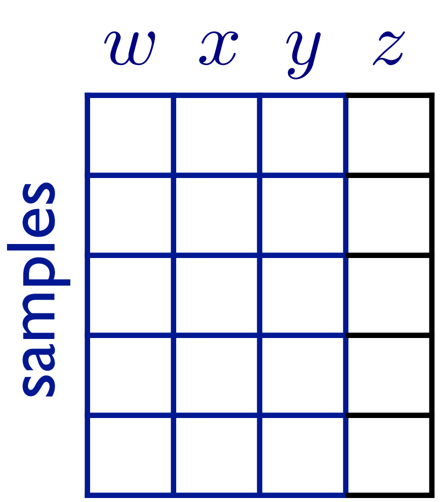
Caltech

Foundations of Causal Discovery

Frederick Eberhardt

Causal Discovery

data sample



Causal Discovery

assumptions, e.g.
- causal Markov
- causal faithfulness
- functional form
- etc.

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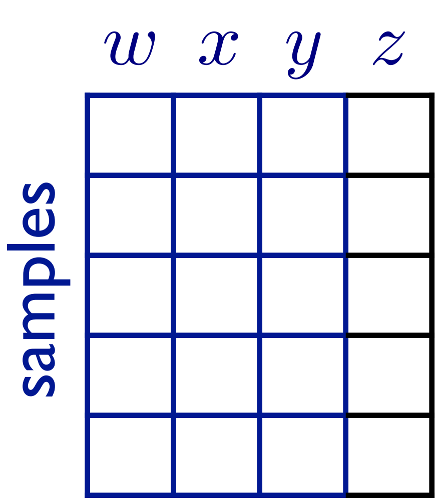

inference algorithm

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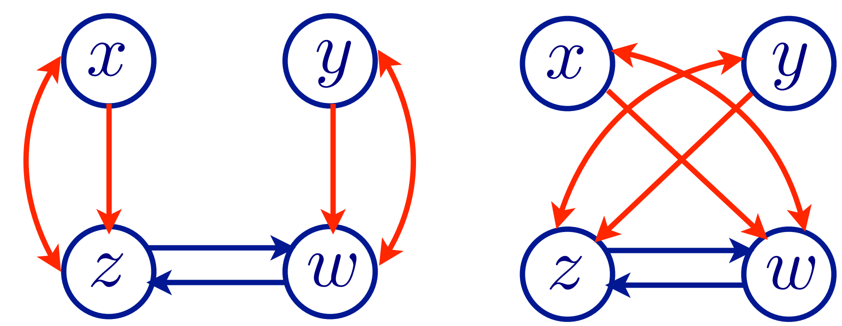

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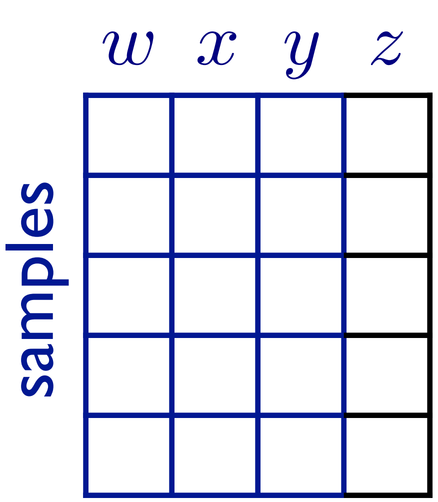

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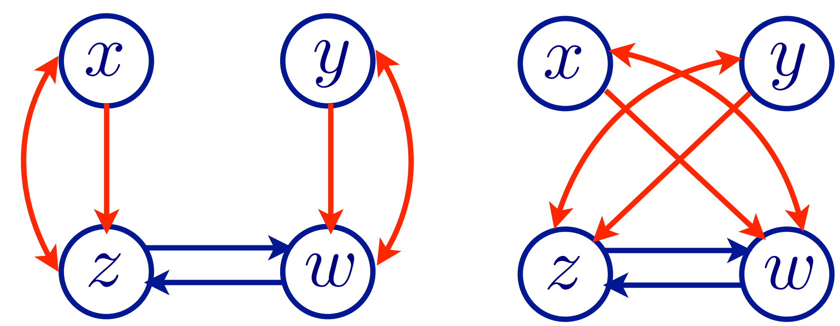

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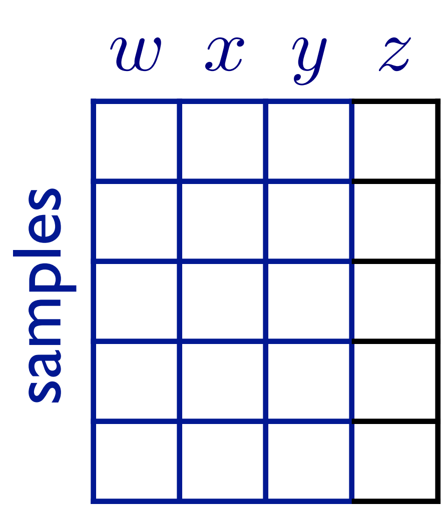


inference algorithm

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

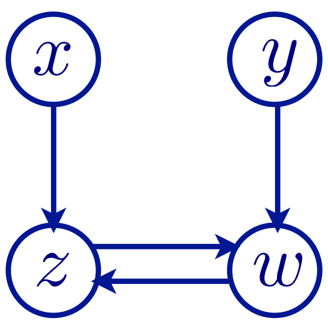
	w	x	y	z
w	0	0	?	?
x	0	0	0	?
y	?	0	0	0
z	?	?	0	0

confounders

Causal Discovery

truth

(unknown)



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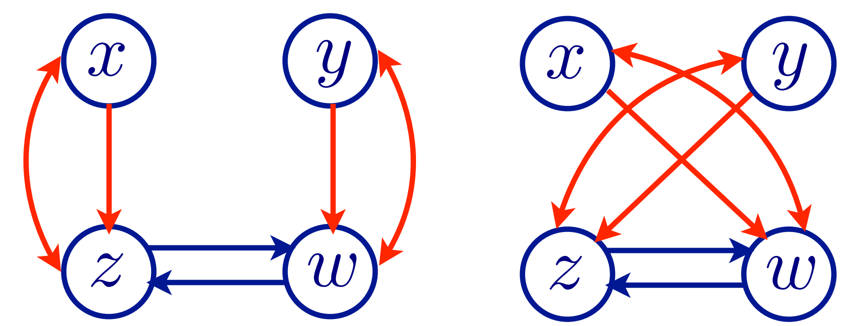

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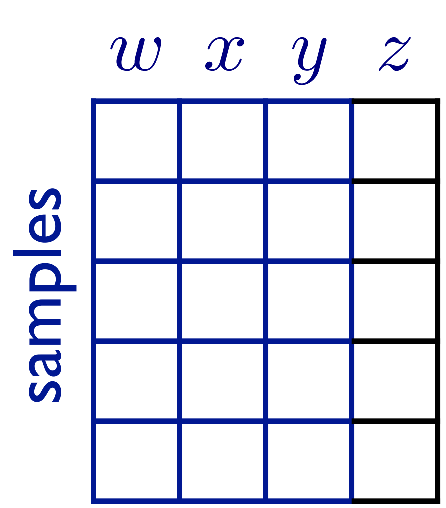

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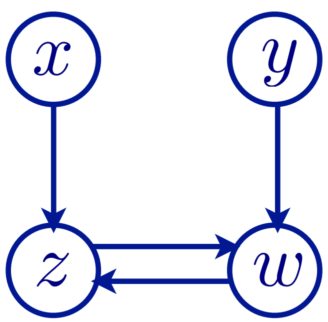

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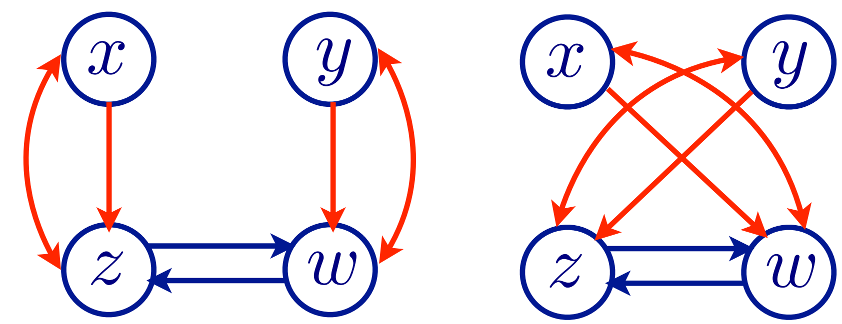

data sample

samples

w	x	y	z

inference algorithm

model specifications

	w	x	y	z
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confounders

Constraint-based Causal Discovery

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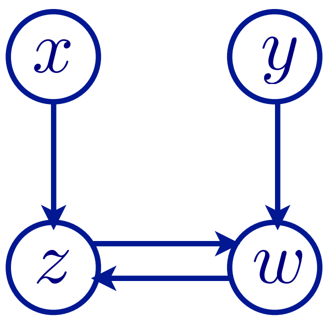

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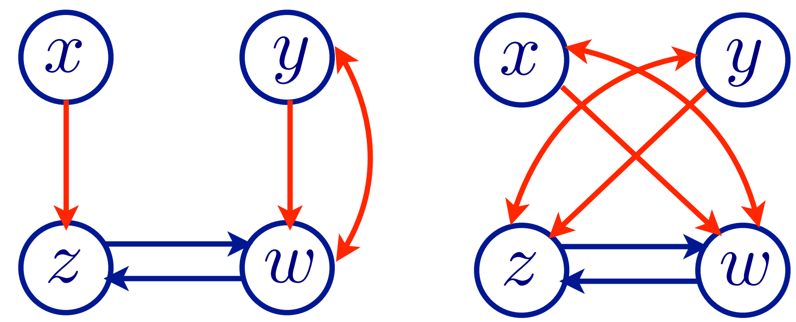

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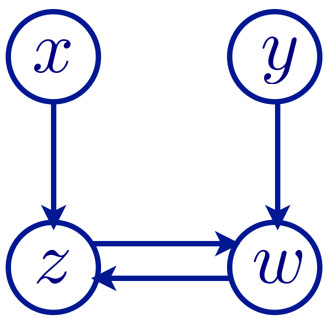

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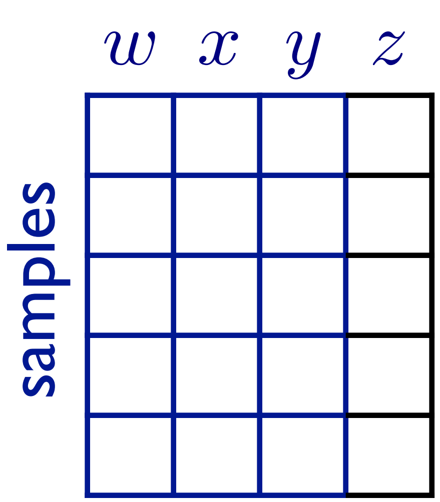

