

General Purpose SAT-Solvers for Causal Discovery

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[joint work with Antti Hyttinen and Matti Jarvisalo]

Causal Discovery

data
sample

	<i>w</i>	<i>x</i>	<i>y</i>	<i>z</i>
samples				

Causal Discovery

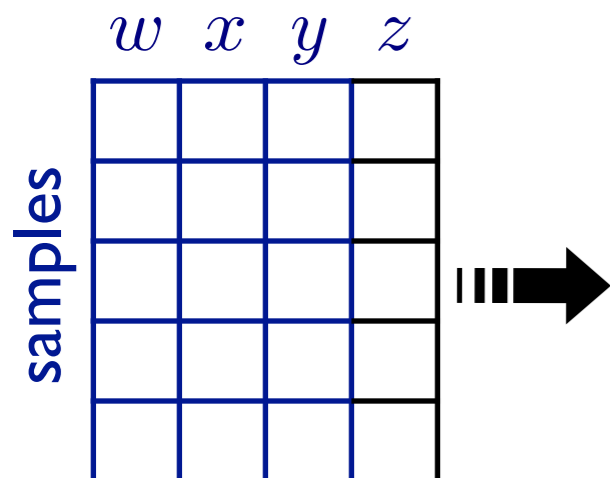
data
sample

assumptions, e.g.

- causal Markov
- causal faithfulness
- functional form
- etc.



inference algorithm



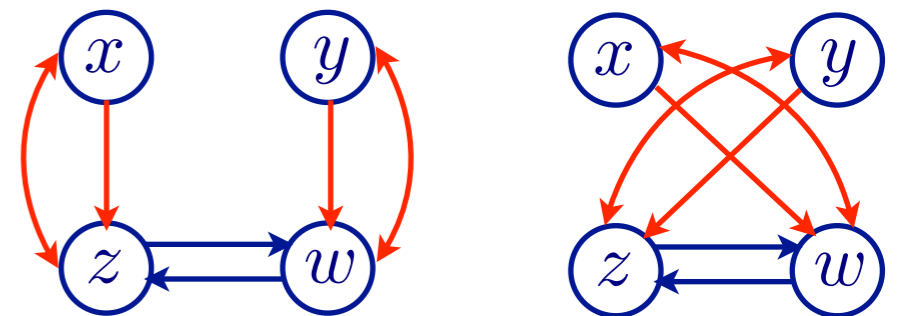
Causal Discovery

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- etc.

equivalence classes



samples

	<i>w</i>	<i>x</i>	<i>y</i>	<i>z</i>



inference algorithm

model specifications

	<i>w</i>	<i>x</i>	<i>y</i>	<i>z</i>
<i>w</i>	0	0	?	a
<i>x</i>	0	0	0	0
<i>y</i>	0	0	0	0
<i>z</i>	b	?	?	0

direct edges

	<i>w</i>	<i>x</i>	<i>y</i>	<i>z</i>
<i>w</i>	0	0	?	?
<i>x</i>	0	0	0	?
<i>y</i>	?	0	0	0
<i>z</i>	?	?	0	0

confounders

General Model Space



General Model Space

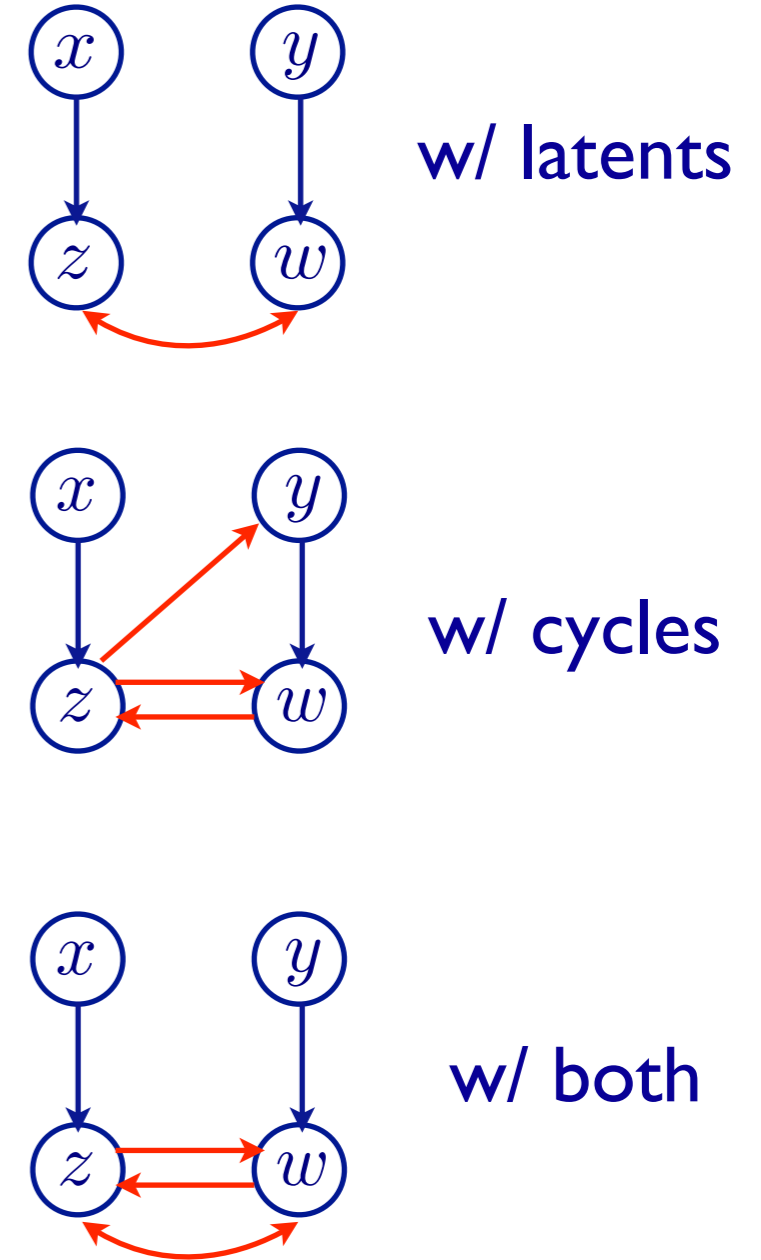
assumption / algorithm	PC / GES	FCI	CCD	LiNGaM	non-linear additive noise
Markov	✓	✓	✓	✓	✓
faithfulness	✓	✓	✓	✗	minimality
causal sufficiency	✓	✗	✓	✓	✓
acyclicity	✓	✓	✗	✓	✓
parametric assumption	✗	✗	✗	linear non-Gaussian	non-linear additive noise

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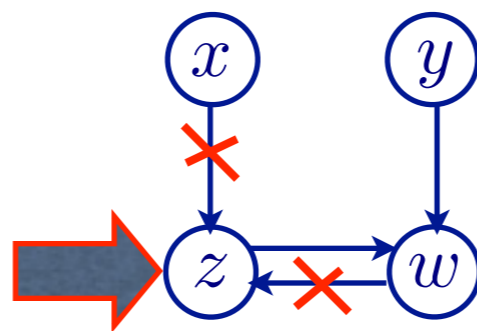
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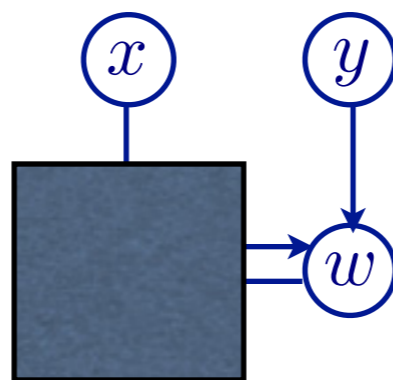


Combining Experiment and Observation

experiment

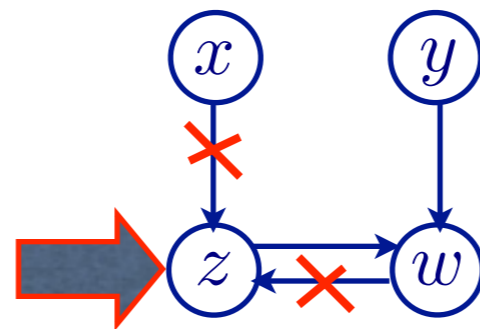


observational study



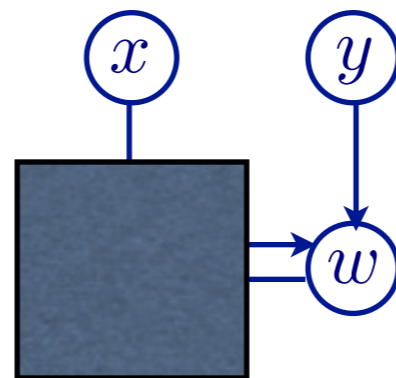
Combining Experiment and Observation

experiment



	w	x	y	z
samples				

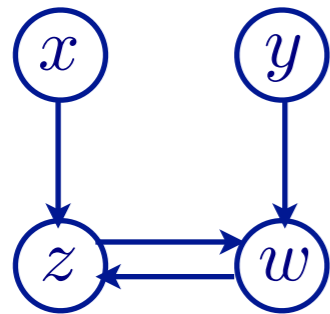
observational study



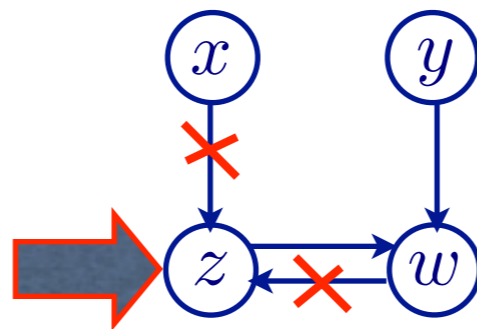
	w	x	y
samples			

Combining Experiment and Observation

true
(unknown)
model



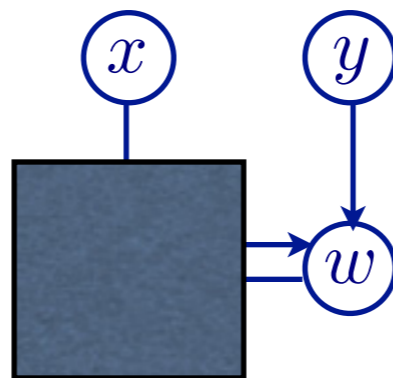
experiment



samples

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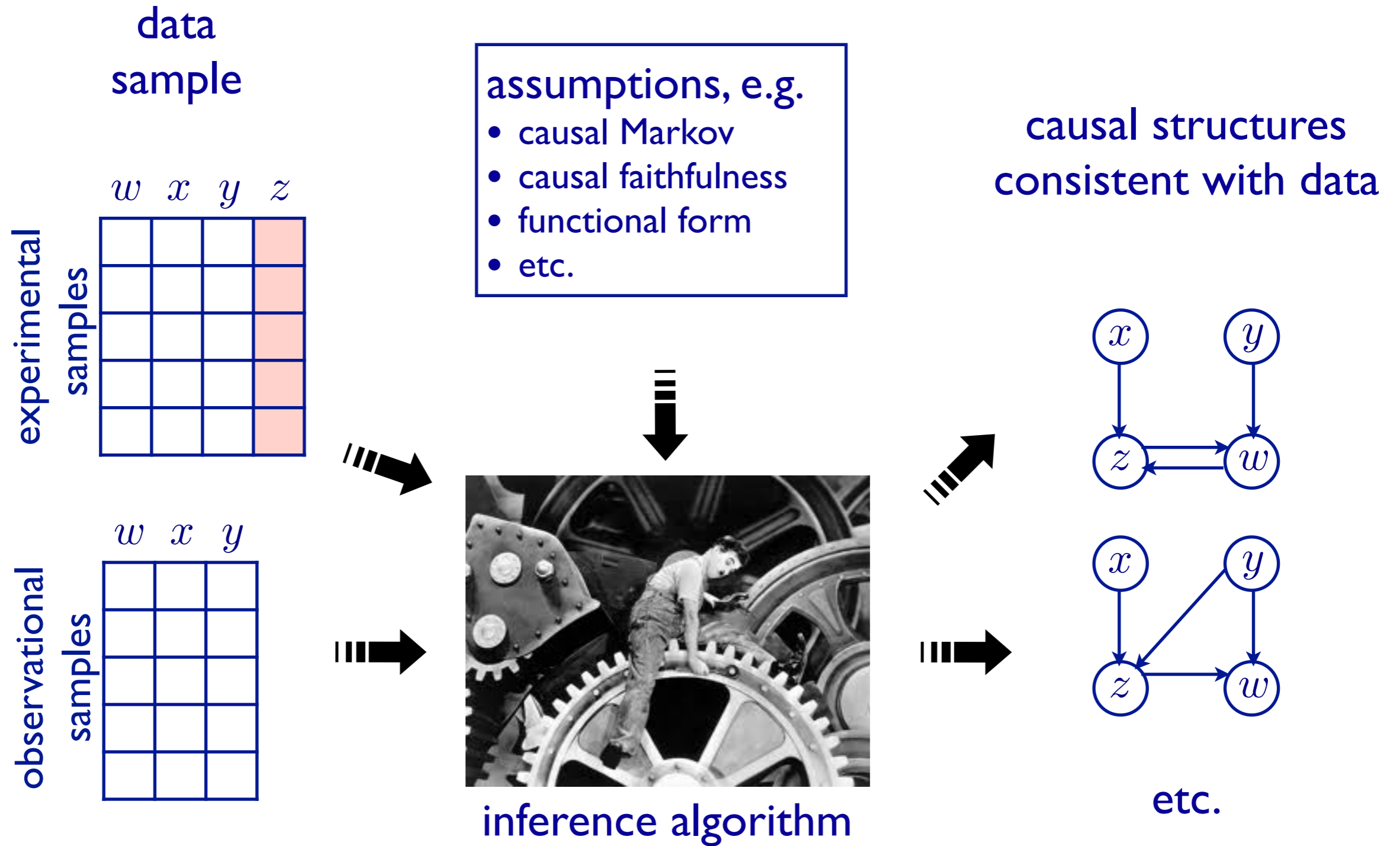
observational study



