} \textcircled{x} \overset{1}{\dashrightarrow} \textcircled{z} \overset{l-1}{\dashleftarrow} \textcircled{y}
 \end{aligned}$$

$$\textcircled{x} \overset{1}{\dashrightarrow} \textcircled{y} \iff \begin{cases} \textcircled{x} \longrightarrow \textcircled{y} & \text{if } y \notin \mathbf{J} \\ 0 & \text{otherwise} \end{cases}$$

$$\textcircled{x} \overset{1}{\dashleftarrow} \textcircled{y} \iff \begin{cases} \textcircled{x} \longleftarrow \textcircled{y} & \text{if } x, y \notin \mathbf{J} \\ 0 & \text{otherwise} \end{cases}$$

$$\textcircled{x} \overset{1}{\dashrightarrow} \textcircled{y} \iff 0$$

$$[x \not\sim y | \mathbf{C} | \mathbf{J}] \Leftrightarrow \bigvee_{l=1}^{l_{\max}} \left( [x \underset{\mathbf{C}, \mathbf{J}}{\overset{l}{>}} y] \vee [y \underset{\mathbf{C}, \mathbf{J}}{\overset{l}{>}} x] \vee [x \underset{\mathbf{C}, \mathbf{J}}{\overset{l}{<}} y] \vee [x \underset{\mathbf{C}, \mathbf{J}}{\overset{l}{-}} y] \right)$$

$$[x \underset{\mathbf{C}, \mathbf{J}}{\overset{l}{>}} y] \Leftrightarrow \bigvee_{z \notin \mathbf{C}} \left( [x \underset{\mathbf{C}, \mathbf{J}}{\overset{1}{>}} z] \wedge [z \underset{\mathbf{C}, \mathbf{J}}{\overset{l-1}{>}} y] \right) \vee \bigvee_{z \in \mathbf{C}} \left( [x \underset{\mathbf{C}, \mathbf{J}}{\overset{1}{>}} z] \wedge [z \underset{\mathbf{C}, \mathbf{J}}{\overset{l-1}{<}} y] \right)$$

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$$[x \underset{\mathbf{C}, \mathbf{J}}{\overset{l}{-}} y] \Leftrightarrow \bigvee_{z \notin \mathbf{C}} \left( [x \underset{\mathbf{C}, \mathbf{J}}{\overset{1}{>}} z] \wedge [z \underset{\mathbf{C}, \mathbf{J}}{\overset{l-1}{-}} y] \right) \vee \bigvee_{z \in \mathbf{C}} \left( [x \underset{\mathbf{C}, \mathbf{J}}{\overset{1}{>}} z] \wedge [y \underset{\mathbf{C}, \mathbf{J}}{\overset{l-1}{>}} z] \right)$$

$$[x \underset{\mathbf{C}, \mathbf{J}}{\overset{1}{>}} y] \Leftrightarrow \begin{cases} [x \rightarrow y] & \text{if } y \notin \mathbf{J} \\ 0 & \text{otherwise} \end{cases}$$

$$[x \underset{\mathbf{C}, \mathbf{J}}{\overset{1}{<}} y] \Leftrightarrow \begin{cases} [x \leftrightarrow y] & \text{if } x \notin \mathbf{J} \text{ and } y \notin \mathbf{J} \\ 0 & \text{otherwise} \end{cases}$$

$$[x \underset{\mathbf{C}, \mathbf{J}}{\overset{1}{-}} y] \Leftrightarrow 0$$

$$[x \not\sim y | \mathbf{C} || \mathbf{J}] \Leftrightarrow \bigvee_{l=1}^{l_{\max}} \left( [x \overset{l}{\underset{\mathbf{C}, \mathbf{J}}{\sim}} y] \vee [y \overset{l}{\underset{\mathbf{C}, \mathbf{J}}{\sim}} x] \vee [x \overset{l}{\underset{\mathbf{C}, \mathbf{J}}{<}} y] \vee [x \overset{l}{\underset{\mathbf{C}, \mathbf{J}}{-}} y] \right)$$