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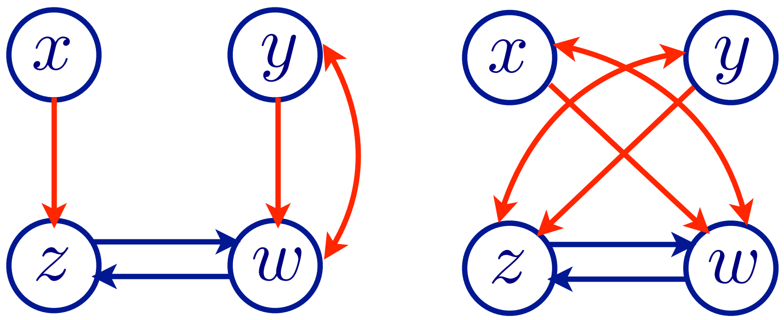

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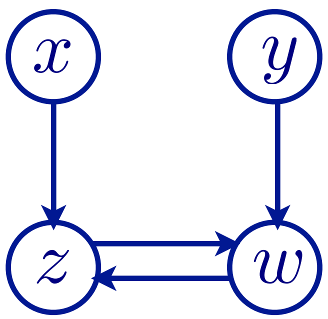

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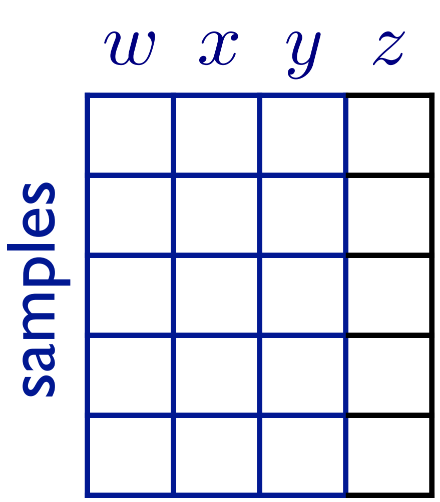
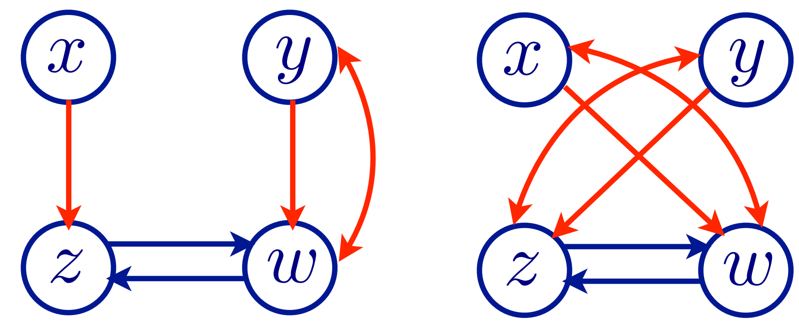


constraints

$$x \perp\!\!\!\perp y \,|\, \{z, w\}$$

probabilistic independence

equivalence classes



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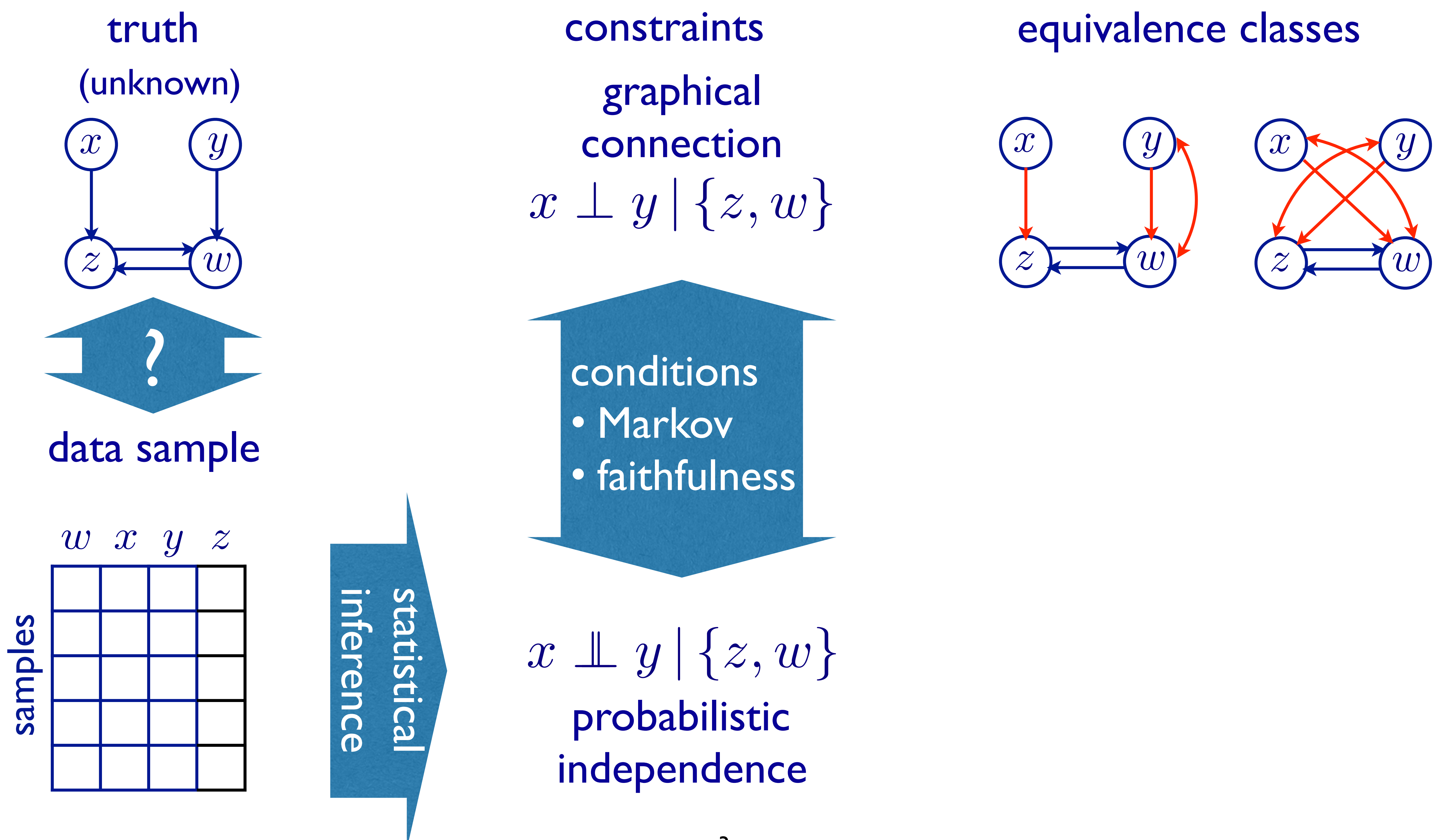

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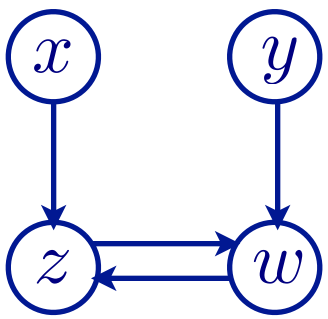

?

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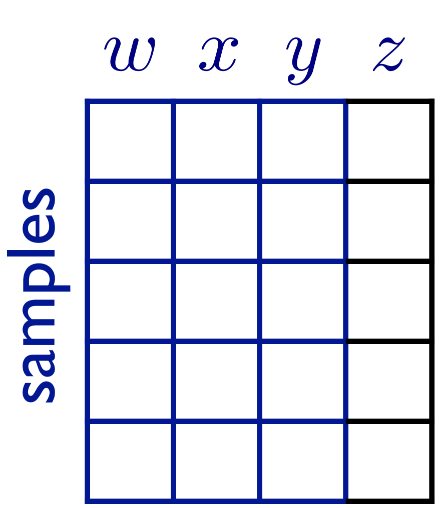