samples

	w	x	y

Causal Discovery

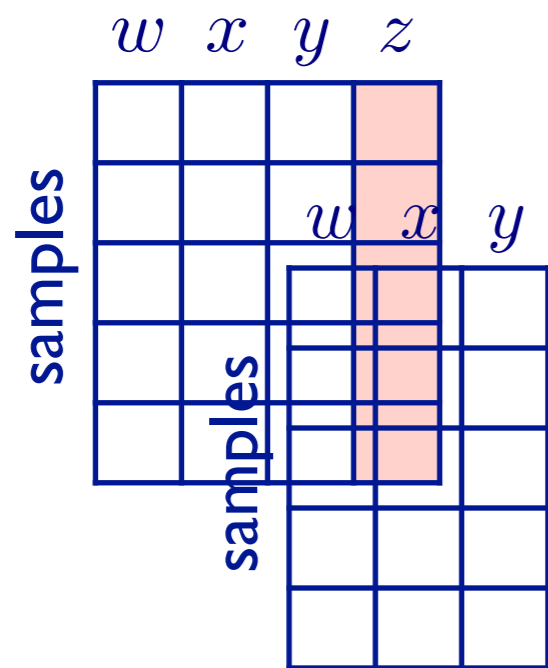


Causal Discovery

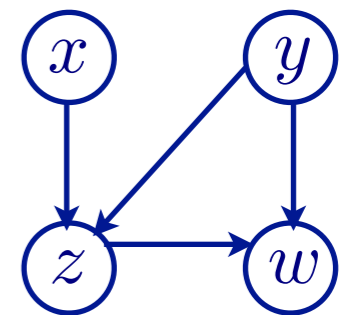
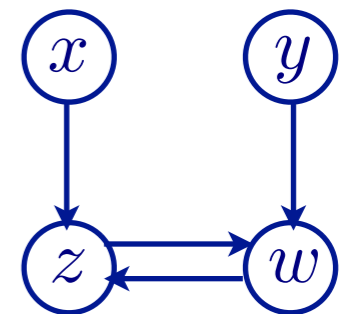
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- etc.

causal structures consistent with data



inference algorithm



etc.

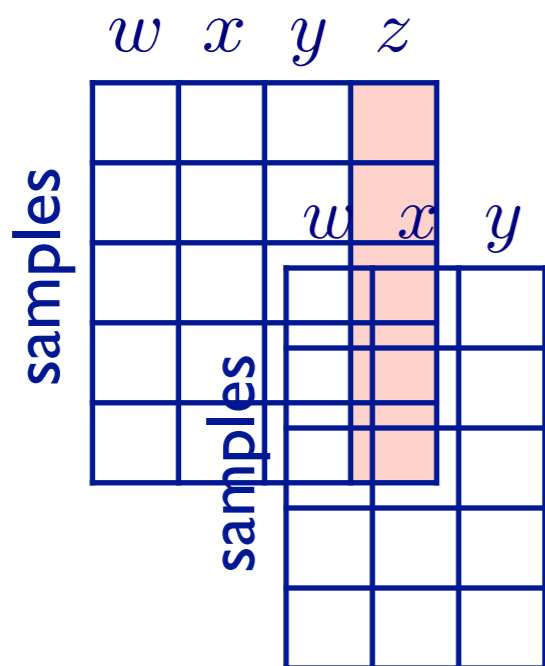
Causal Discovery

background knowledge

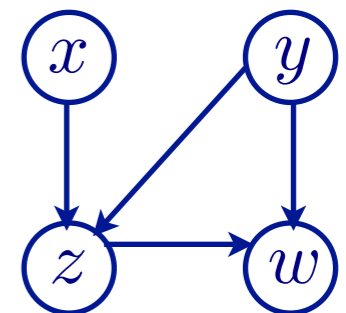
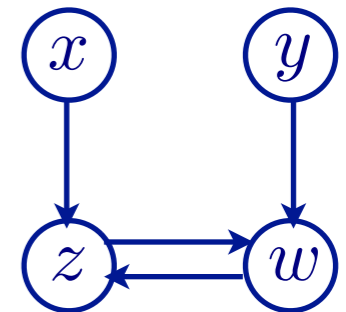
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Causal Discovery

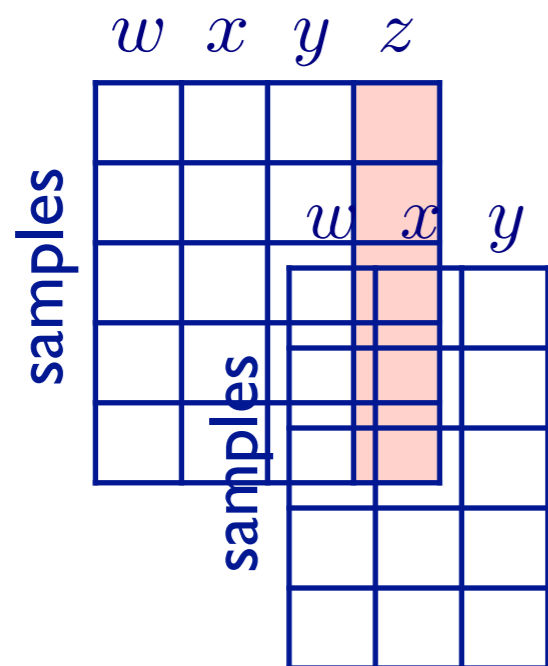
background knowledge

- edge presences/ absences

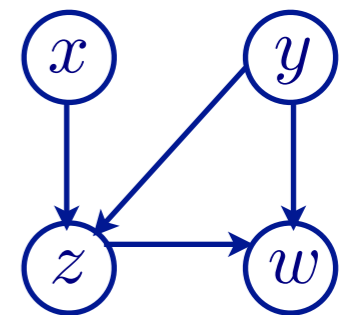
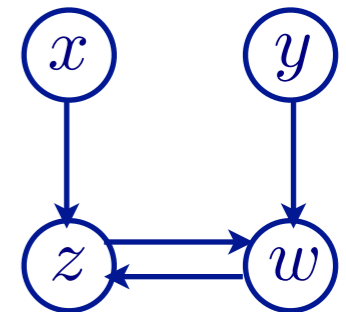
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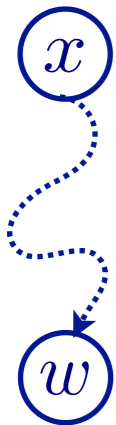
inference algorithm



etc.

Causal Discovery

background knowledge

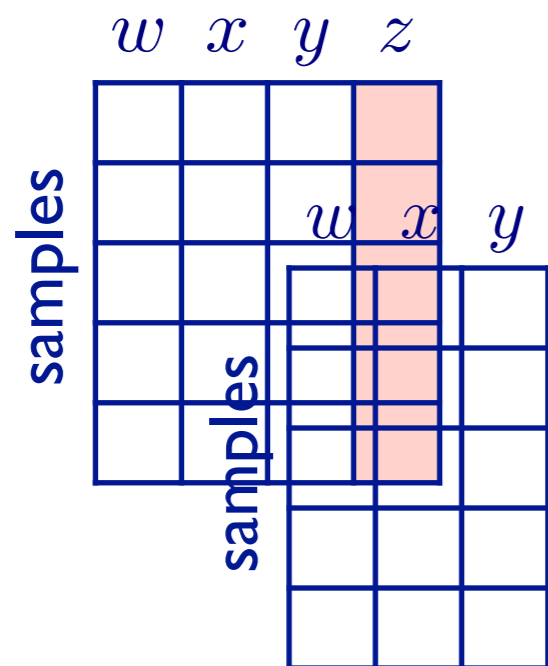


- edge presences/ absences
- pathways

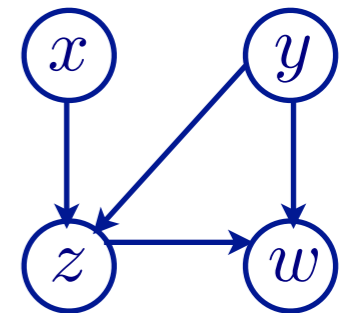
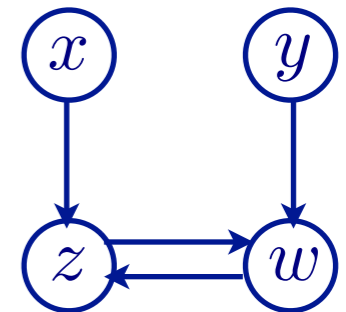
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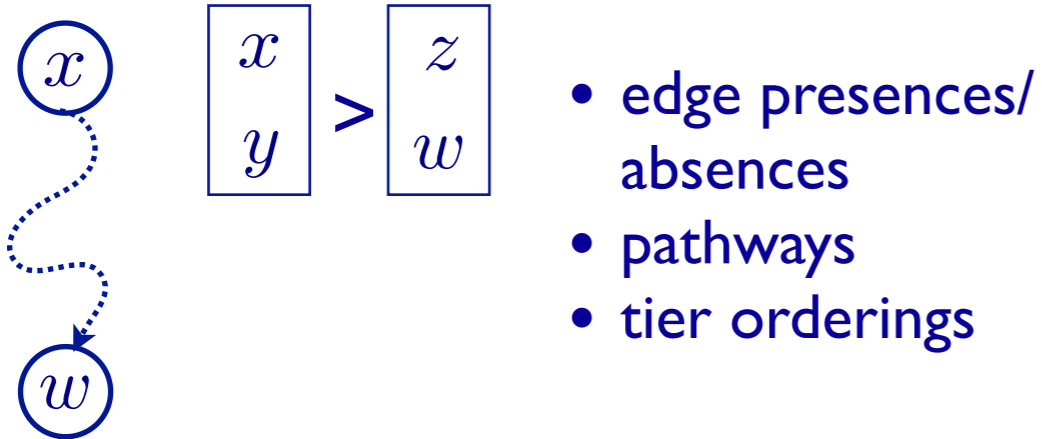
inference algorithm



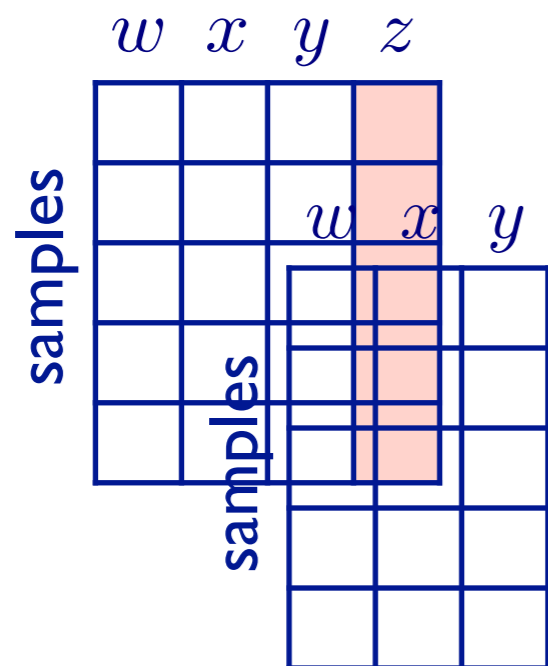
etc.

Causal Discovery

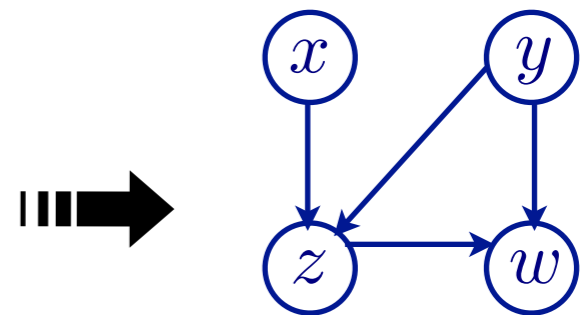
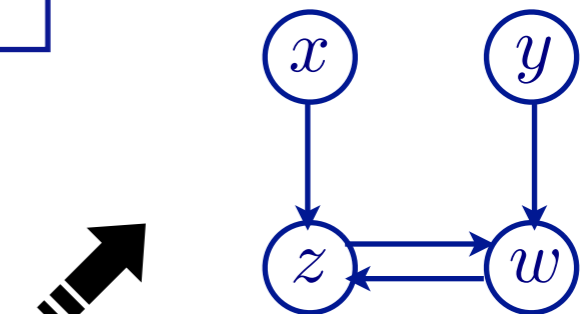
background knowledge



causal structures consistent with data



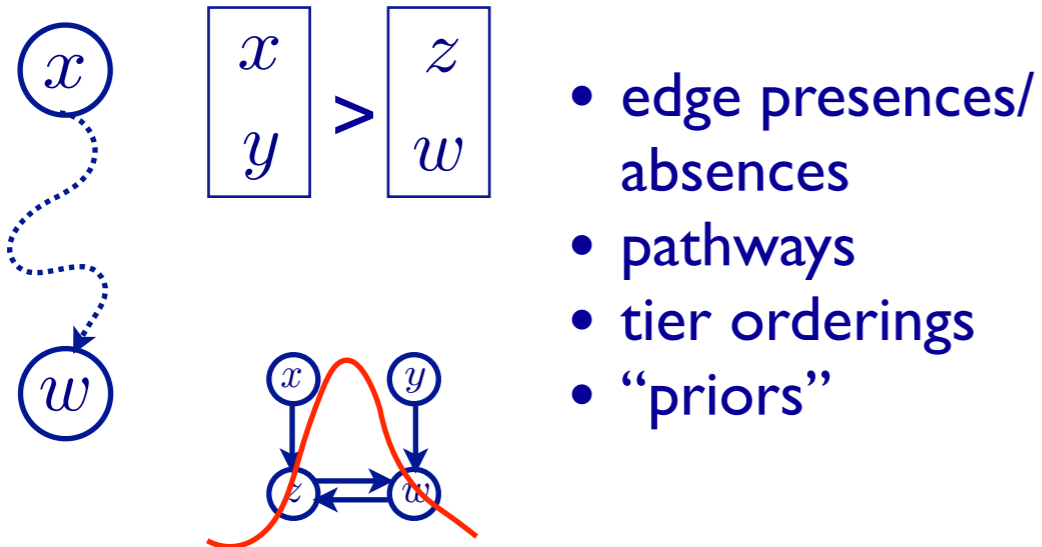
inference algorithm



etc.