$$[x \overset{l}{\underset{\mathbf{C}, \mathbf{J}}{\sim}} y] \Leftrightarrow \bigvee_{z \notin \mathbf{C}} \left( [x \overset{1}{\underset{\mathbf{C}, \mathbf{J}}{\sim}} z] \wedge [z \overset{l-1}{\underset{\mathbf{C}, \mathbf{J}}{\sim}} y] \right) \vee \bigvee_{z \in \mathbf{C}} \left( [x \overset{1}{\underset{\mathbf{C}, \mathbf{J}}{\sim}} z] \wedge [z \overset{l-1}{\underset{\mathbf{C}, \mathbf{J}}{<}} y] \right)$$

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$$[x \overset{1}{\underset{\mathbf{C}, \mathbf{J}}{<}} y] \Leftrightarrow \begin{cases} [x \leftrightarrow y] & \text{if } x \notin \mathbf{J} \text{ and } y \notin \mathbf{J} \\ 0 & \text{otherwise} \end{cases}$$

$$[x \overset{1}{\underset{\mathbf{C}, \mathbf{J}}{-}} y] \Leftrightarrow 0$$

longest path  
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 $l_{\max} = 2n-4$   
where  $n = |\mathbf{V}|$

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For a network of  $n=10$  variables



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- ~ 5million path variables
- **Gigabytes** of CNF formulas, but only define those that you need!

# Algorithm

Proceed in order of conditioning set size

- heuristically find unknown d-separation / d-connection relations and determine them.
- Encode the relations into the working formula  $F$ , including definitions as needed.
- Determine the “backbone” of  $F$  using the SAT-solver, i.e. for each pair of variables  $(x,y)$  in  $\mathbf{V}$  and for each edge type determine whether it is
  - present in all causal structures consistent with the input.
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you can compute the backbone over any graphical feature that you are interested in

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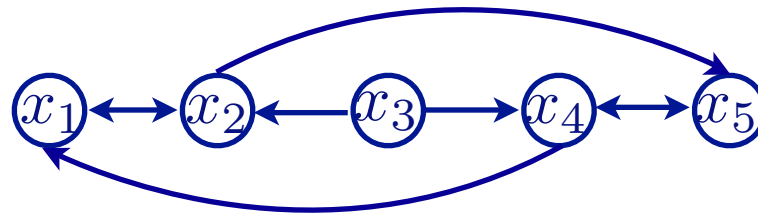
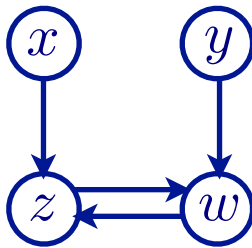
# Compare to FCI or CCD

- Both FCI and CCD use a representation of the current equivalence class to inform the choice of next independence test
- For our search space we have no such representation
  - recall the blow-up of the equivalence class in the search space of **acyclic** models in overlapping data sets for the ION and IOD algorithm (see Tillman et al. 2009, Triantafillou et al. 2010)



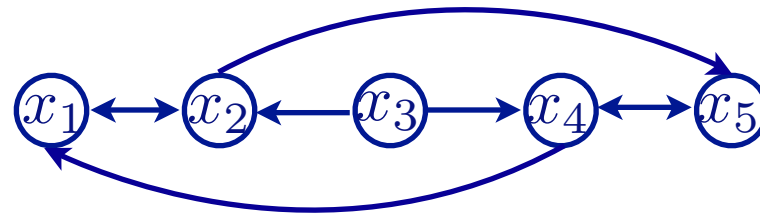
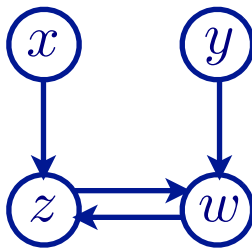
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- in restricted search spaces we can copy the test schedules of e.g. PC, FCI, CCD or ION for efficiency (while integrating background or experimental constraints)

# Handling Statistical Errors

- do what any other constraint based methods do
    - retract and return “don’t knows” when conflicts arise
    - focus on reliable tests first and stop
    - different cut-offs for d-separation vs. d-connection
    - try doing some type of false discovery rate control
- ➡ use weighted maxSAT techniques

# Conclusion

- a constraint based inference procedure for a search space that includes causal models **with latents and cycles**
- combination of input obtained from **experimental or observational overlapping** data sets
- inclusion of **wide variety of background knowledge**
  - change to a query based approach to causal discovery
  - code package available

# References to Related Work

Claassen, T. and Heskes, T. (2011). A logical characterization of constraint-based causal discovery. In Proc. UAI 2011.