d-separation

statistical inference

constraints

graphical connection

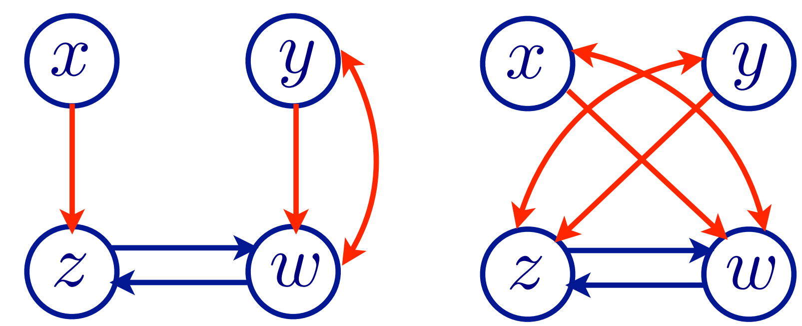
$$x \perp y \,|\, \{z, w\}$$

conditions
- Markov
- faithfulness

$$x \perp\!\!\!\perp y \,|\, \{z, w\}$$

probabilistic independence

equivalence classes



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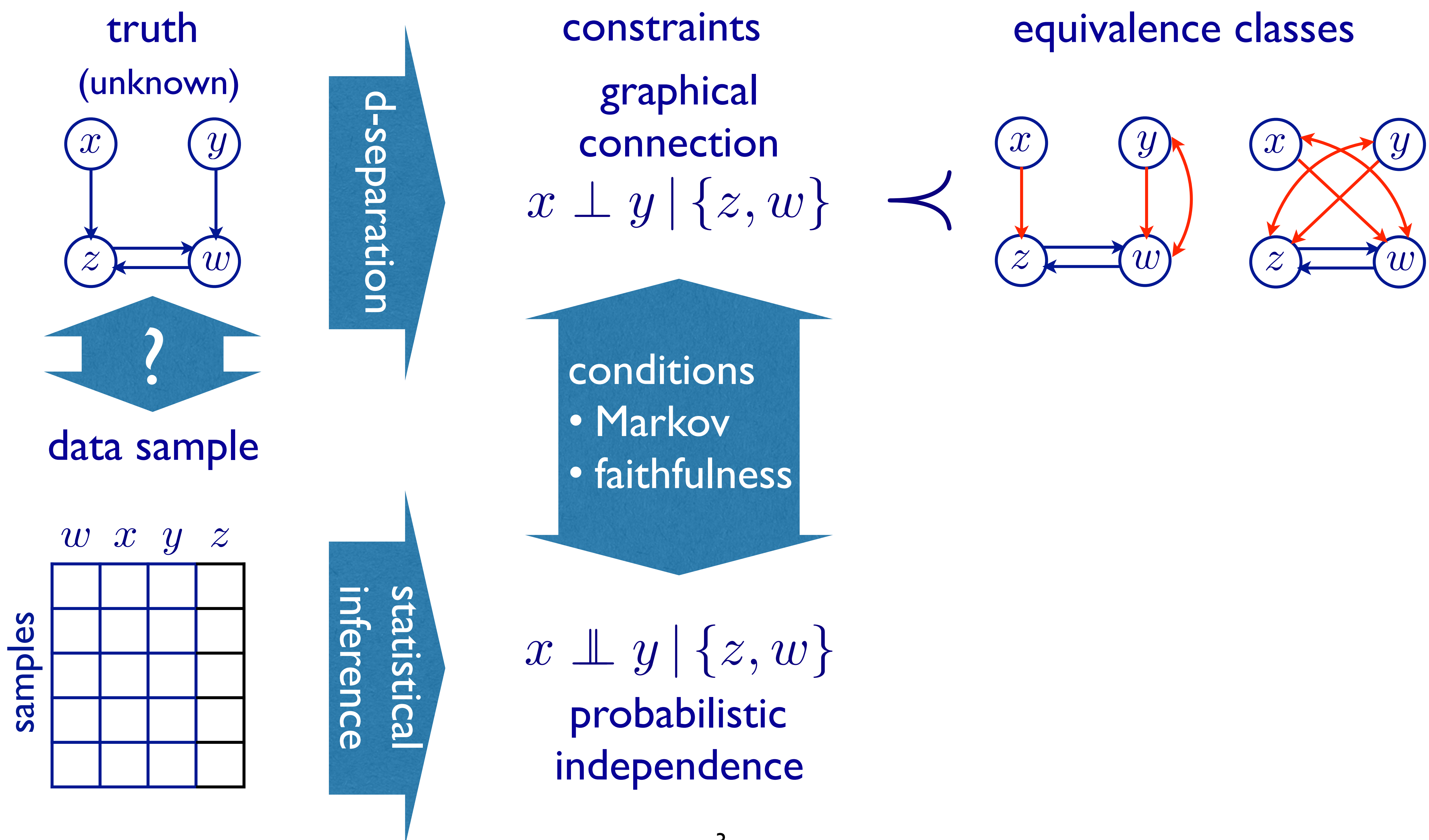

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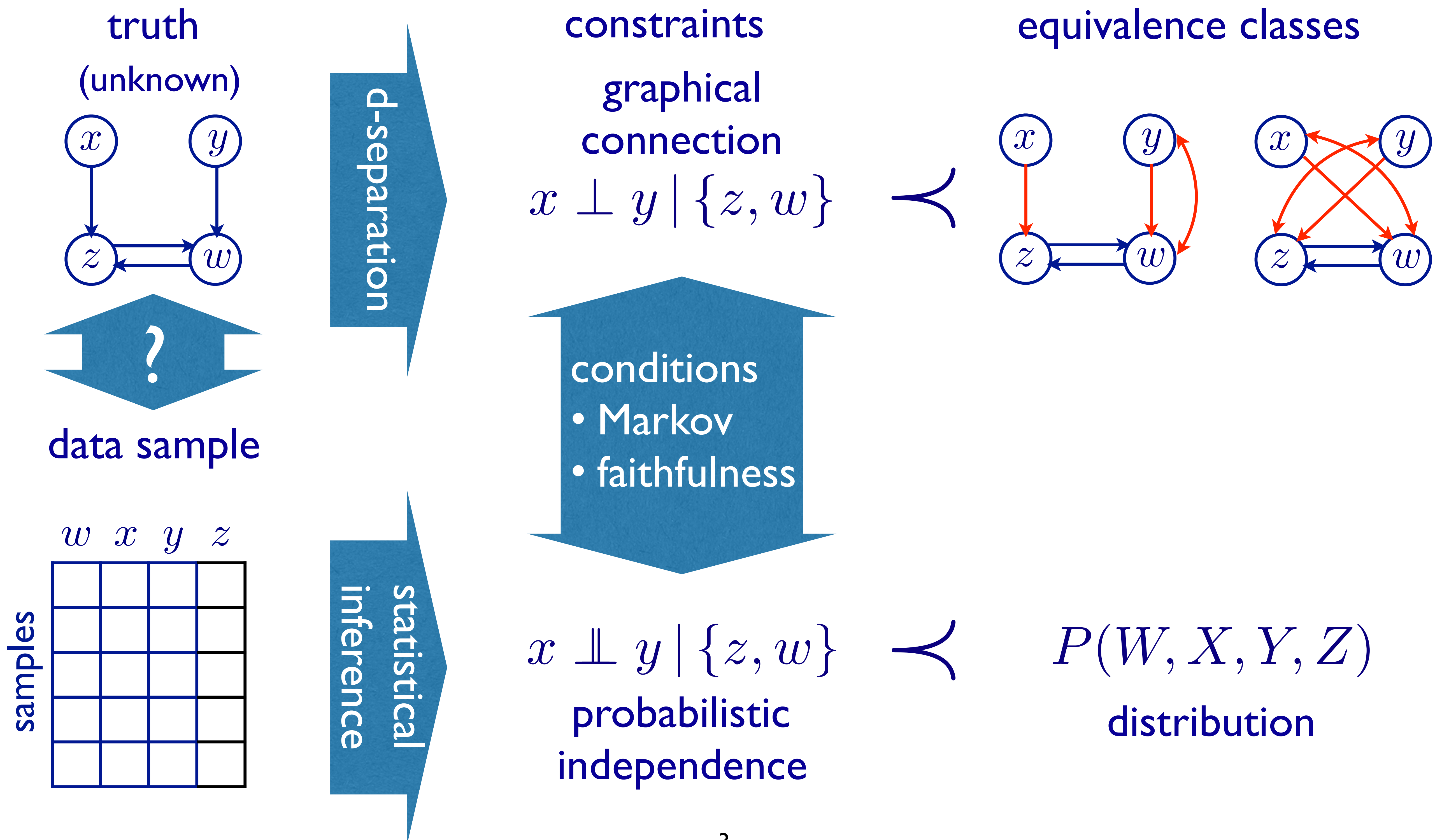
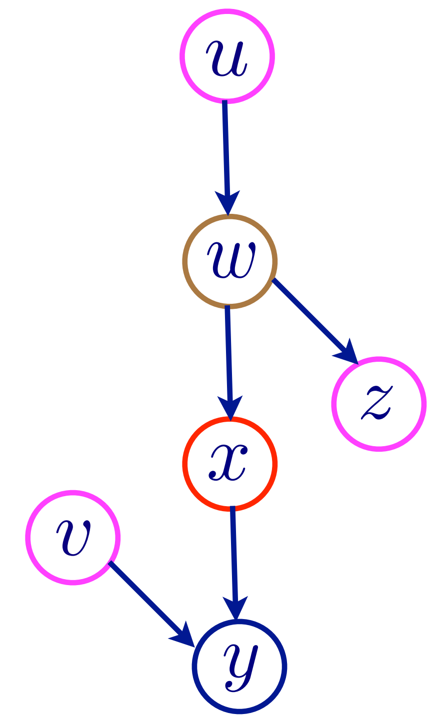


Causal Markov

x is independent of its non-descendents given its parents in the causal graph



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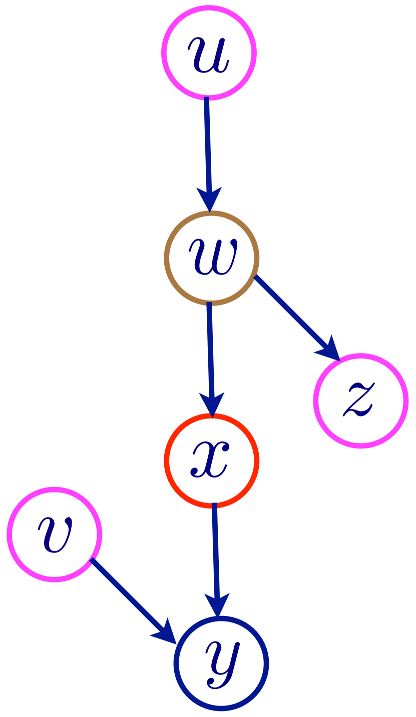

Violations of Causal Markov

- quantum mechanics
- [unmeasured common causes]
- [mixtures of populations]
- [variables are not distinct, or too coarsely grained]

Causal Faithfulness

If x is independent of y given **C** in the probability distribution then x is d-separated from y given **C** in the graph.

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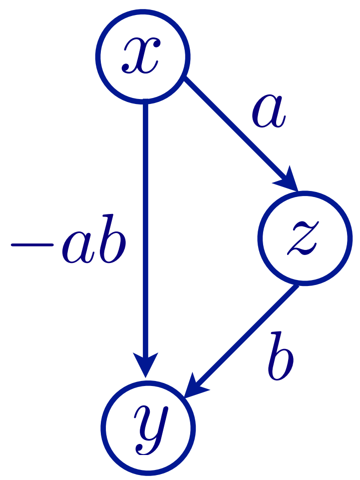
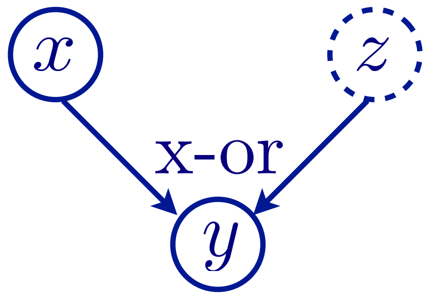


Violations of Causal Faithfulness

- canceling pathways
- matching pennies cases
- [small sample sizes and near violations of faithfulness]



Assumptions

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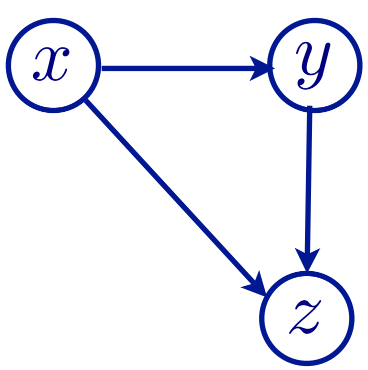

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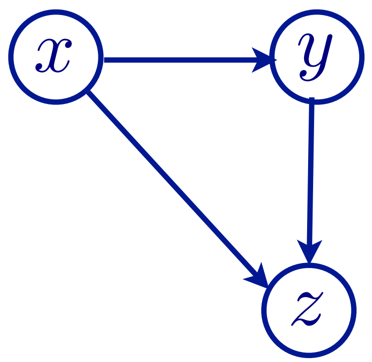