Causal Discovery

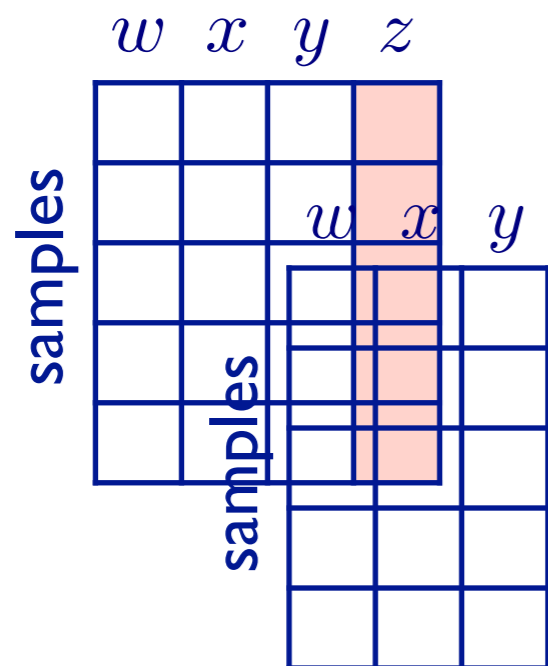
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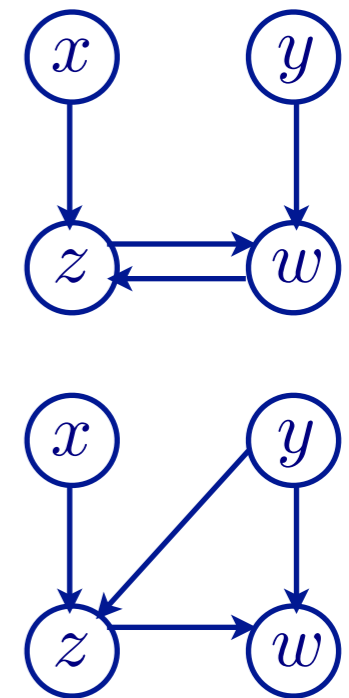
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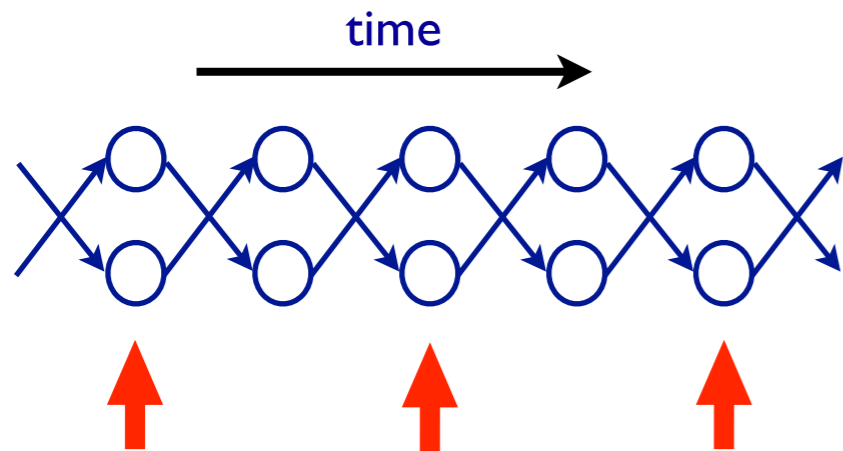
inference algorithm



etc.

Settings: examples

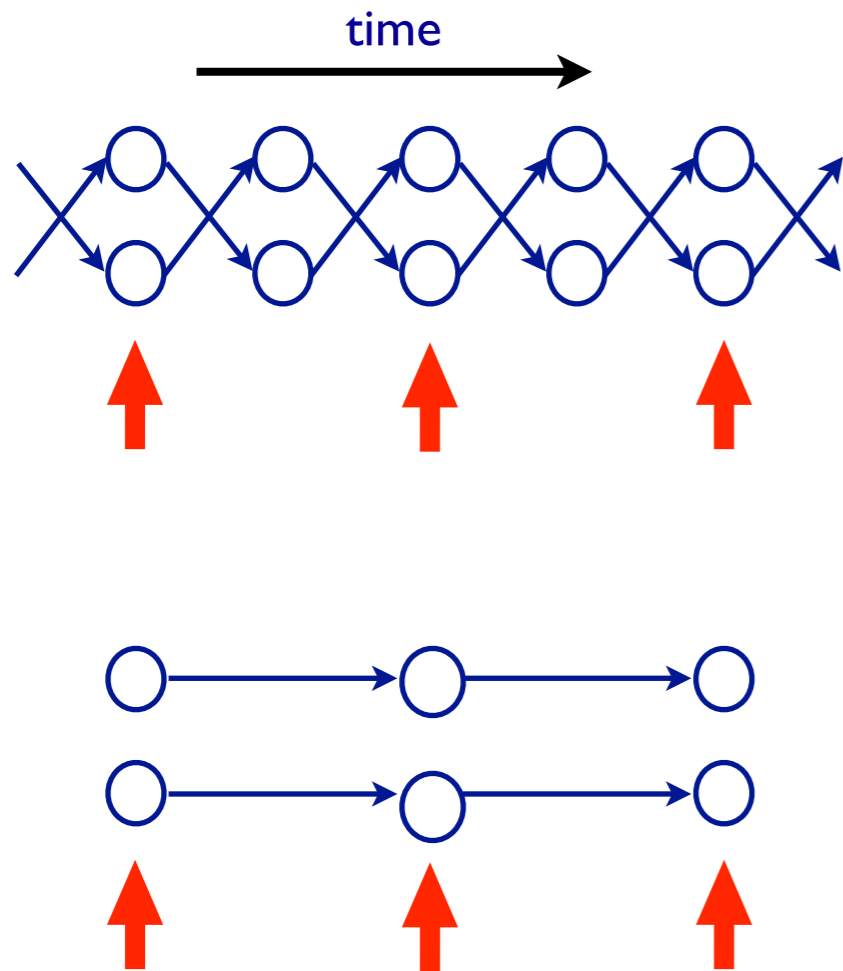
subsampled time series



(cf. work by Plis & Danks)

Settings: examples

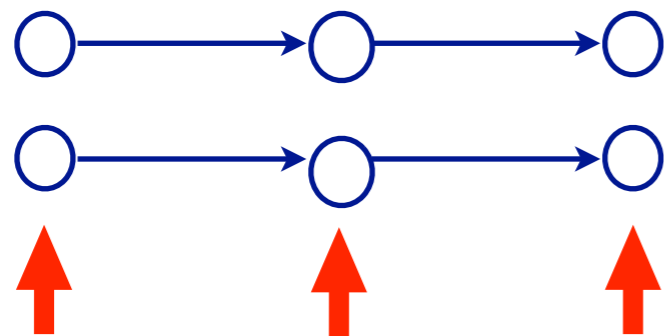
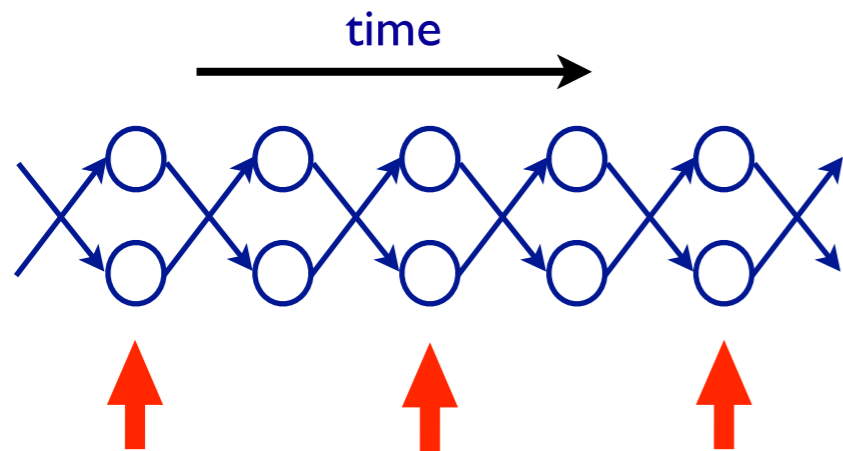
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Settings: examples

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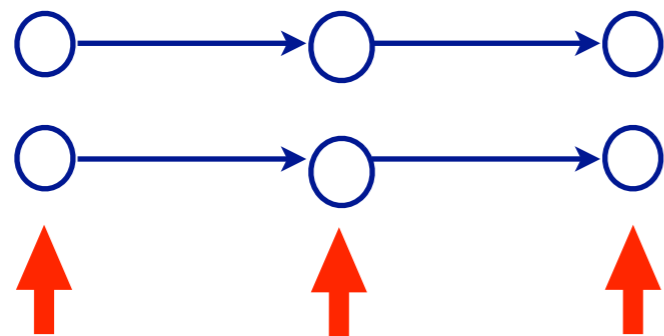
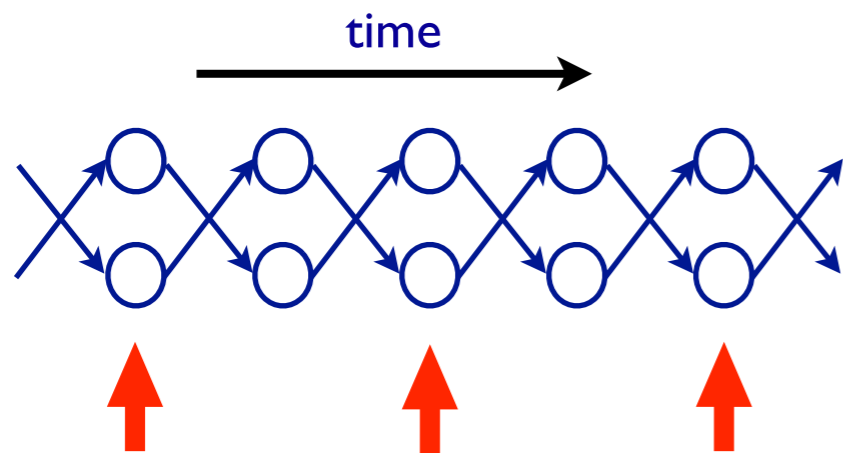
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inference algorithm

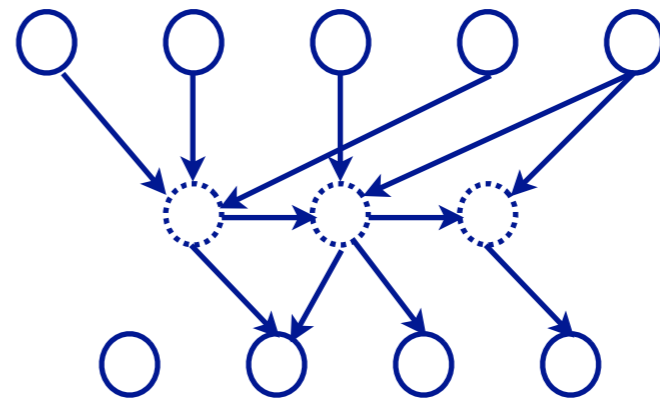
Settings: examples

subsampled time series



(cf. work by Plis & Danks)

biological settings



(cf. work by Murray-Watters & Glymour)



inference algorithm

Causal Effects

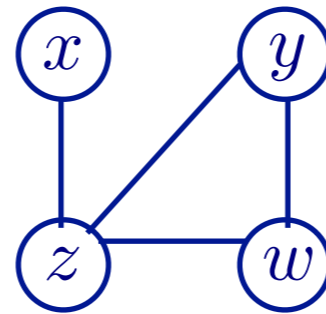


inference algorithm

Causal Effects



inference algorithm

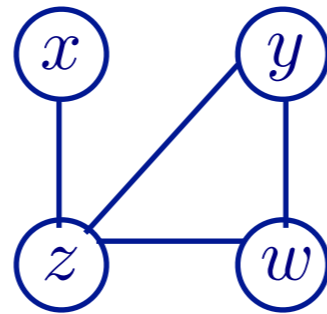


equivalence class

Causal Effects



inference algorithm



equivalence class



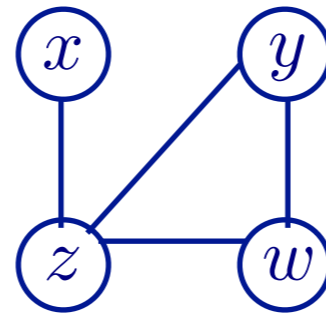
$$P(y|do(w))$$

causal effect

Causal Effects



inference algorithm



equivalence class



$$P(y|do(w))$$

causal effect

How to apply the do-calculus in settings when the causal structure is underdetermined?

High-Level

High-Level

data
sample

	<i>w</i>	<i>x</i>	<i>y</i>	<i>z</i>
samples				

	<i>w</i>	<i>x</i>	<i>y</i>
samples			

High-Level

data
sample

assumptions, e.g.