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Triantafillou, S., Tsamardinos, I., and Tollis, I. G. (2010). Learning causal structure from overlapping variable sets. In Proc. AISTATS, pages 860–867.

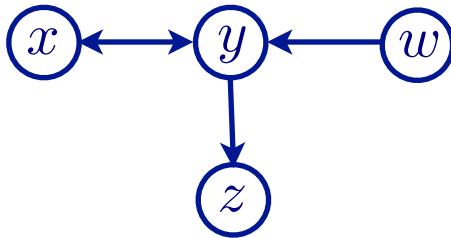
Tsamardinos, I., Triantafillou, S., and Lagani, V. (2012). Towards integrative causal analysis of heterogeneous data sets and studies. *Journal of Machine Learning Research*, 13:1097–1157.

Our research was supported by the Academy of Finland, HIIT and the James S. McDonnell Foundation.



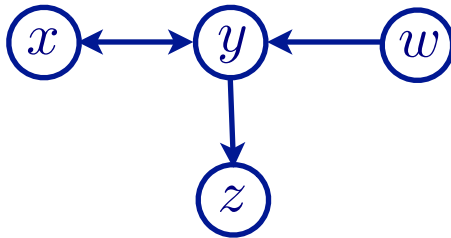
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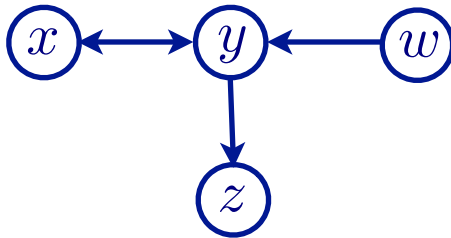
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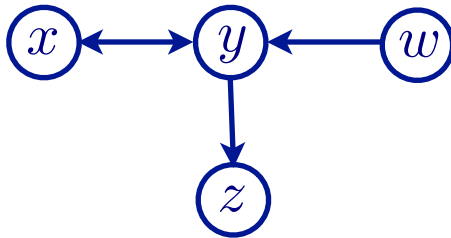
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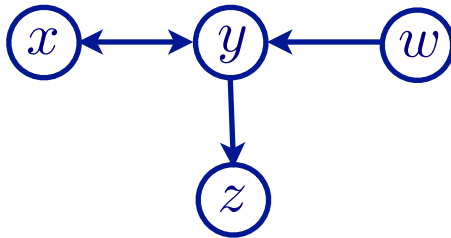
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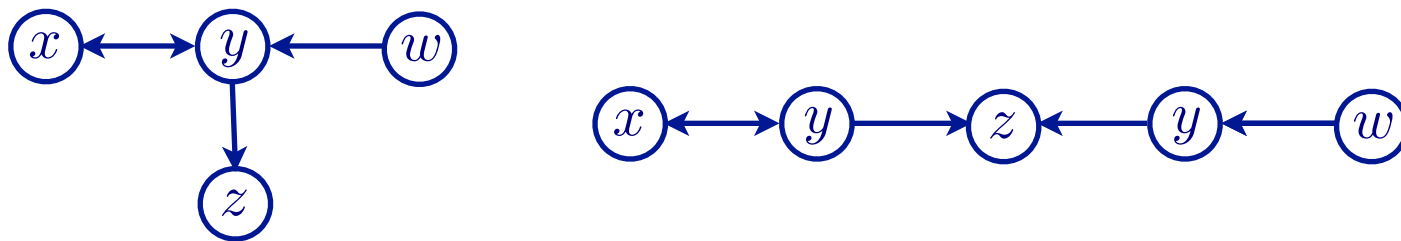
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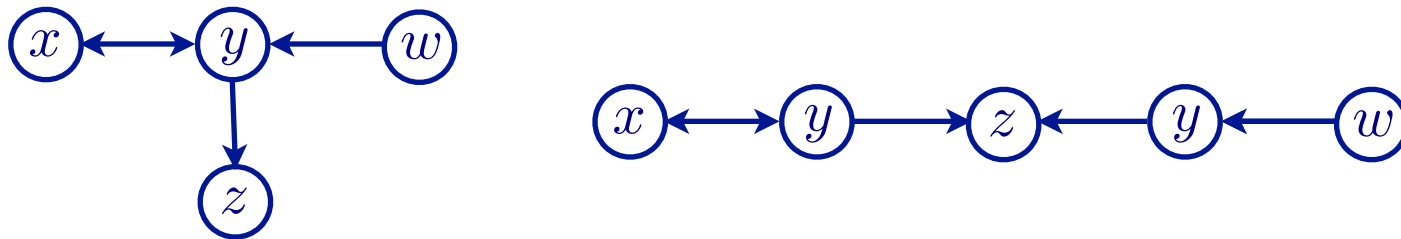
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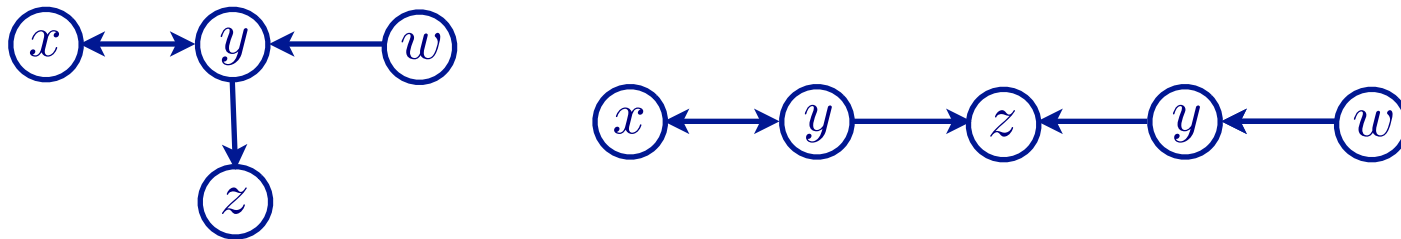