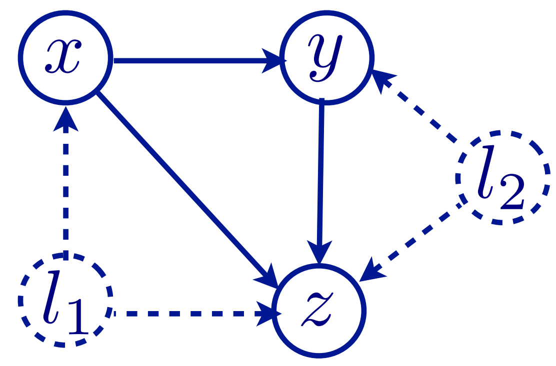

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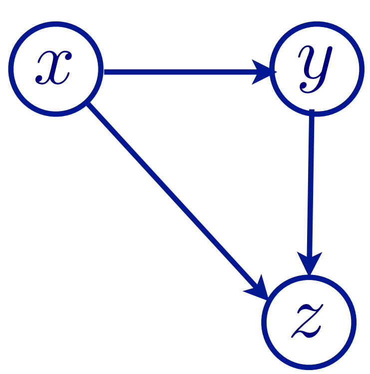

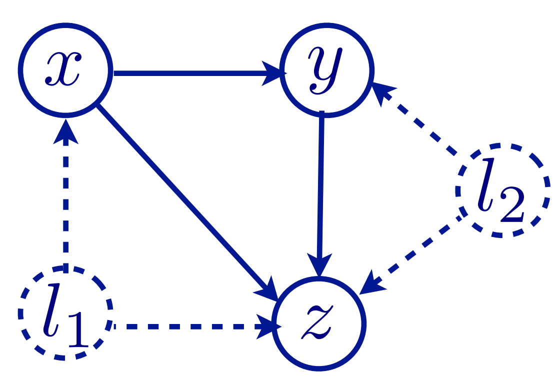

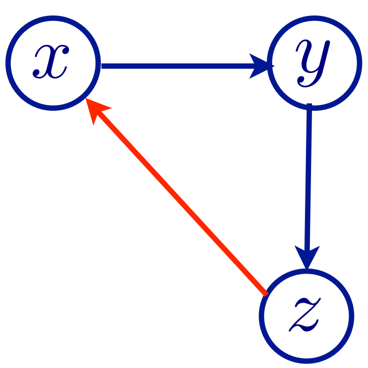

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All graphs in an equivalence class have:

- same adjacencies (“skeleton”)
- same unshielded colliders

[Verma & Pearl 1990, Frydenberg 1990]

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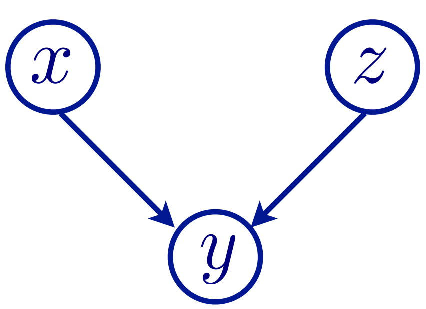

unshielded collider

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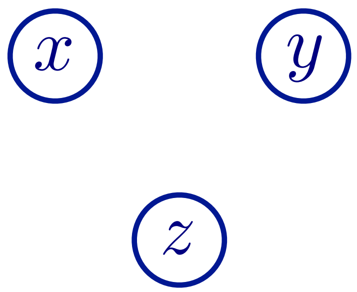

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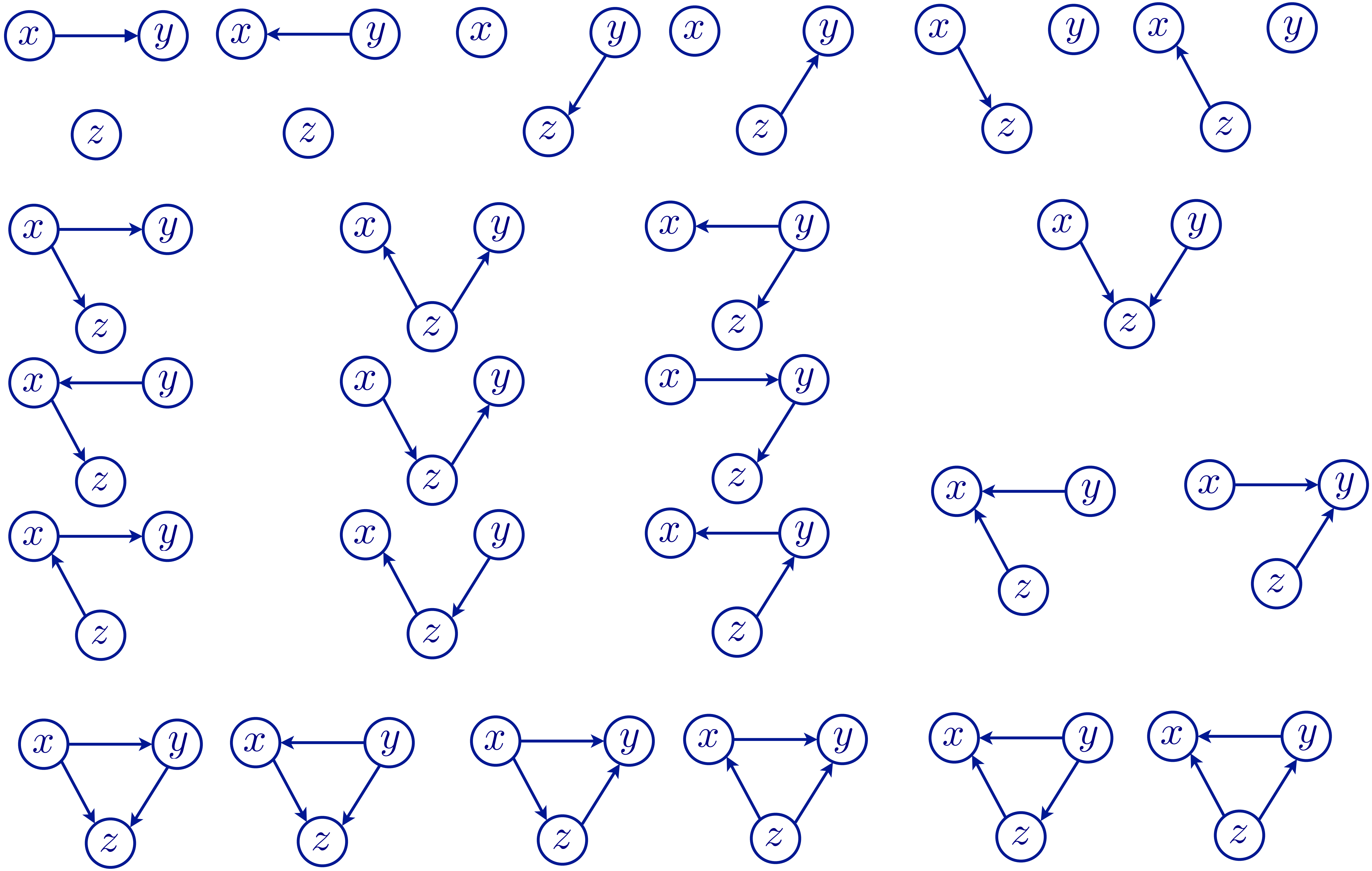

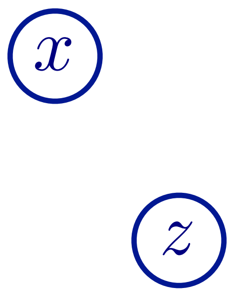

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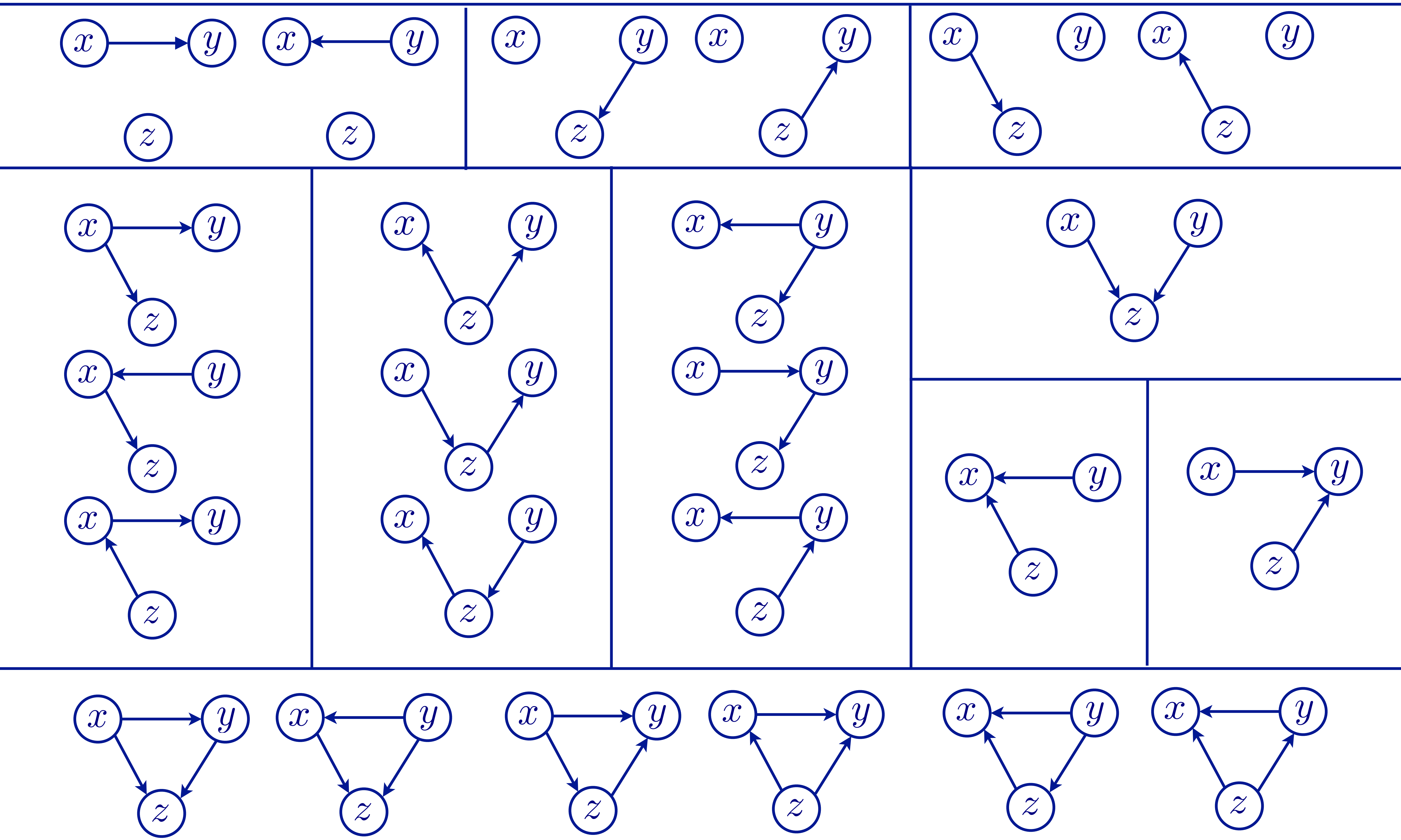