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- causal faithfulness
- etc.

w *x* *y* *z*

samples

w *x* *y*

samples

High-Level

data
sample

assumptions, e.g.

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- etc.

background
knowledge, e.g.

- pathways
- tier ordering
- “priors”
- etc.

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samples

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setting

- subsampled time series
- tier structure

w x y z

samples

w x y

samples

High-Level

data
sample

assumptions, e.g.

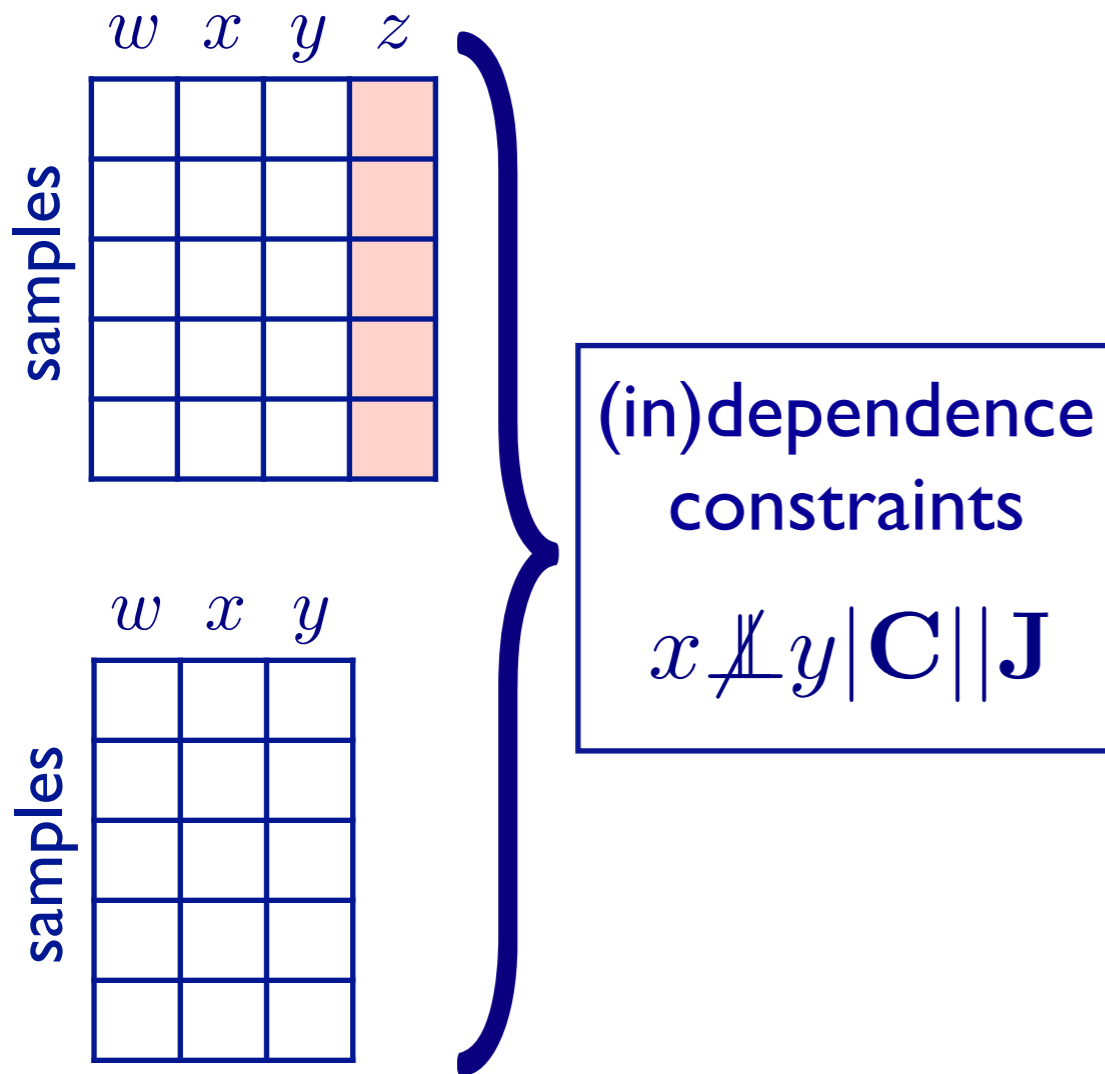
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<i>w</i>	<i>x</i>	<i>y</i>	<i>z</i>

samples

<i>w</i>	<i>x</i>	<i>y</i>

(in)dependence
constraints

$$x \not\perp y | \mathbf{C} || \mathbf{J}$$

Encode these as
logical constraints on
the underlying graph
structure

High-Level

data sample

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(in)dependence constraints

$$x \not\perp y \mid \mathbf{C} \mid \mathbf{J}$$

Encode these as logical constraints on the underlying graph structure

(max) SAT-solver

d-separation and independence

- Under the assumption of **causal Markov** and **causal Faithfulness**:

$$x \not\perp y \mid \mathbf{C} \parallel \mathbf{J} \iff x \perp y \mid \mathbf{C} \parallel \mathbf{J}$$

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x and y are d-connected
given **C** when variables
in **J** are subject to
intervention



x and y are dependent
given **C** when variables
in **J** are subject to
intervention

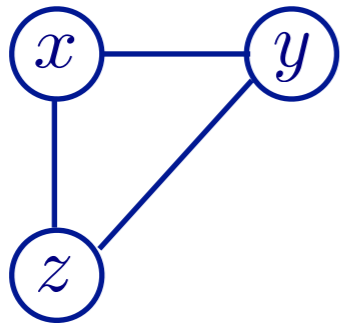
Example with 3 variables: x, y, z

$$x \perp y$$

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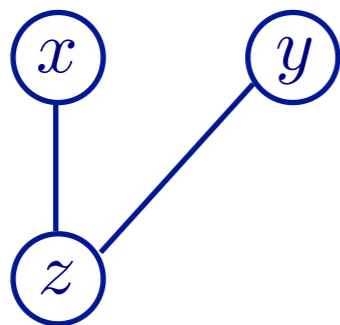
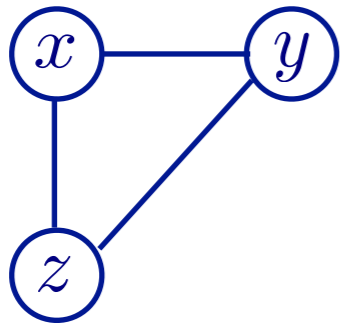
PC-algorithm



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$$x \perp\!\!\!\perp y$$

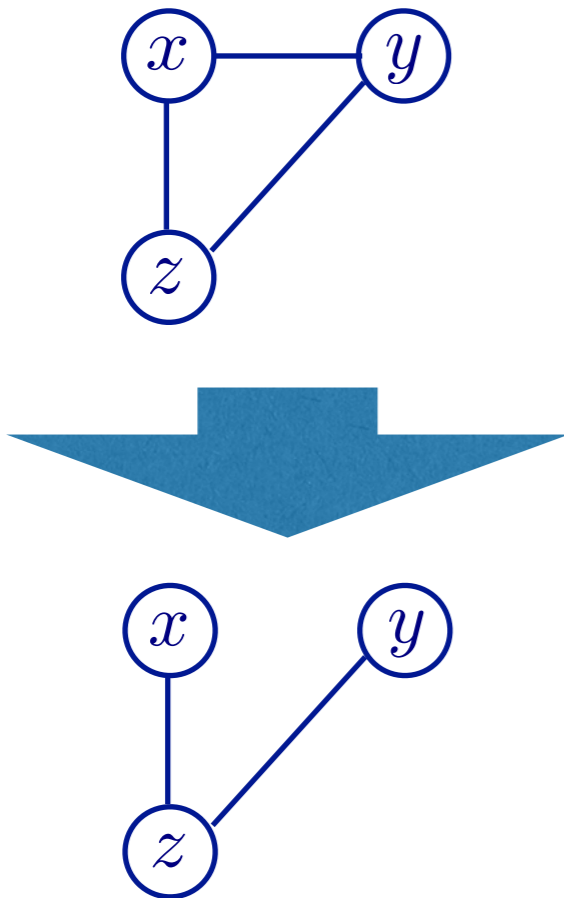
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PC-algorithm



SAT-algorithm

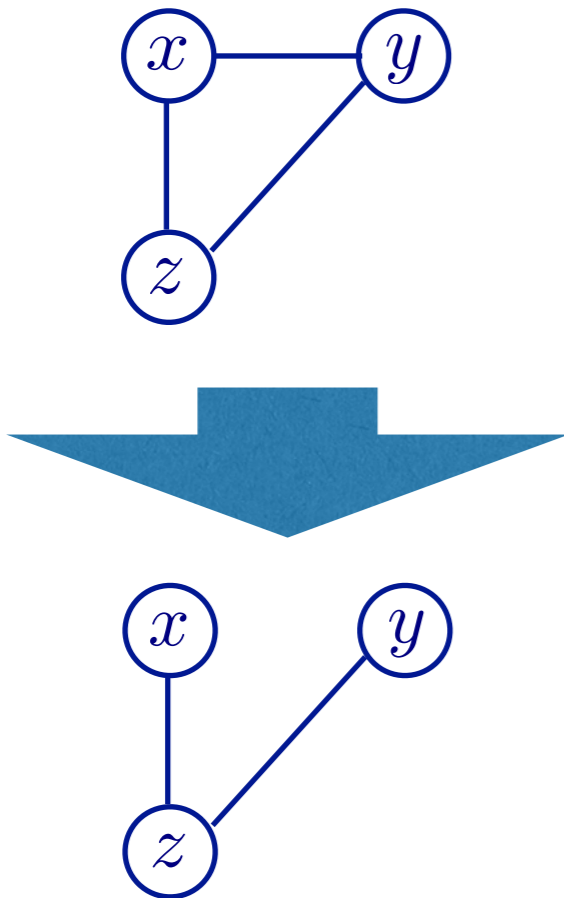
define atoms

- $A := "x \rightarrow y \in G"$
- $B := "y \rightarrow x \in G"$
- $C := "z \rightarrow x \in G"$
- $D := "z \rightarrow y \in G"$
- ...

Example with 3 variables: x, y, z

$$x \perp\!\!\!\perp y$$

PC-algorithm



SAT-algorithm

define atoms

$$\left\{ \begin{array}{l} A := "x \rightarrow y \in G" \\ B := "y \rightarrow x \in G" \\ C := "z \rightarrow x \in G" \\ D := "z \rightarrow y \in G" \\ \dots \end{array} \right.$$

encode constraint

$$\left\{ \begin{array}{ll} \neg A \wedge \neg B & // \text{direct edges} \\ \wedge \neg(C \wedge D) & // \text{common causes} \\ \wedge \neg\dots & // \text{indirect paths} \end{array} \right.$$

SAT-based Causal Discovery

- **Formulate the independence constraints in propositional logic**

$$x \perp\!\!\!\perp y \iff \neg A \wedge \neg B \dots$$

$$A = 'x \rightarrow y \text{ is present}'$$

SAT-based Causal Discovery

- Formulate the independence constraints in propositional logic
- Encode the constraints into one formula.

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SAT-based Causal Discovery

- Formulate the independence constraints in propositional logic
- Encode the constraints into one formula.
- Find satisfying assignments using a SAT-solver

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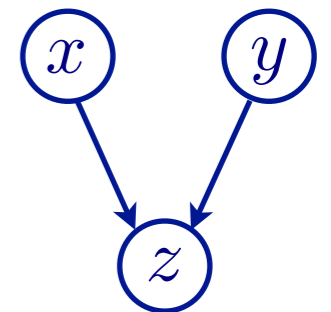
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$$A = \textit{false}$$

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...



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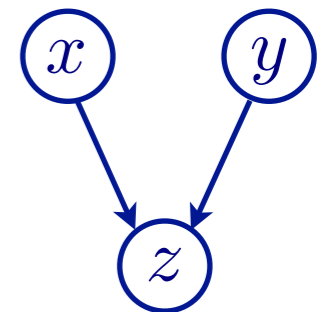
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➡ very general setting (allows for cycles and latents) and trivially complete

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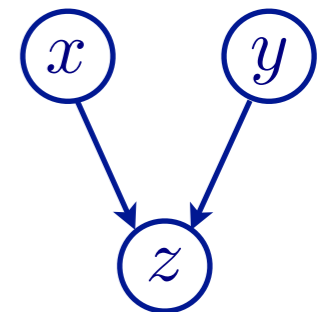
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...