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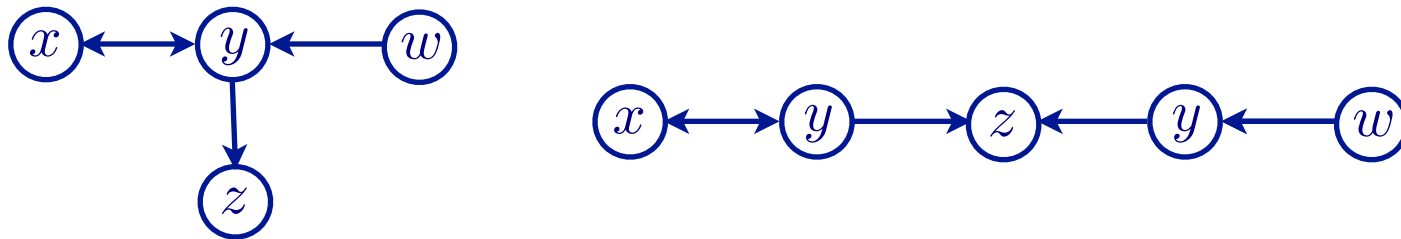
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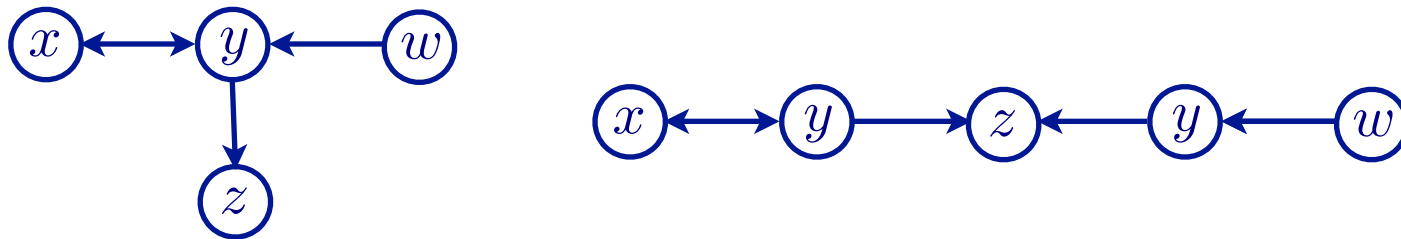
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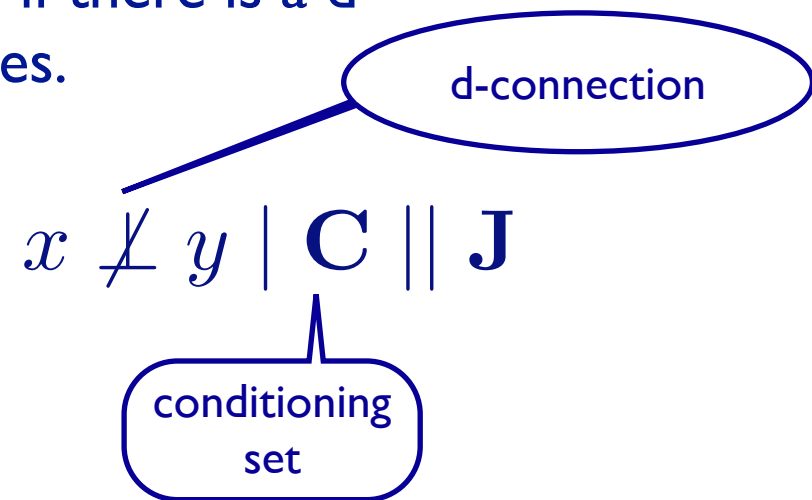