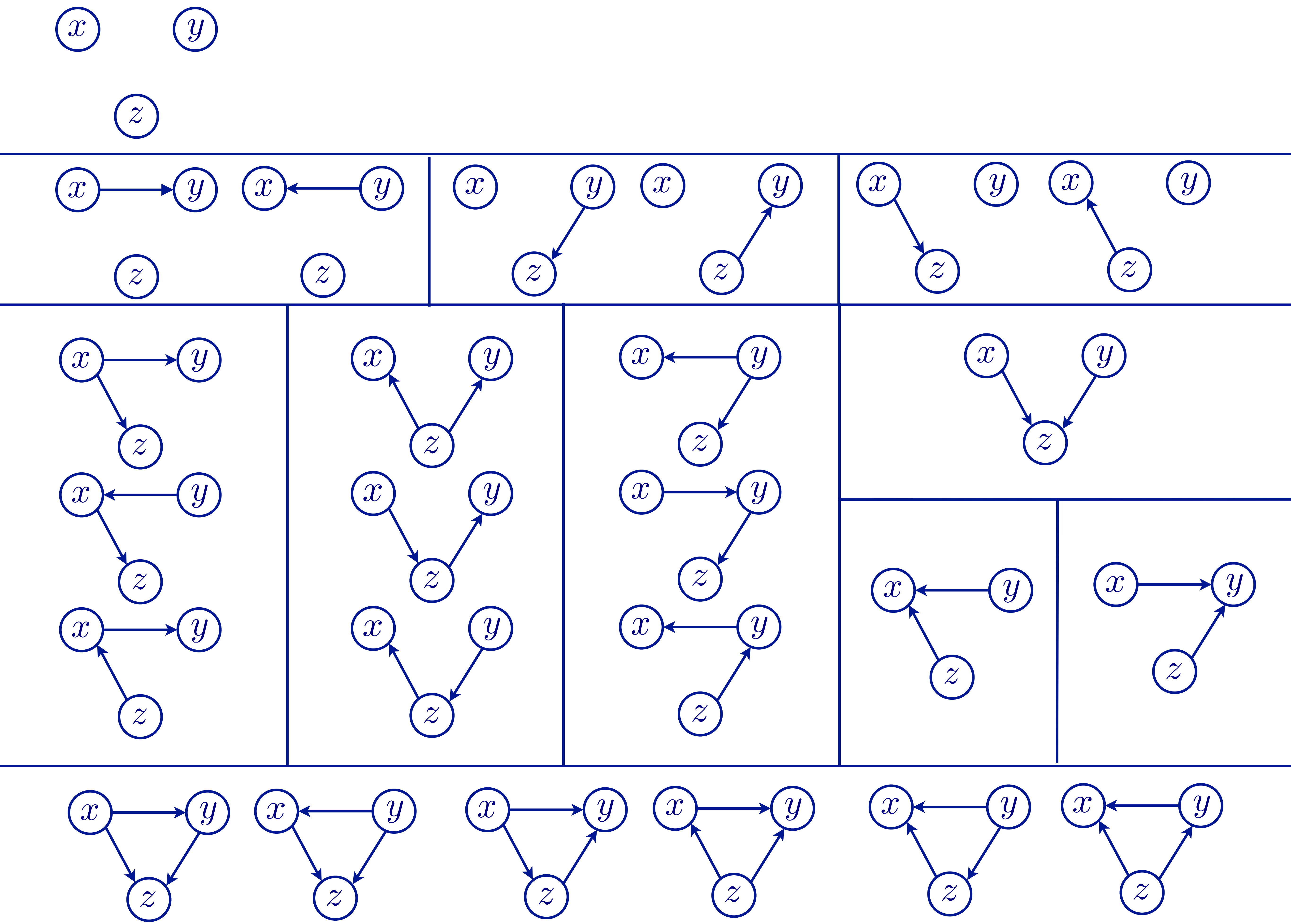

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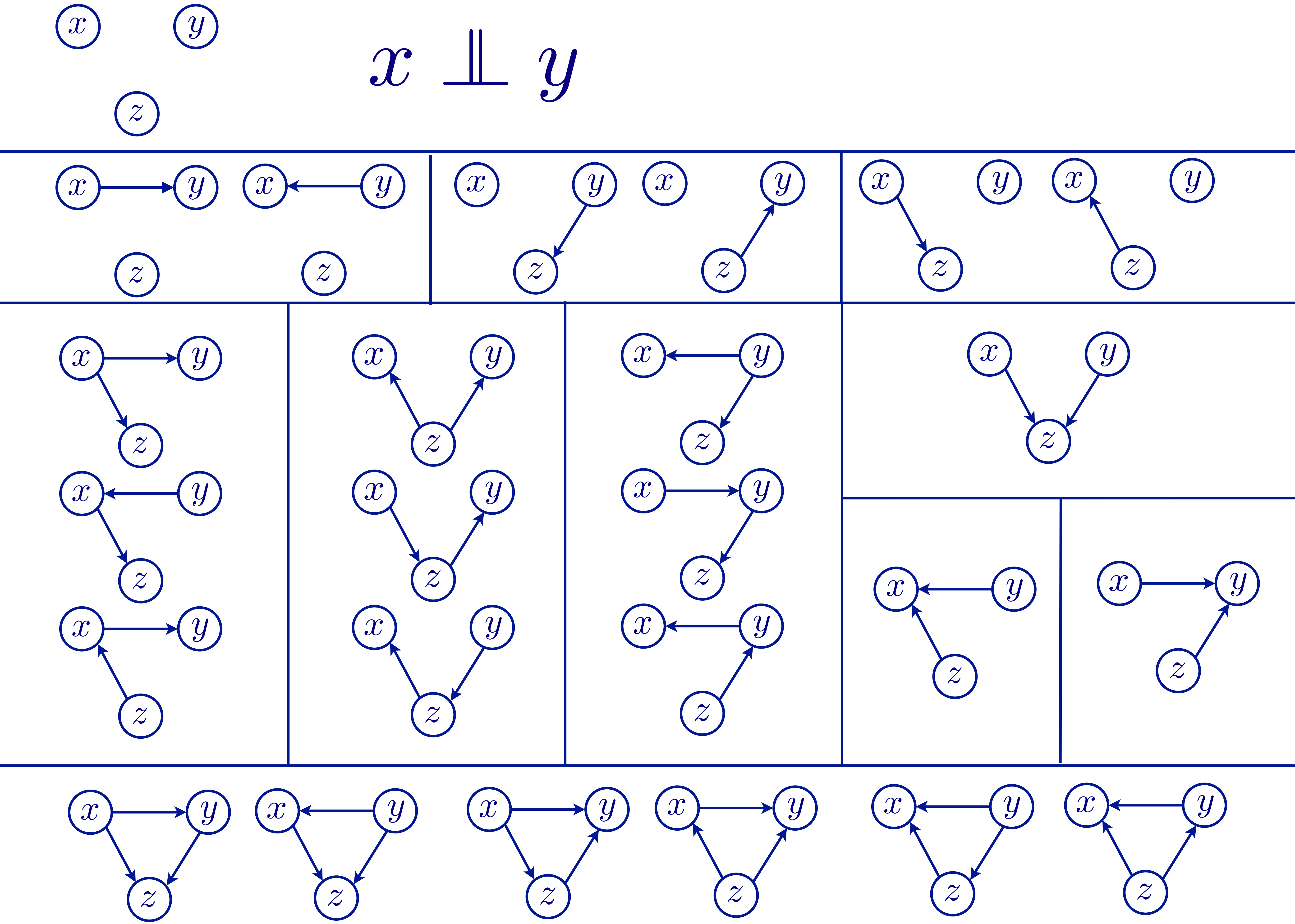

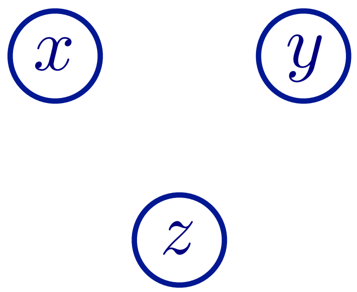

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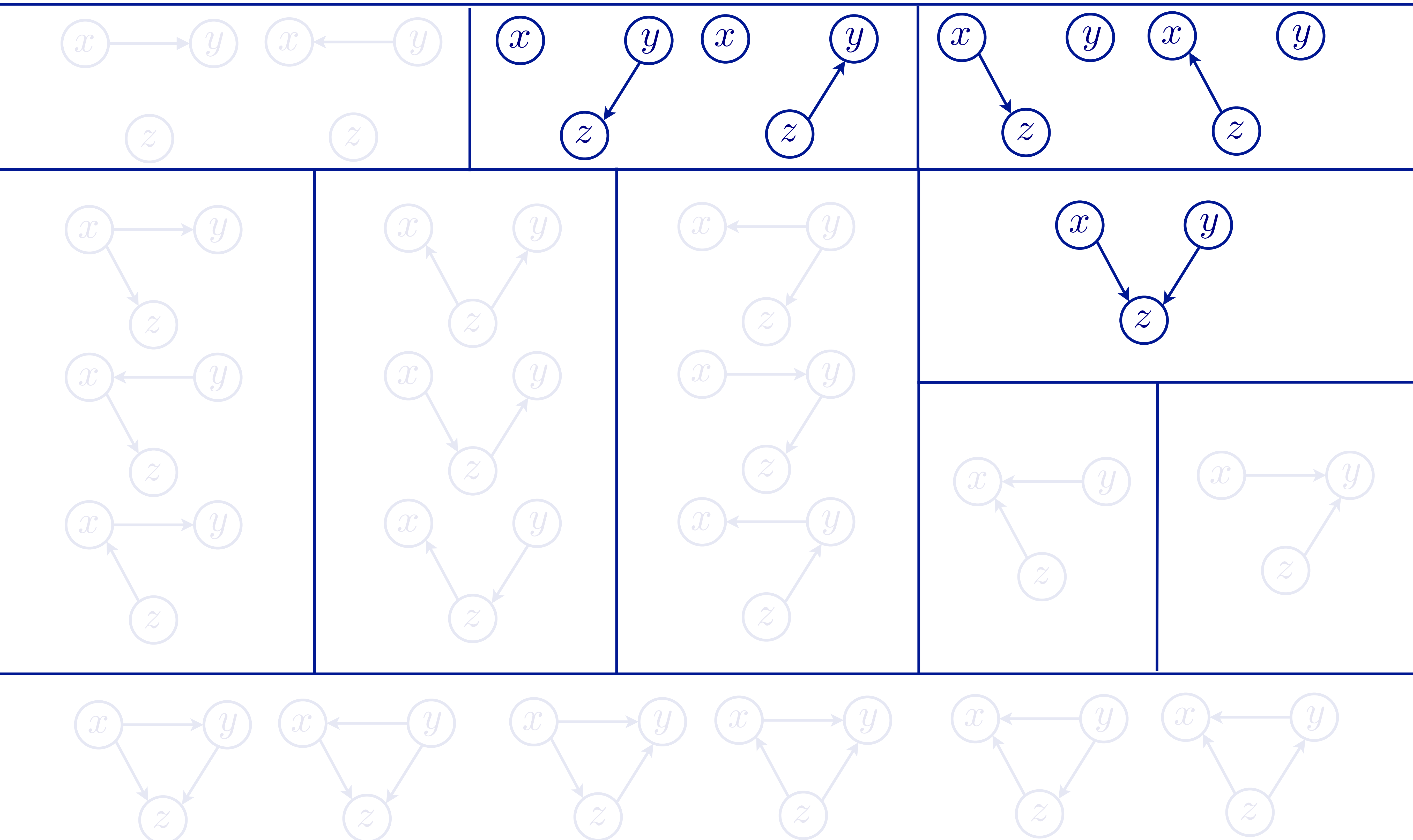