➡ very general setting (allows for cycles and latents) and trivially complete

➡ **BUT:** erroneous test results induce conflicting constraints:
UNsatisfiable

Conflicts and Errors

- **Statistical independence tests produce errors**

constraint

$$x \not\perp z$$

$$y \not\perp z$$

$$x \perp y$$

$$x \perp y | z$$

Conflicts and Errors

- Statistical independence tests produce errors

➔ **Conflict:** no graph can produce the set of constraints

constraint

$$x \not\perp z$$

$$y \not\perp z$$

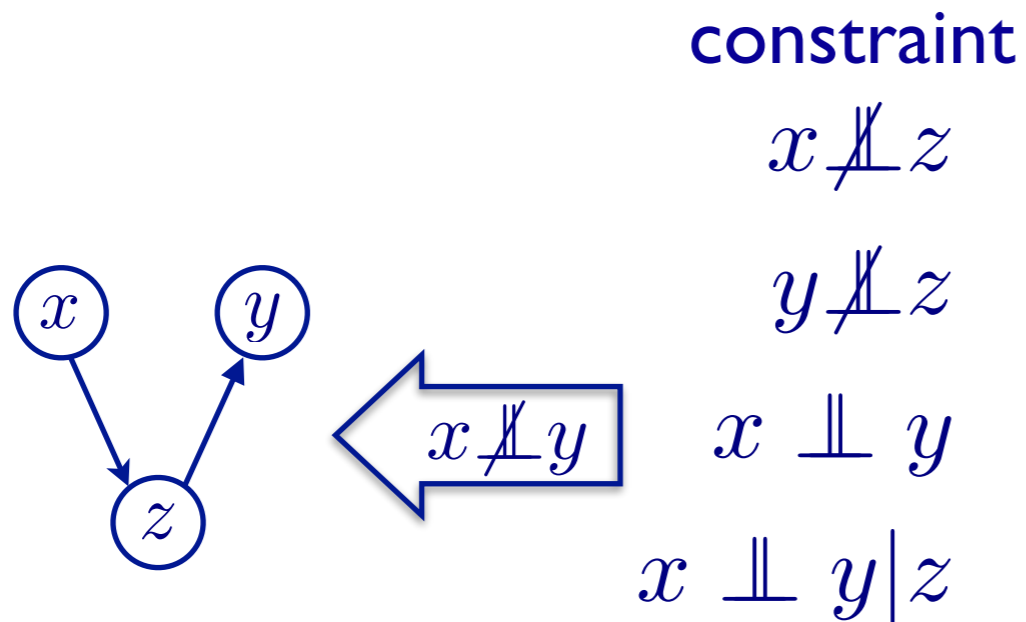
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Conflicts and Errors

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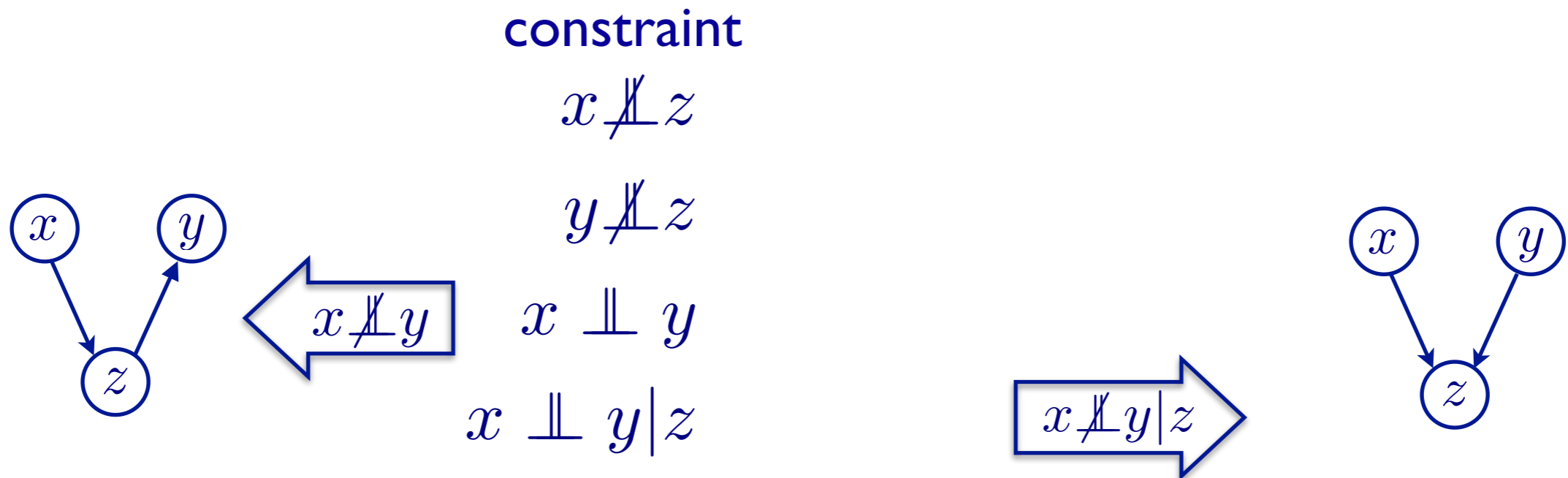
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Conflicts and Errors

- Statistical independence tests produce errors

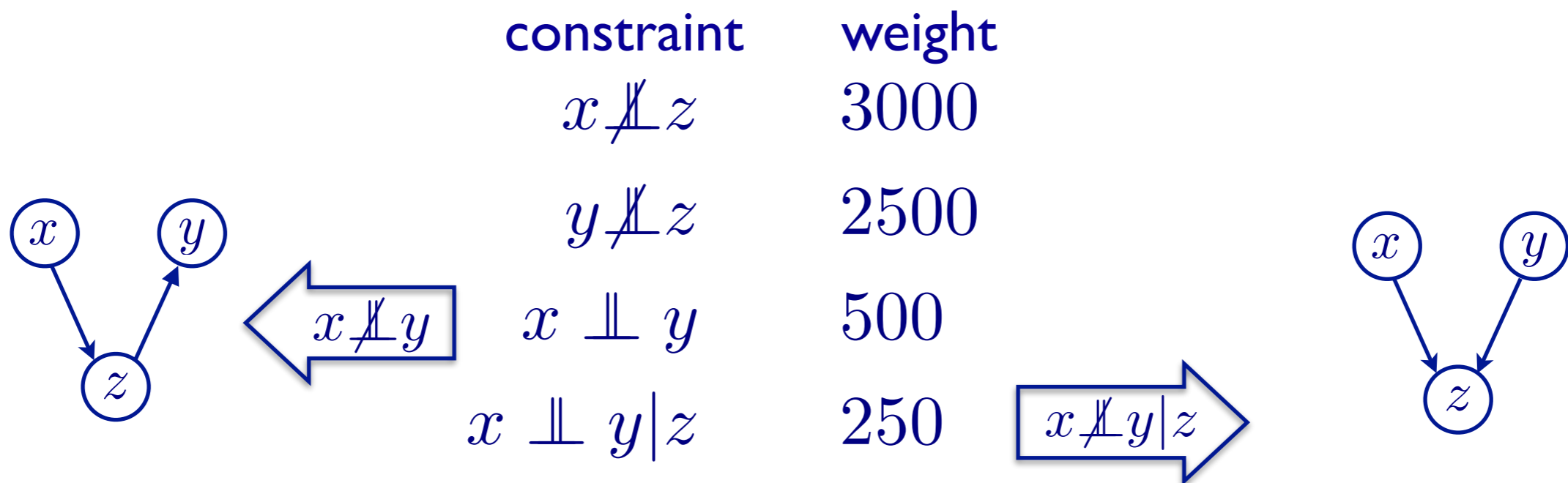
➡ **Conflict:** no graph can produce the set of constraints



Conflicts and Errors

- Statistical independence tests produce errors

➡ **Conflict:** no graph can produce the set of constraints



Constraint Satisfaction Approach

- **INPUT:** (in)dependence constraints weighted according to reliability

$$\min_G \sum_{k : \text{constraint } k \text{ is not satisfied by } G} w(k)$$

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What are suitable weights?

Weighting Schemes

- Constant weights
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 - Model selection with Bayes rule:

$$\begin{array}{ccc} x \not\perp y | C & & x \perp y | C \\ P(x|C)P(y|x, C) & \text{VS.} & P(x|C)P(y|C) \end{array}$$

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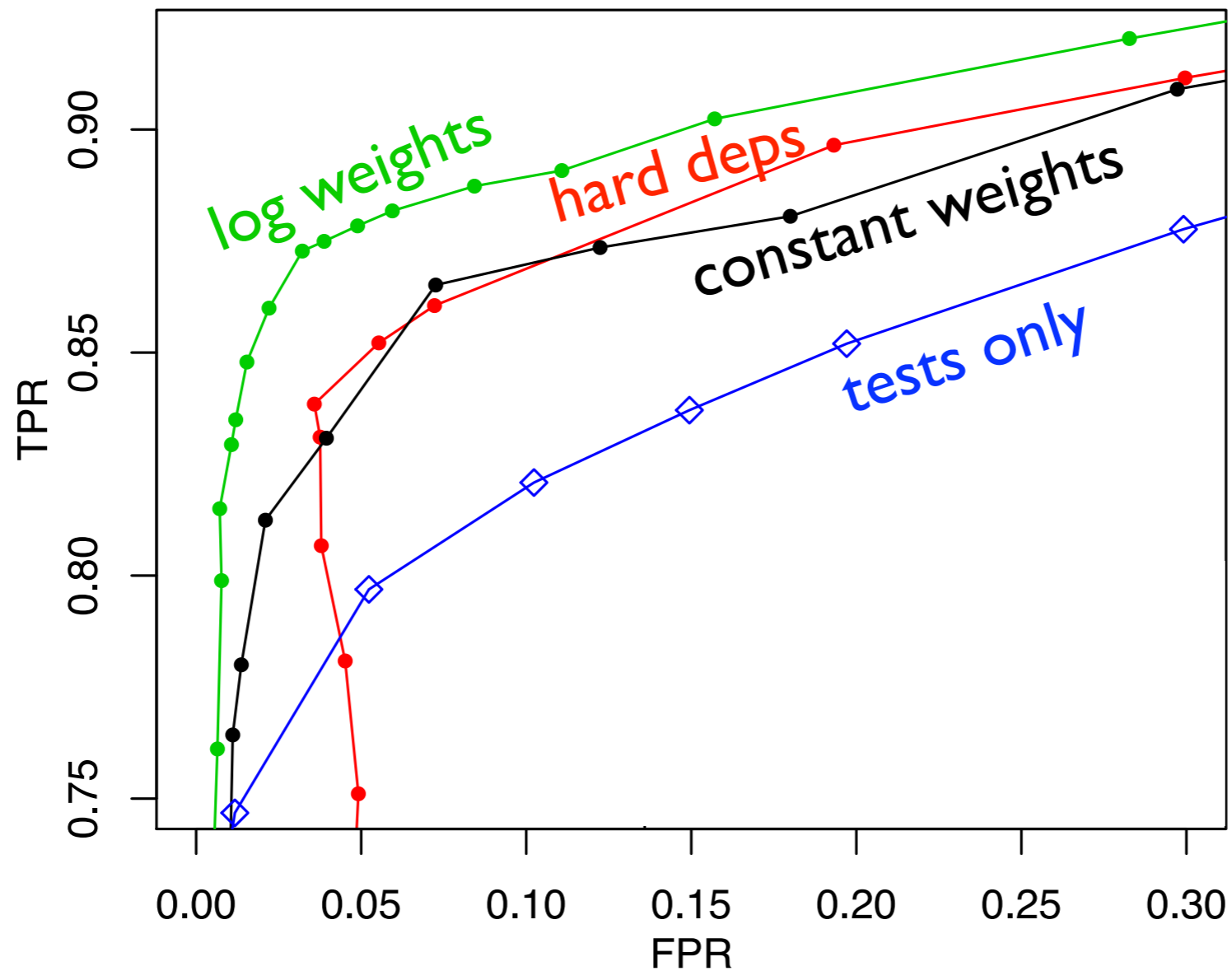
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- probabilistic classifier: find G such that if it were true, test results would be optimal in the sense of a proper score

Optimization

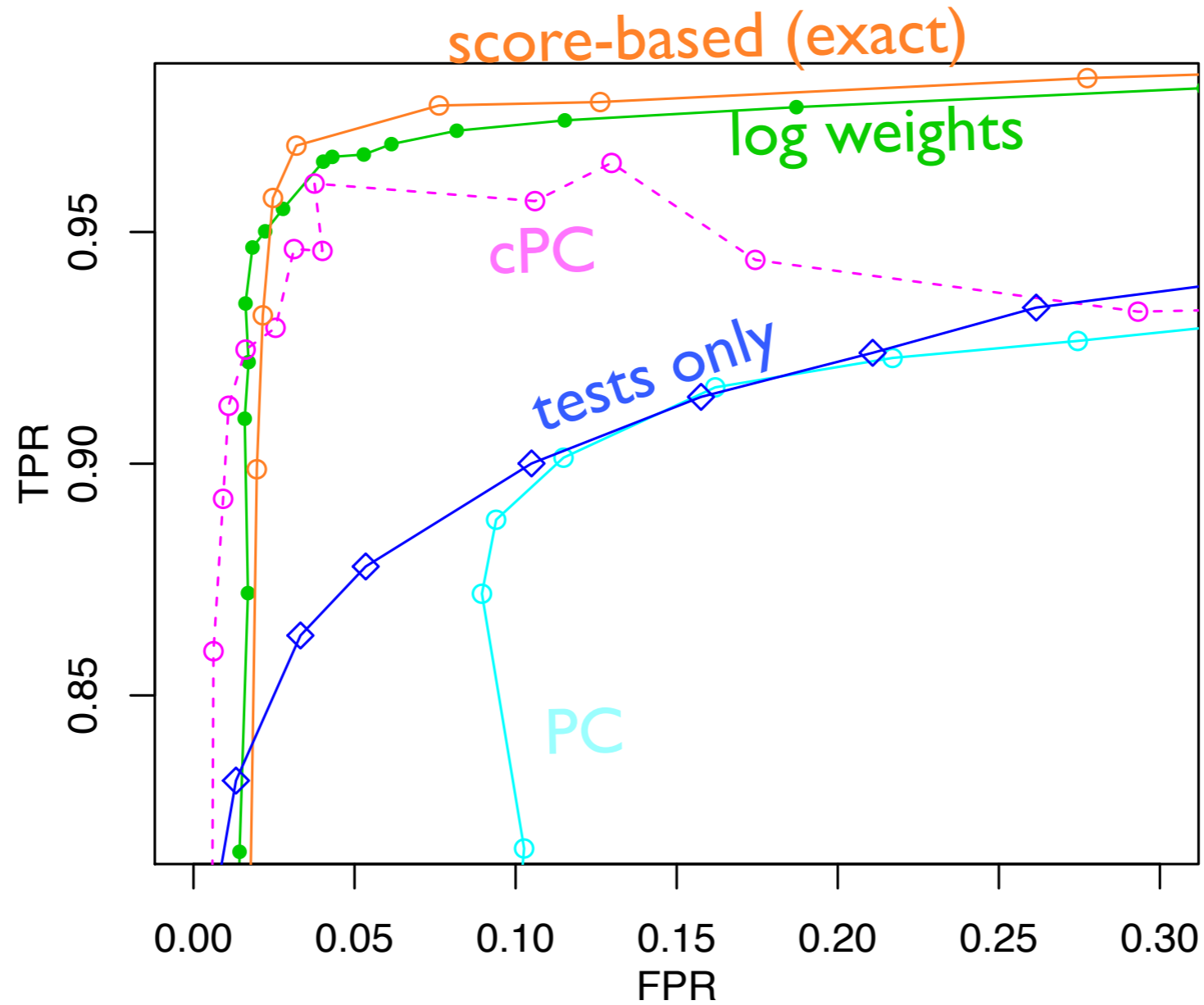
- Answer Set Programming (ASP) is a modern declarative programming paradigm
 - solver used: Clingo
 - SAT-solver and branch and bound algorithm
 - finds globally optimal weighted maxSAT solution