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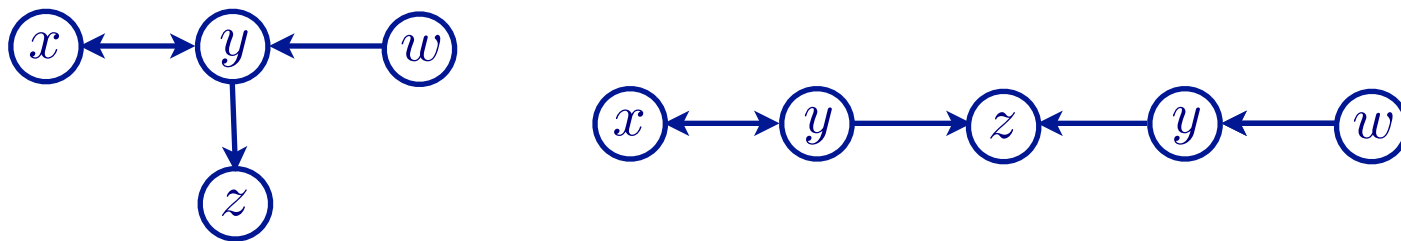
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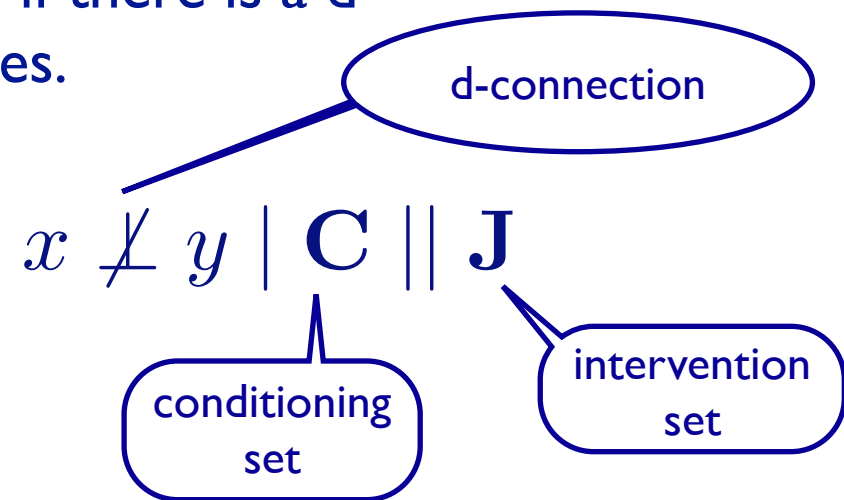
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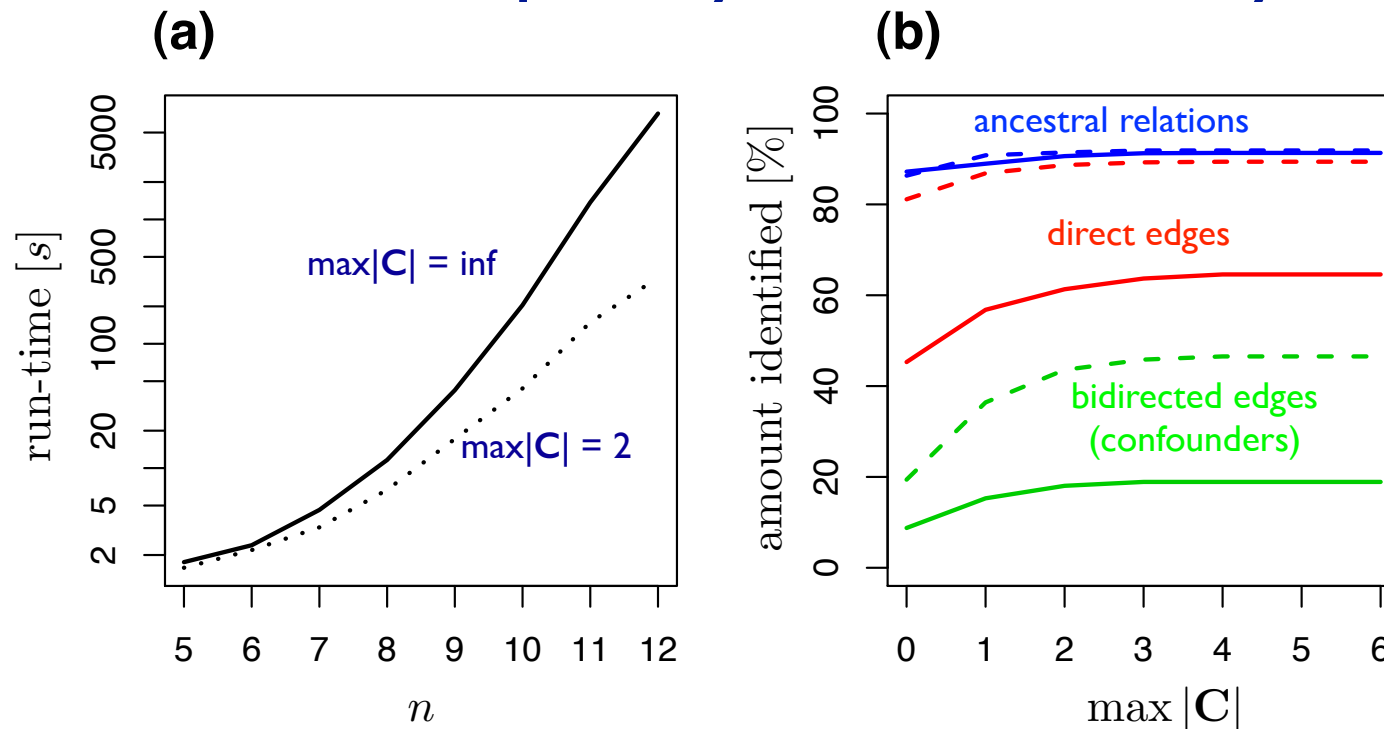