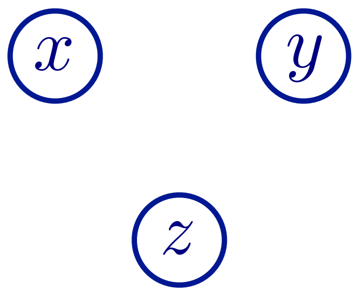

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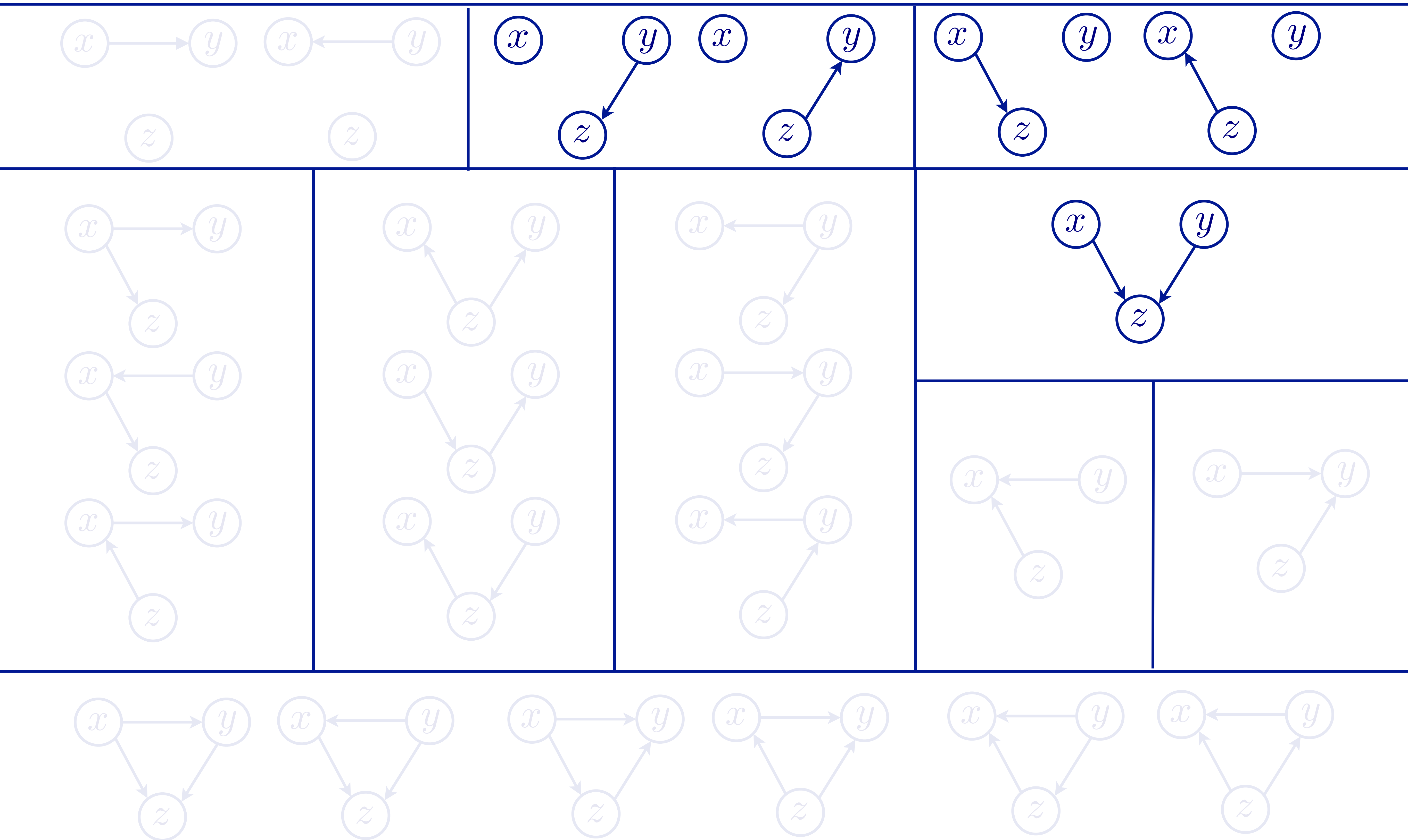

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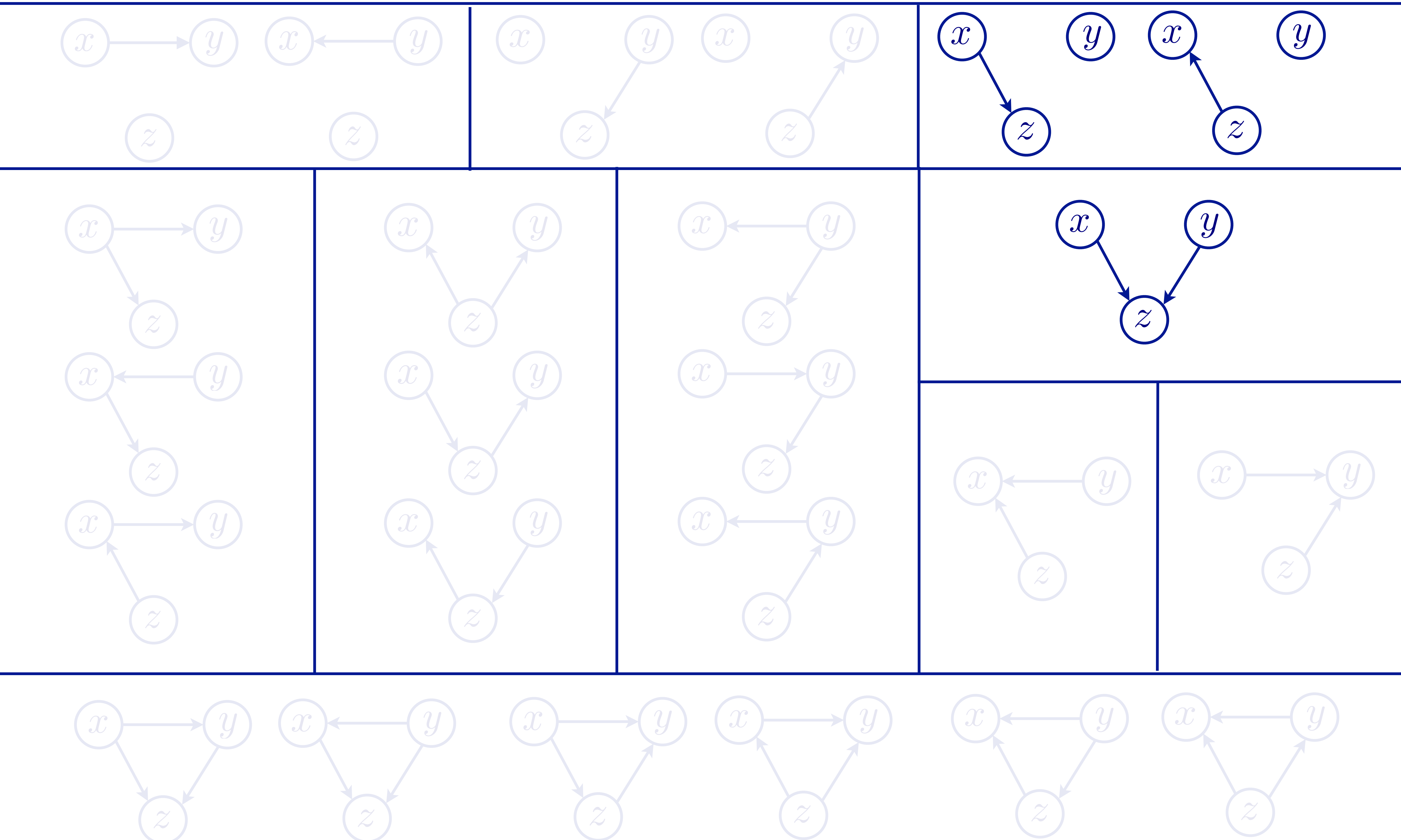