Simulation I: cycles and latents



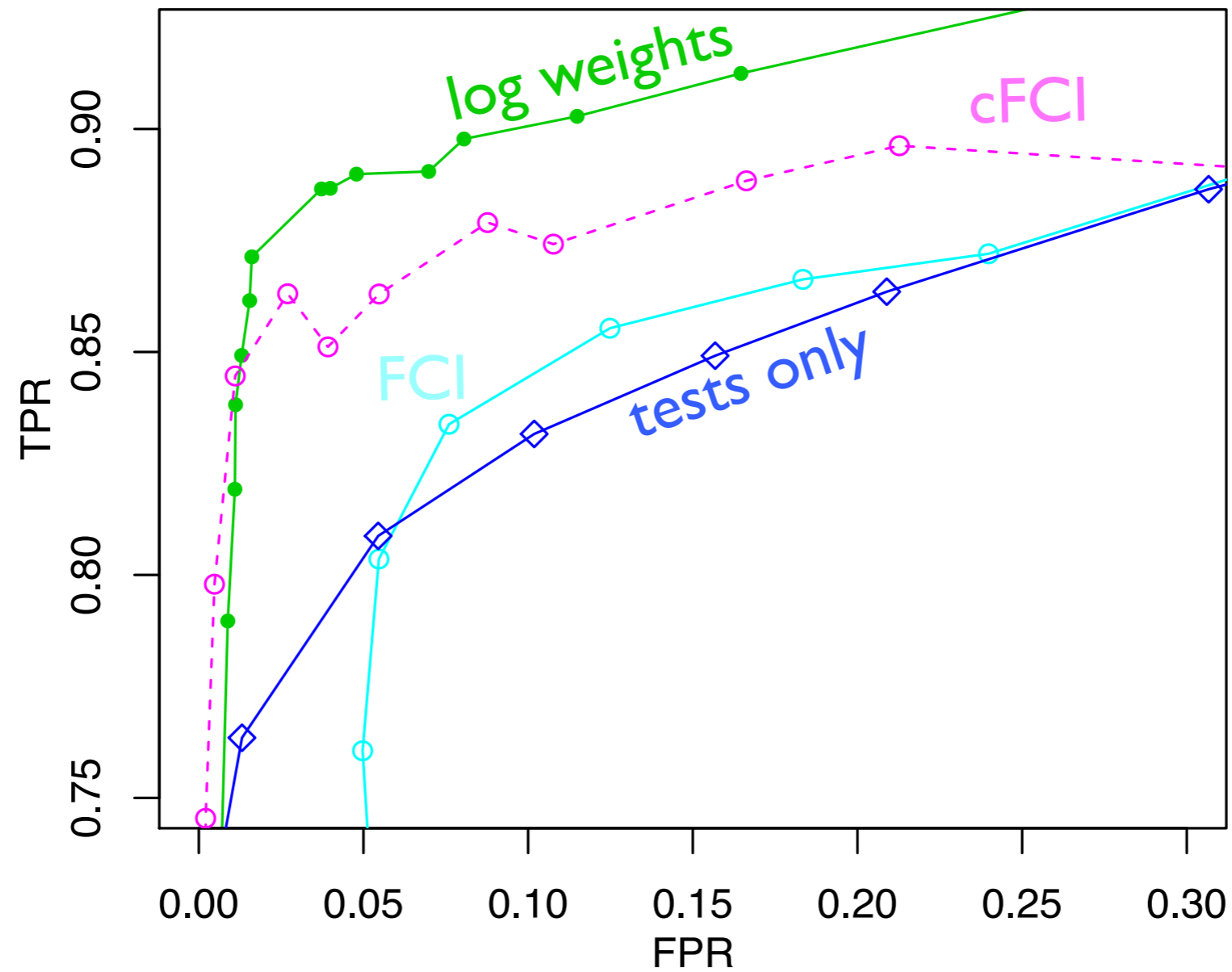
- ROC of dependences, passive observational data set, 6 observed variables, average degree 2; 500 samples, 200 models, linear Gaussian parameterization

Simulation 2: no cycles, no latents



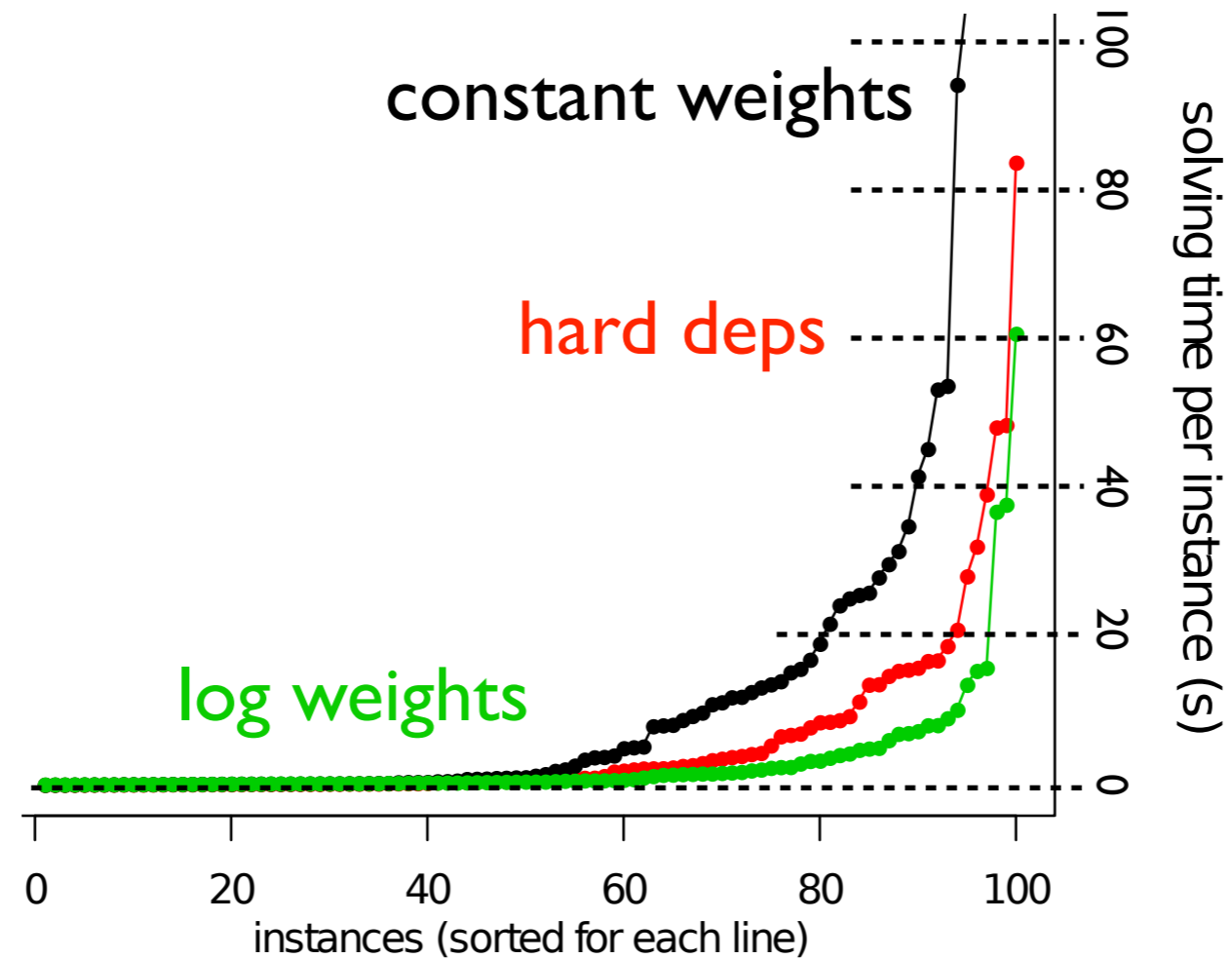
- cPC returns a fully determined output only 58/200 times at its optimum

Simulation 3: no cycles, but latents



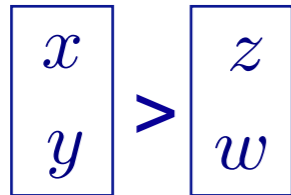
- cFCI only returns unambiguous results 61/200 times at its optimum

Simulation 4: Scalability



- up to 7 variables and only a few data sets for now (9×10^{18} graphs)

Background Knowledge

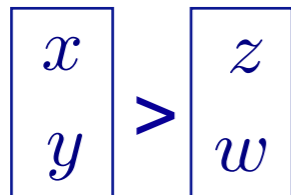


“priors”

Background Knowledge

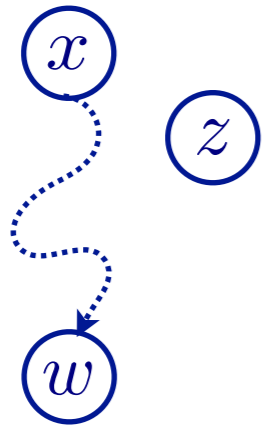


$$x \not\perp w \mid x$$

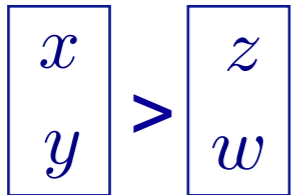


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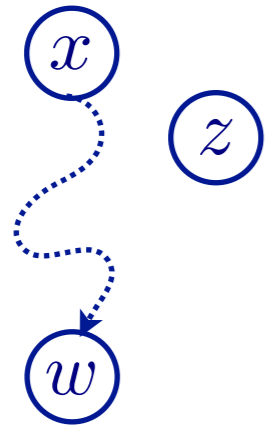


$$x \not\perp w \mid x z$$

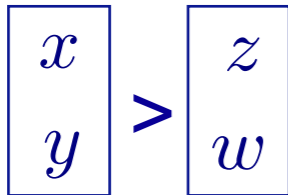


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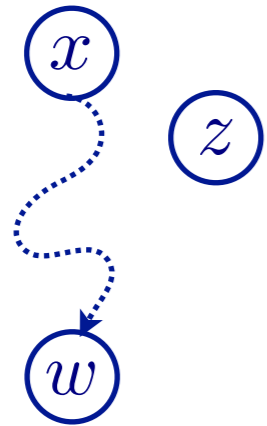


$x \perp w \mid x z$ *weight* = 0.8

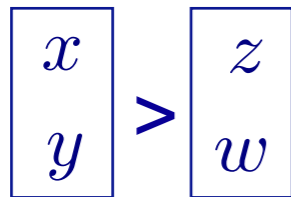


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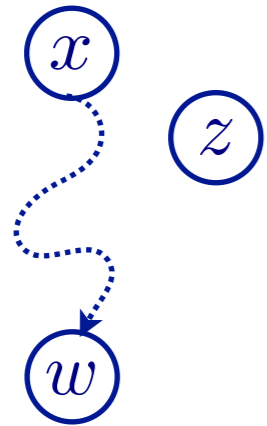
$$x \not\perp w \mid x z \quad \text{weight} = 0.8$$



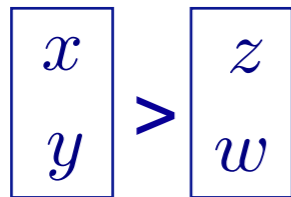
$$(x > z) \wedge (x > w) \\ \wedge (y > z \wedge (y > w))$$

“priors”

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$$x \not\perp w \mid x \ z \quad \text{weight} = 0.8$$