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# Simulations: Complexity & Identifiability

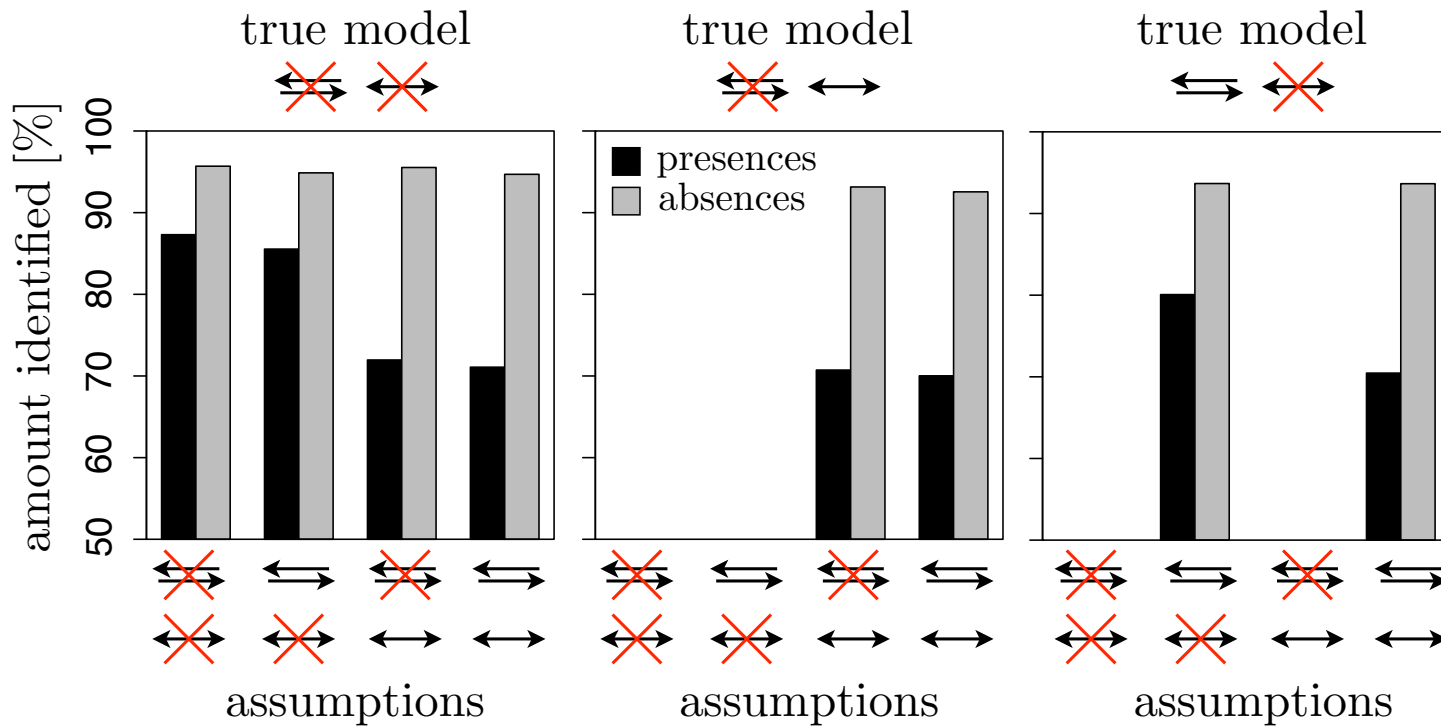


(a) Median runtime of the procedure as a function of the total number of nodes in the model.

(b) Proportion of edges (solid lines) and absences of edges (dashed) identified as a function of  $\max|\mathbf{C}|$

100 graphs, edge probability 0.2, 10 overlapping experiments with equal probability for each node to be observed, intervened or hidden.

# Simulations: Search Space Assumptions



- Proportion of directed edge presences and absences identified, under various model space assumptions, for acyclic true models without latent variables (left), acyclic models with latents (center), and cyclic models without latents (right).

# Test Pruning Heuristic

- Given an intermediary solution of **present, absent & unknown** edges:
  - Consider a minimal model: all unknown edges absent
  - Consider a maximal model: all unknown edges present
  - Search for d-separation relations in which the minimal and maximal model differ
  - Omit tests that contain nodes that cannot be on a d-connecting path (e.g. nodes known to be disconnected)