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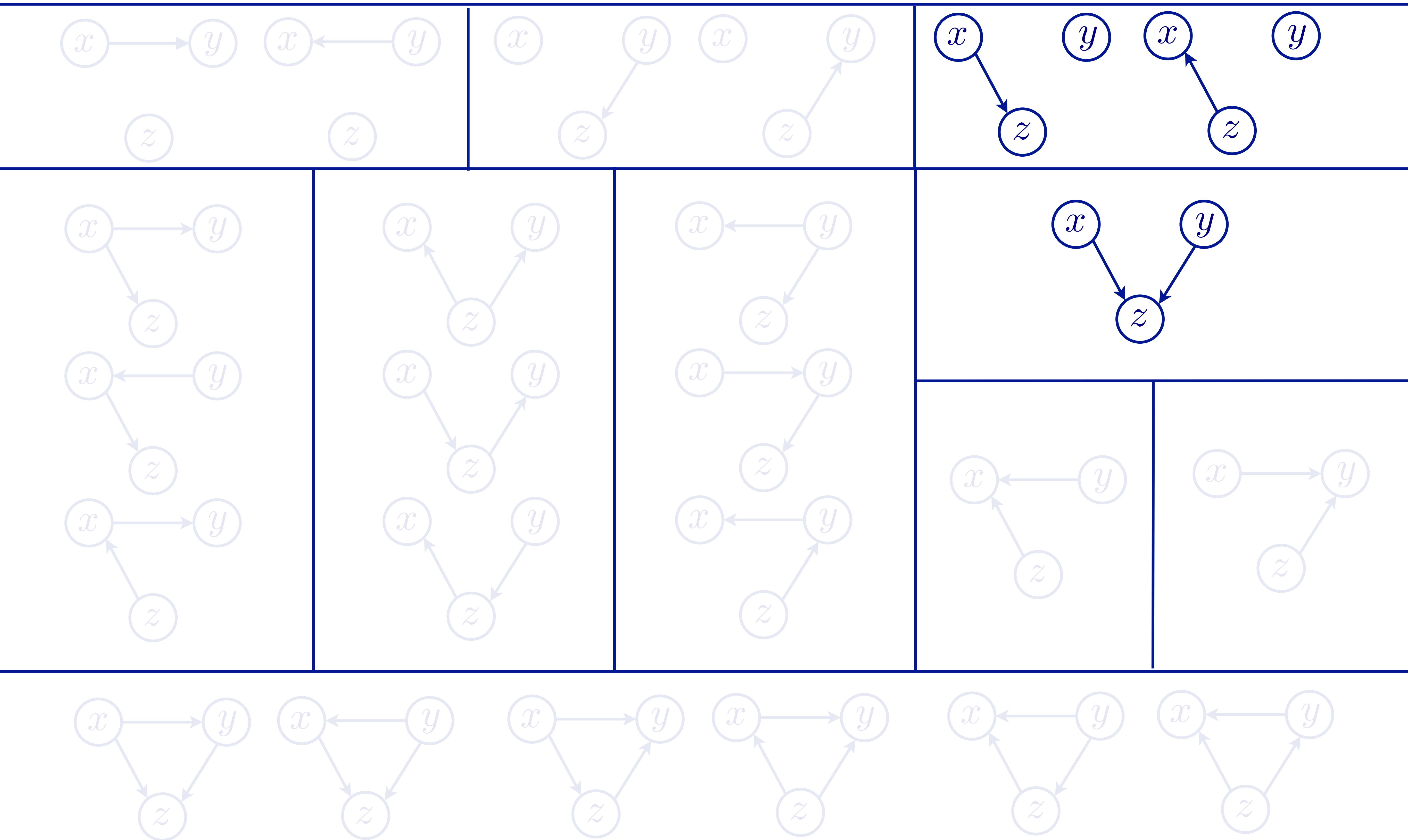

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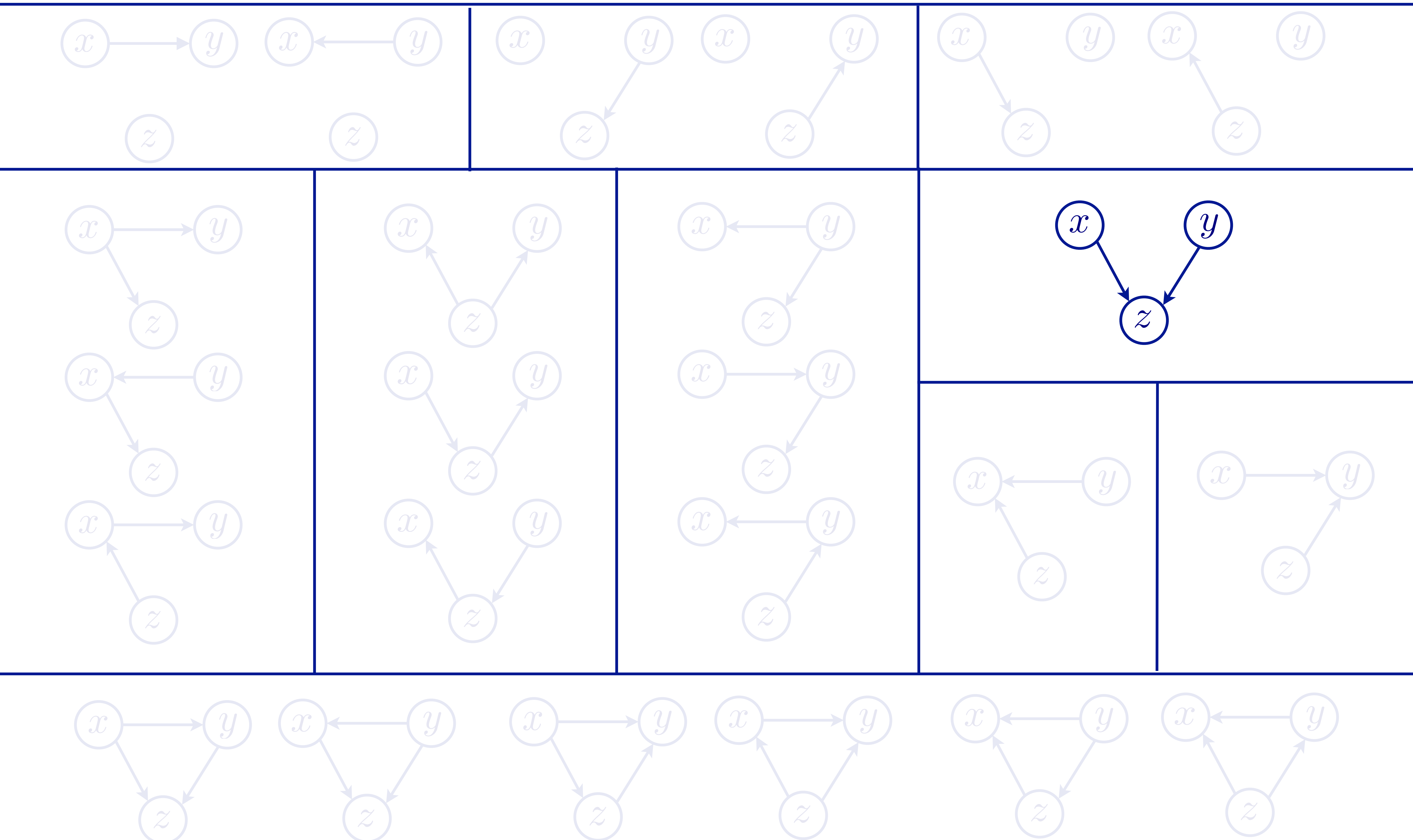

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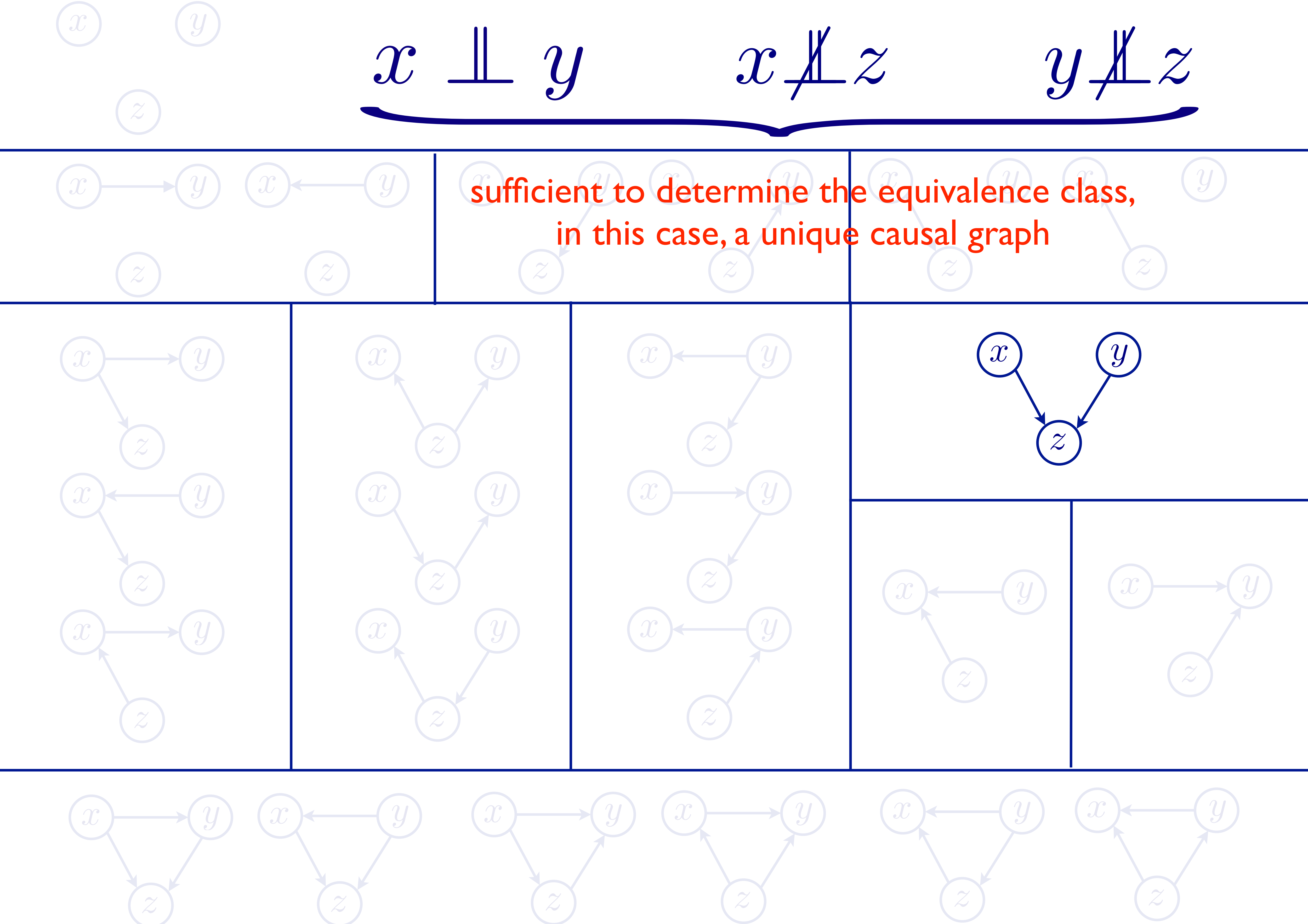
sufficient to determine the equivalence class,
in this case, a unique causal graph