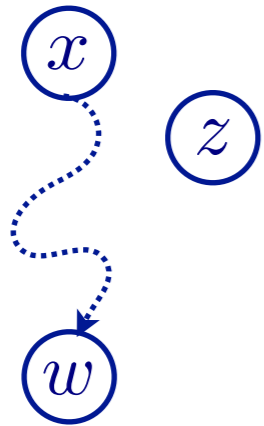


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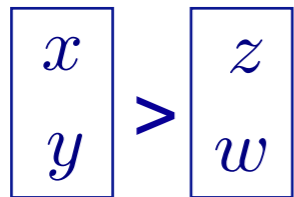
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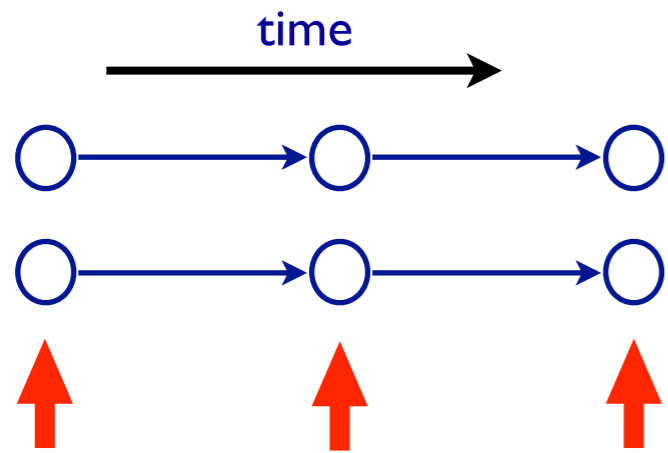
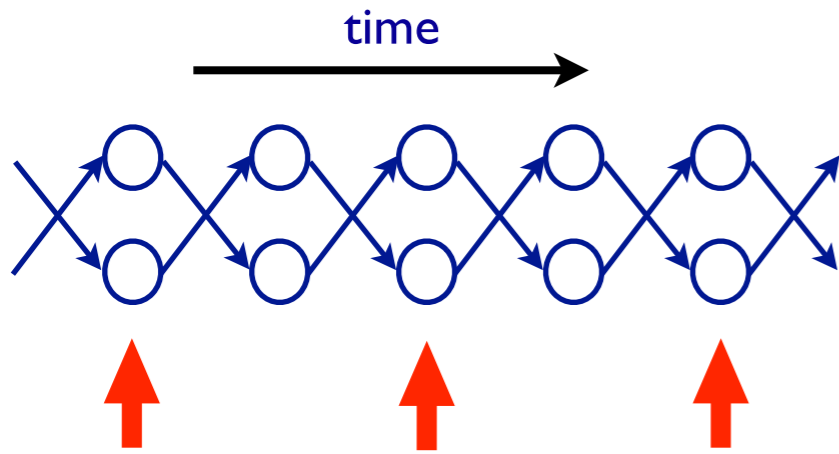
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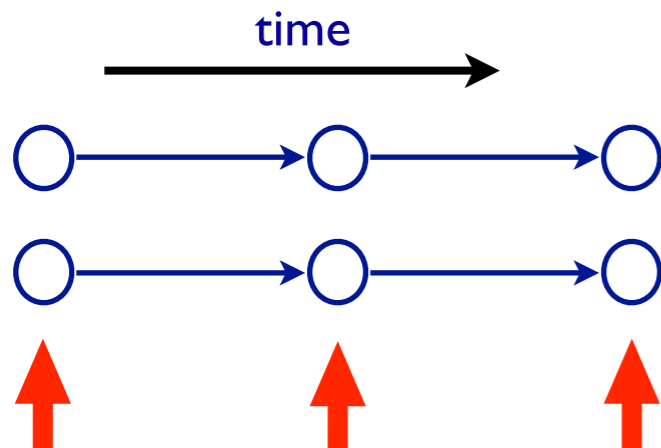
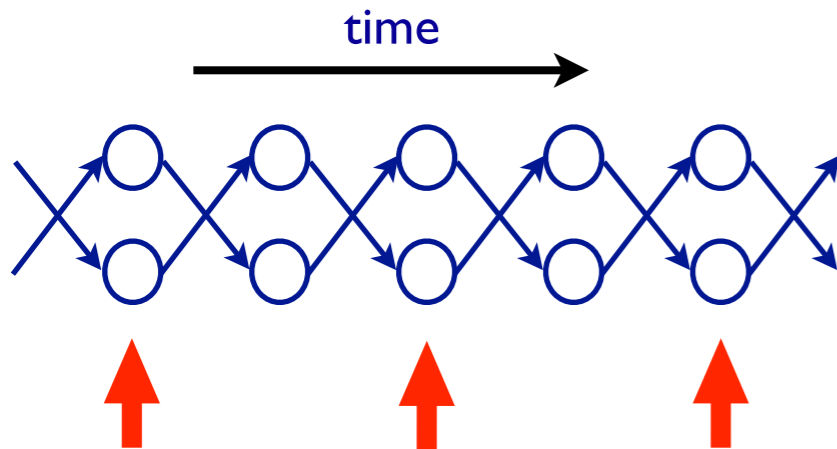


- specific probabilities for each graph
- soft sparsity constraint
- ...

Settings



Settings



```
urange(1..5).
```

```
1 { u(U): urange(U) } 1.
```

```
{ edge1(X,Y) } :- node(X), node(Y).
```

```
path(X,Y,1) :- edge1(X,Y).
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path(X,Y,L) :- path(X,Z,L-1), edge1(Z,Y),  
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conflu(X,Y) :- path(Z,X,L), path(Z,Y,L),  
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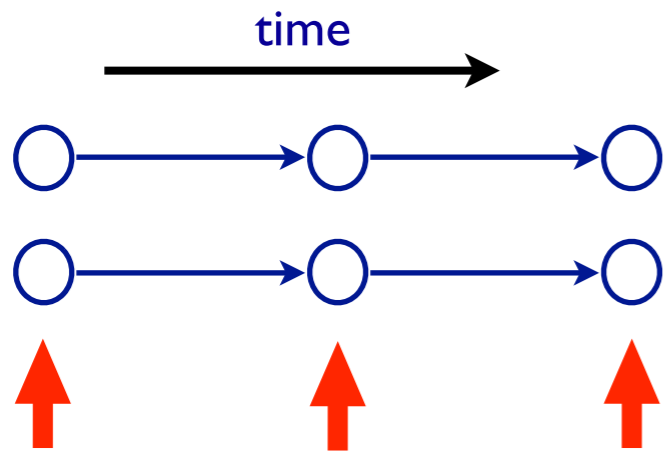
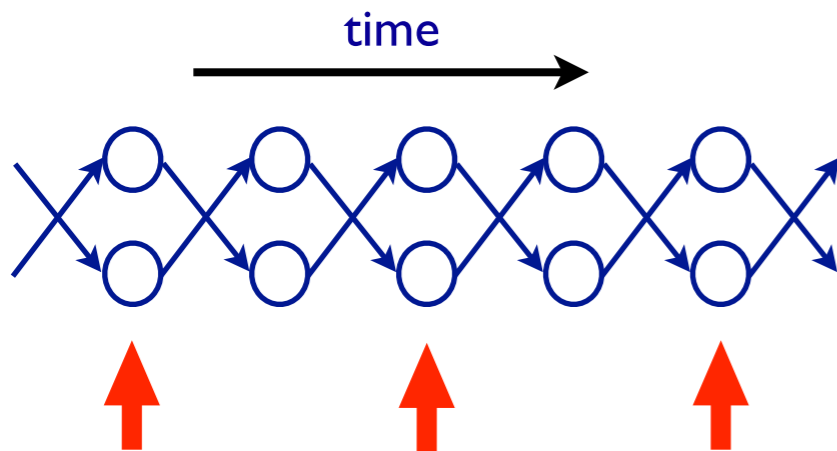
```
:- edgeu(X,Y), not edge1u(X,Y).
```

```
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```

```
:- confu(X,Y), not conflu(X,Y).
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Settings



def. of how confounders arise due to subsampling

range for rate of subsampling

subsampling rate is unique

def. of edge in graph

recursive def. of path

def. of edge in subsampled graph

constraints on how edges in subsampled graph relate to edges in true graph

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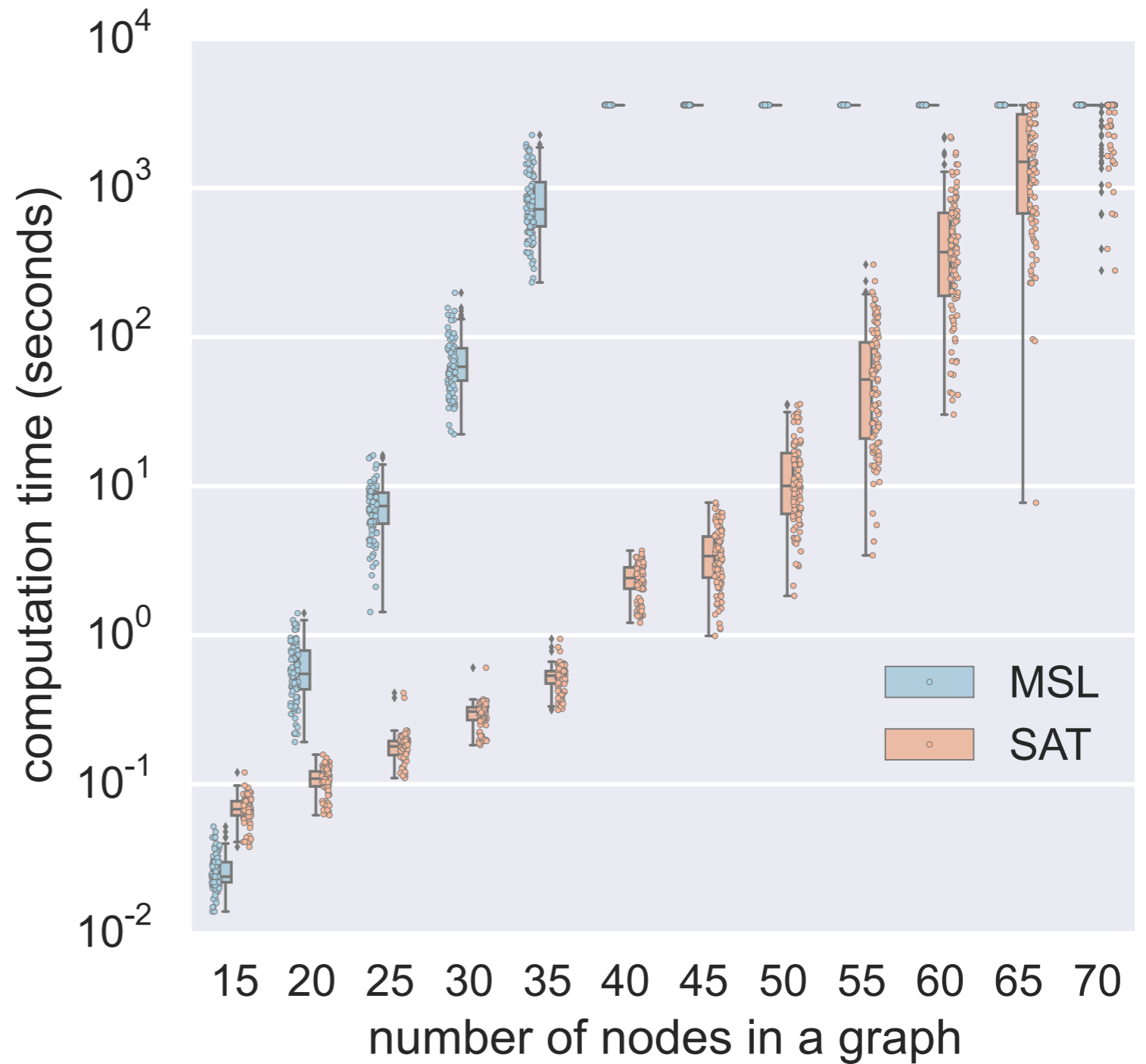
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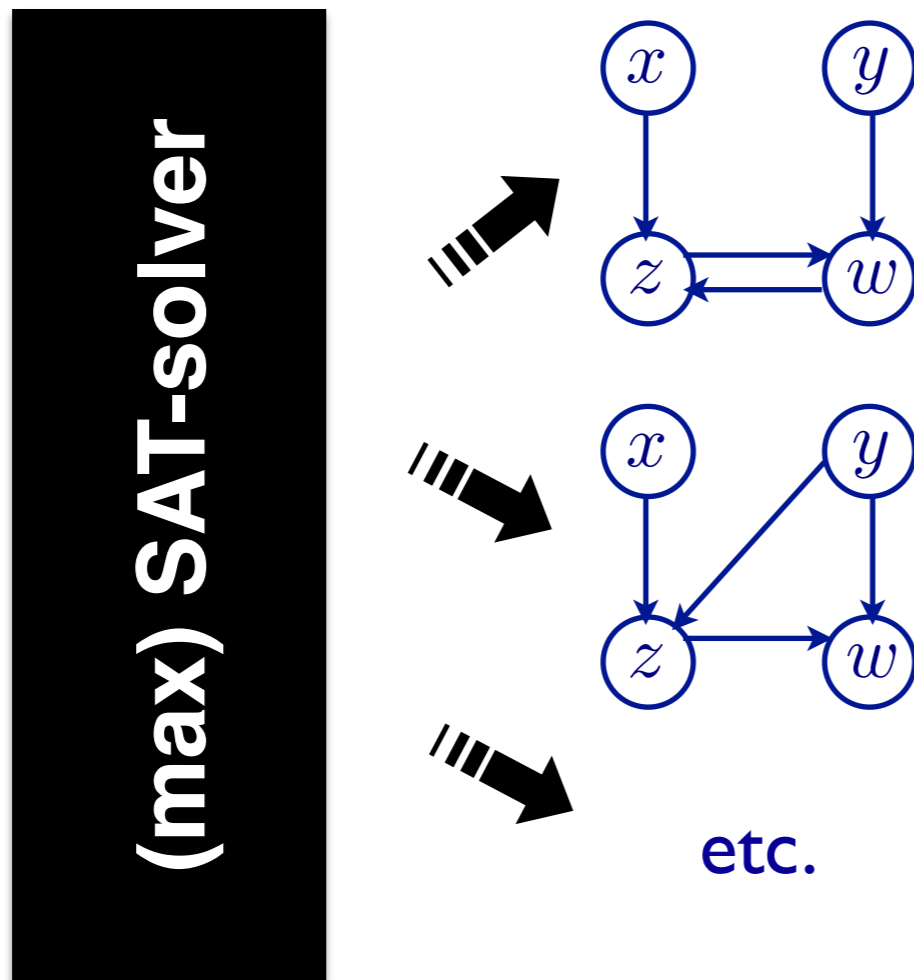
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Runtime comparison

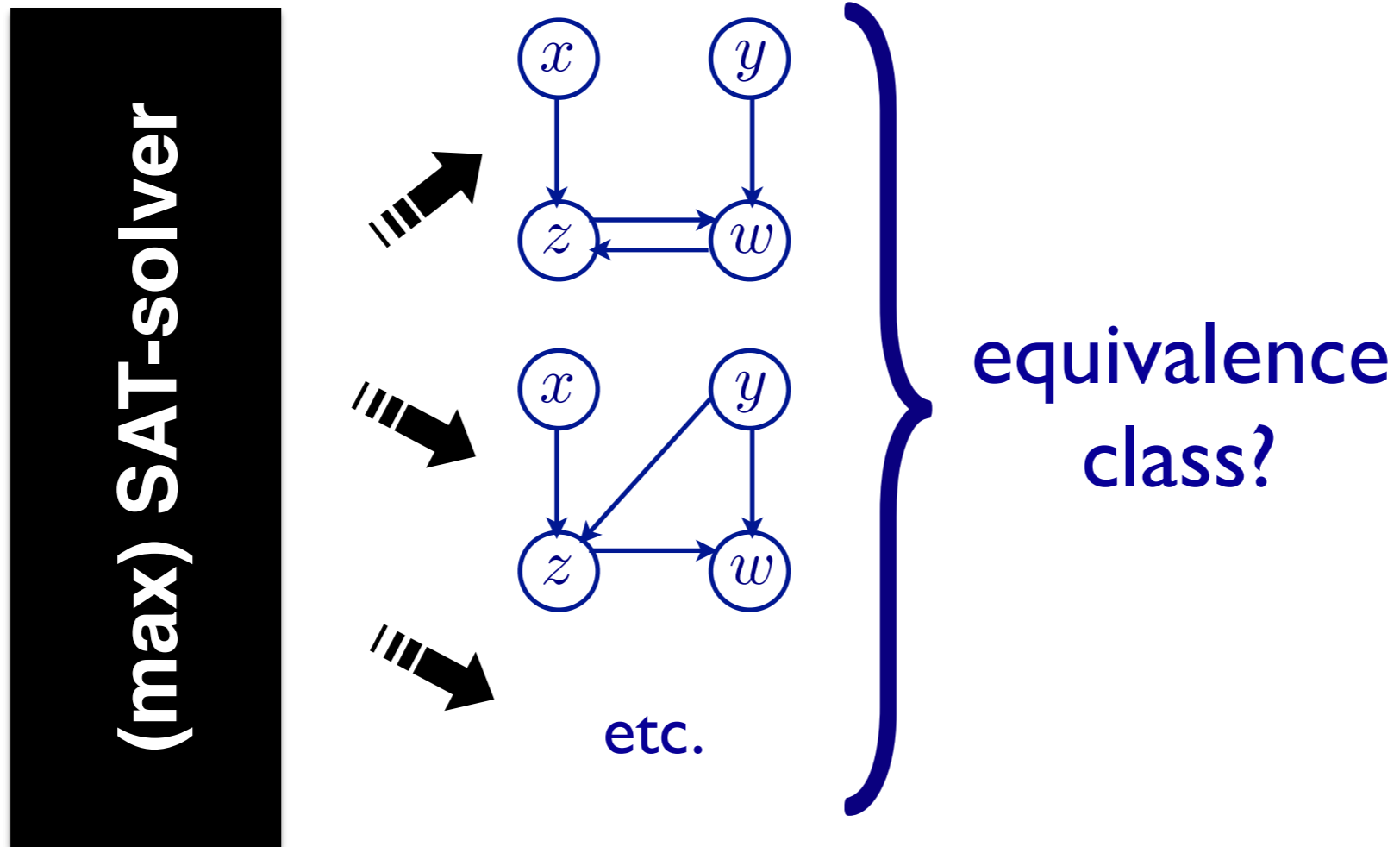
For a graph determined at subsampling rate 2, infer the equivalence class of graphs at the system time scale (1-step)



Output of Causal Search Algorithms



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Query:

(max) SAT-solver

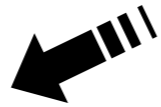


Output of Causal Search Algorithms

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- list the structures in the equivalence class

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Output of Causal Search Algorithms

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Query:

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 - edges, confounders
 - ancestral relations
 - pathways

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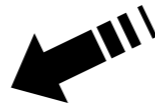


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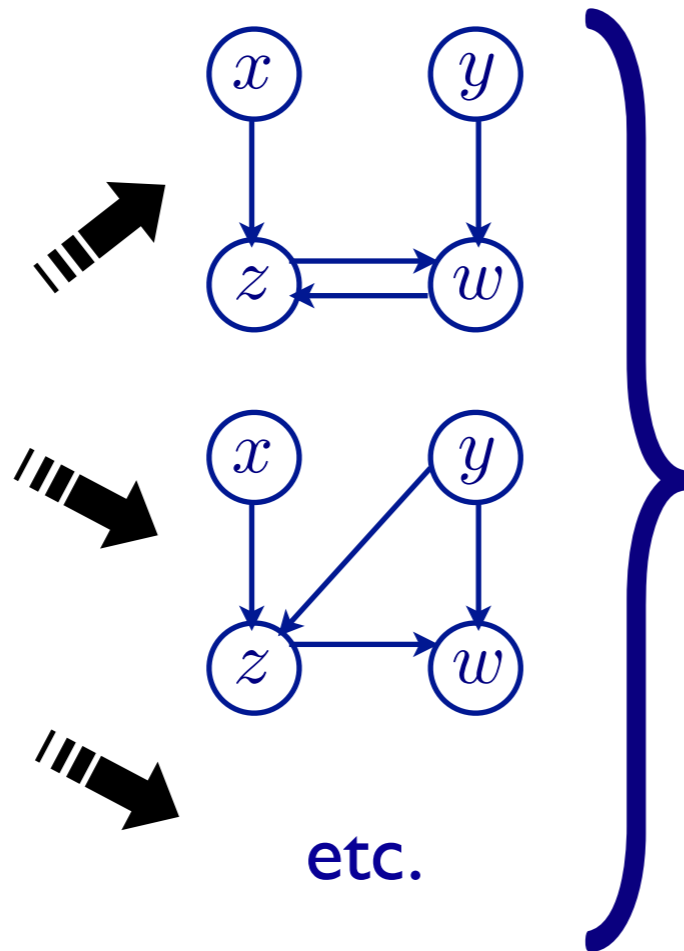
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Response:

- enumeration of solutions
- “backbone” of the SAT-instance
- ...

Computing Causal Effects

(max) SAT-solver



equivalence class?

$P(y|do(x))$?

equivalence
class? $\rightarrow P(y|do(x)) ?$

equivalence
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- enumerate each graph in the equivalence class and run the Tian-Shpitser algorithm to determine the causal effect?

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- Alternative:

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do-calculus

Rule 1 (insertion/deletion of observations)

$$P(y|do(x), z, w) = P(y|do(x), w) \text{ if } Y \perp\!\!\!\perp Z|X, W||X$$

Rule 2 (action/observation exchange)

$$P(y|do(x), do(z), w) = P(y|do(x), z, w) \text{ if } Y \perp\!\!\!\perp I_Z|X, Z, W||X$$

Rule 3 (insertion/deletion of actions)

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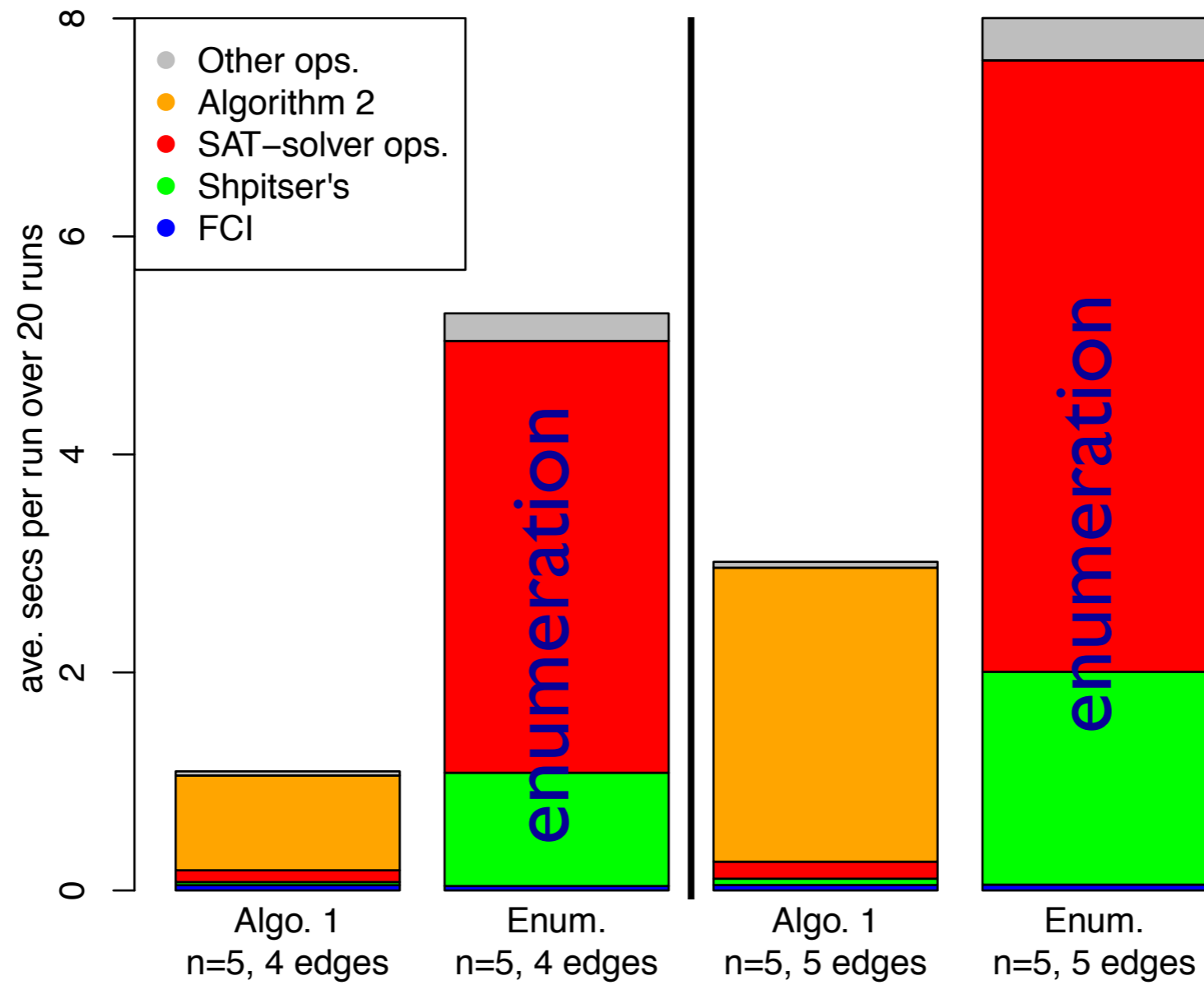
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- ➔ search in the equivalence class over the possible applications of the *do*-calculus rules by *querying* the satisfaction of their conditions

Algorithm for the *do*-calculus when the graph is unknown

- determine the equivalence class implicitly using a SAT-solver
- query one solution graph G
- run the Tian-Shpitser-algorithm on G to determine whether the causal effect $P(y|do(w))$ is determined for G
- if it is, determine which *do*-calculus rules were applied and record the constraints C_1, \dots, C_n that were used
 - add $\neg C_1 \vee \dots \vee \neg C_n$ as a constraint to refine the current equivalence class
- if not, determine the “hedge” H and add $\neg H$ to refine the current equivalence class
- repeat until the equivalence is exhausted
- return the set of estimates of the causal effect and NA if it cannot be determined in one member of the equivalence class

Comparison of our approach to enumeration



In sum: *do*-calculus using a SAT-solver

- enables computation of the causal effect when the graph structure is underdetermined

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In sum: *do*-calculus using a SAT-solver

- enables computation of the causal effect when the graph structure is underdetermined
- ➡ how should one estimate a causal effect when the equivalence class of causal structures was determined on the basis of a set of conflicted constraints?
- some avenues one can explore with the query-based approach:
 - explore more closely the conditions involved in determining the causal effect
 - find multiple different estimators
 - even though the overall graph structure may not be determinable without resolving conflicts, some causal effects may be

Conclusion

- the use of general purpose SAT-solvers provides an extraordinarily versatile tool for causal discovery
- it opens new avenues for handling background knowledge and the computation of causal effects when the causal structure is underdetermined
- it provides a query based approach in contrast to a representation of an equivalence class of causal structures
- it suggests that current general purpose constraint solvers outperform domain specific approaches

References

- Hyttinen, Eberhardt & Järvisalo (2015). *Do-calculus when the true graph is unknown*. UAI 2015.
- Hyttinen, Eberhardt & Järvisalo (2014). *Constraint-based Causal Discovery: Conflict Resolution with Answer Set Programming*. UAI 2014.
- Hyttinen, Hoyer, Eberhardt & Järvisalo (2013). *Discovering Cyclic Causal Models with Latent Variables: A General SAT-Based Procedure*. UAI 2013.
- {Hyttinen, Plis, Danks, Eberhardt & Järvisalo} (work in progress). *Causal Discovery from Subsampled Time Series Data by Constraint Optimization*.

Other relevant work that is closely related:

- Triantafillou & Tsamardinos (2015). *Constraint-based Causal Discovery from Multiple Interventions Over Overlapping Variable Sets*. JMLR 16(Nov):2147–2205.
- Claassen & Heskes (2011). *A logical characterization of constraint-based causal discovery*. UAI 2011.
- Triantafillou, Tsamardinos & Tollis (2010). *Learning Causal Structure from Overlapping Variable Sets*. AISTATS 2010.

Thank you!