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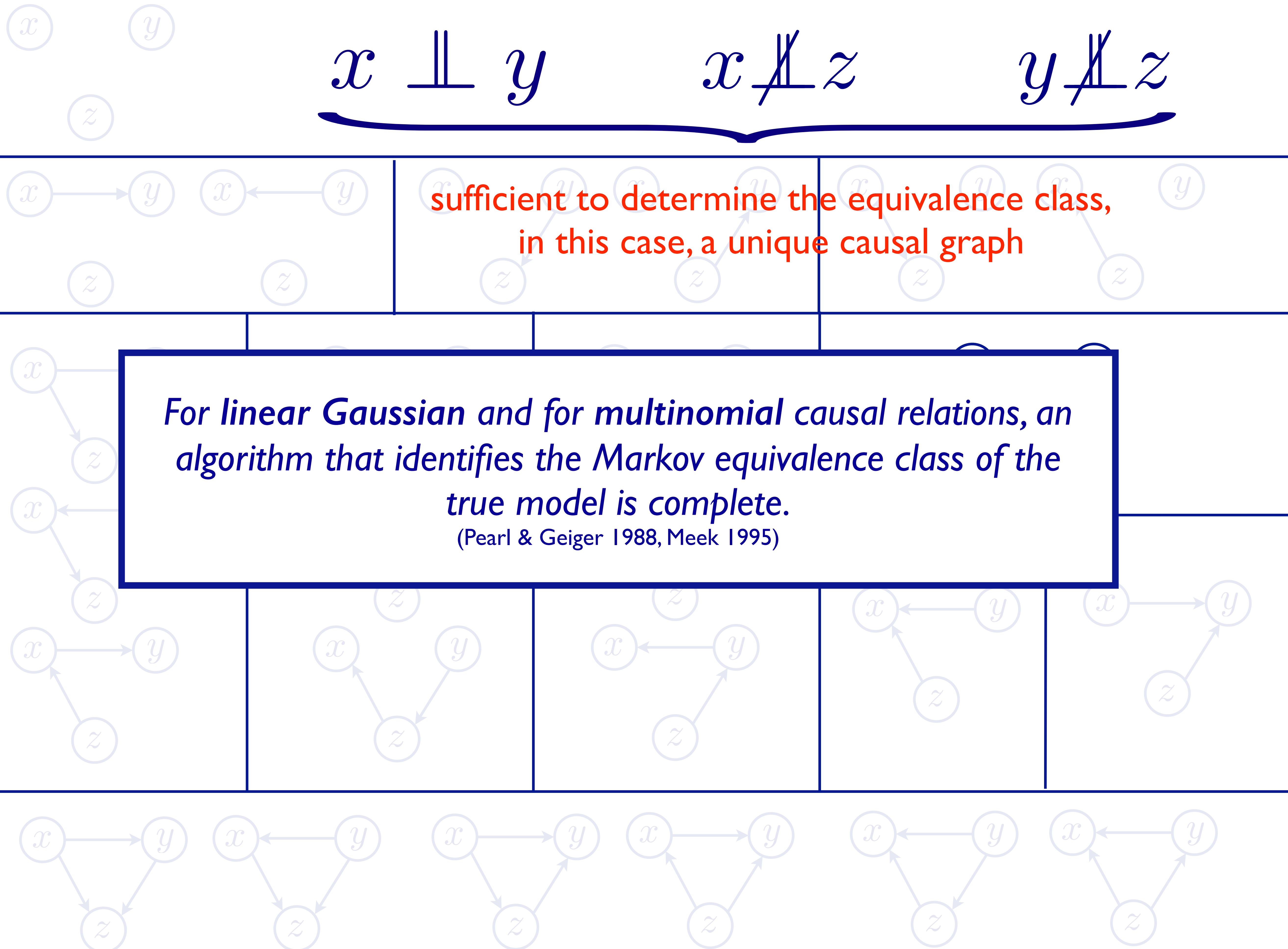

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*For **linear Gaussian** and for **multinomial** causal relations, an algorithm that identifies the Markov equivalence class of the true model is complete.*

(Pearl & Geiger 1988, Meek 1995)

Staying in business

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  - allow for unmeasured common causes
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Zhalama talk

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Tank talk

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Limitations

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(Pearl & Geiger 1988, Meek 1995)

Linear non-Gaussian method (LiNGaM)

- Linear causal relations:

$$x_i = \sum_{x_j \in \mathbf{Pa}(x_i)} \beta_{ij} x_j + \epsilon_j$$

- Assumptions:
  - causal Markov
  - causal sufficiency
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[Shimizu et al., 2006]

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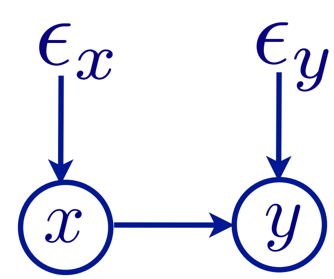
▸ If $\epsilon_j \sim$ non-Gaussian, then the true graph is **uniquely identifiable** from the joint distribution.

[Shimizu et al., 2006]

Two variable case

True model

$$y = \beta x + \epsilon_y$$



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$$\begin{tikzcd} \epsilon_x \arrow[d] & \epsilon_y \arrow[d] \\ x \arrow[r] & y \end{tikzcd}$$

$$x \perp\!\!\!\perp \epsilon_y$$

Two variable case

True model

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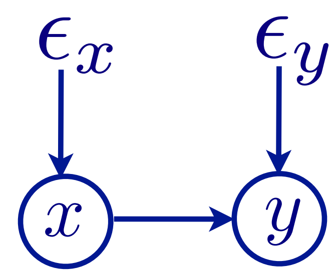

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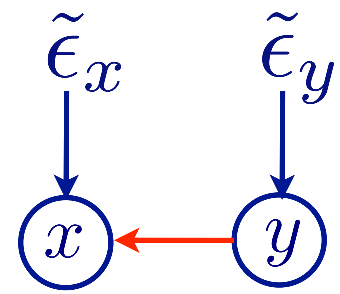

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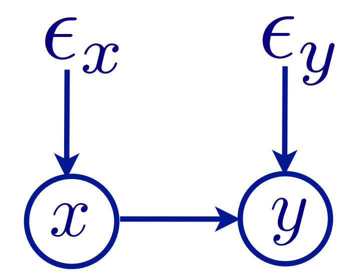

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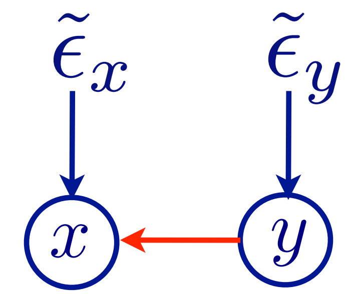

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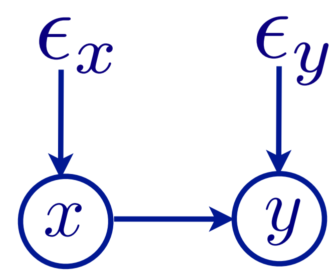

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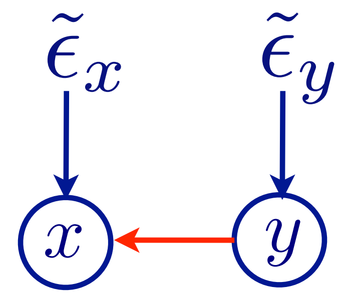

$$y \perp\!\!\!\perp \tilde{\epsilon}_x$$

$$\begin{aligned}
\tilde{\epsilon}_x &= x - \theta y \\
&= x - \theta(\beta x + \epsilon_y) \\
&= (1 - \theta\beta)x - \theta\epsilon_y
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Why Normals are unusual

Forwards model $y = \beta x + \epsilon_y$

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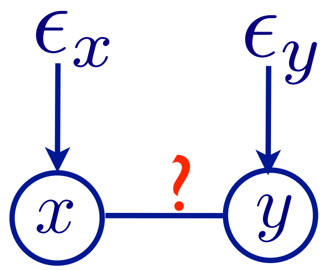

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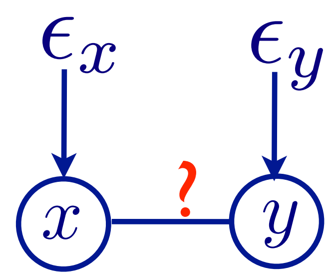

Theorem 1 (Darmois-Skitovich) *Let $X_1, \ldots, X_n$ be independent, non-degenerate random variables. If for two linear combinations*

$$
\begin{aligned}
l_1 &= a_1 X_1 + \ldots + a_n X_n, \quad a_i \neq 0 \\
l_2 &= b_1 X_1 + \ldots + b_n X_n, \quad b_i \neq 0
\end{aligned}
$$

are independent, then each X_i is normally distributed.

algorithm/ assumption
Markov faithfulness causal sufficiency acyclicity parametric assumption
output

algorithm/ assumption	PC / GES	FCI	CCD
Markov	✓	✓	✓
faithfulness	✓	✓	✓
causal sufficiency	✓	✗	✓
acyclicity	✓	✓	✗
parametric assumption	✗	✗	✗
output	Markov equivalence	PAG	PAG

algorithm/ assumption	PC / GES	FCI	CCD	LiNGaM	lvLiNGaM	cyclic LiNGaM
Markov	✓	✓	✓	✓	✓	✓
faithfulness	✓	✓	✓	✗	✓	~
causal sufficiency	✓	✗	✓	✓	✗	✓
acyclicity	✓	✓	✗	✓	✓	✗
parametric assumption	✗	✗	✗	linear non-Gaussian	linear non-Gaussian	linear non-Gaussian
output	Markov equivalence	PAG	PAG	unique DAG	set of DAGs	set of graphs

Limitations

*For **linear Gaussian** and for **multinomial** causal relations, an algorithm that identifies the Markov equivalence class of the true model is complete.*

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Bivariate Linear Gaussian case

True model

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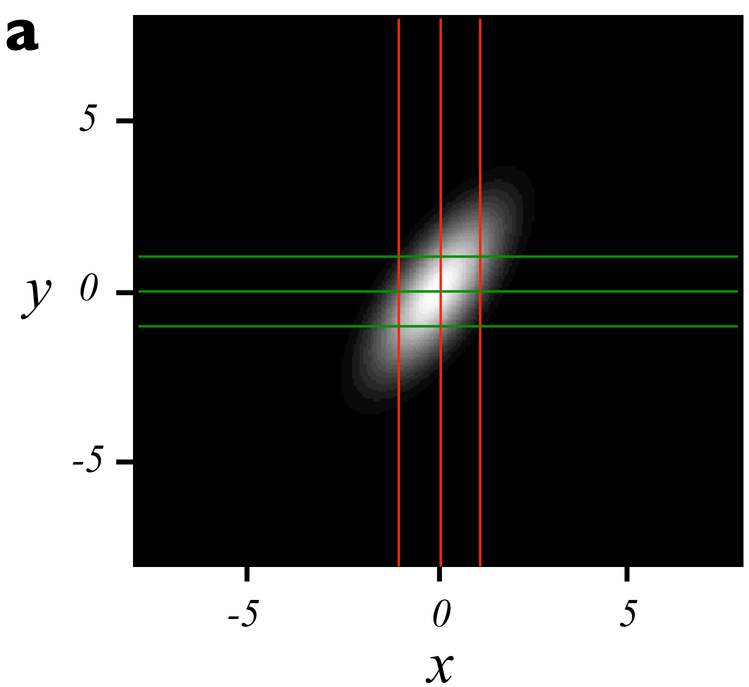
$$\epsilon_x, \epsilon_y \sim \text{indep. Gaussian}$$



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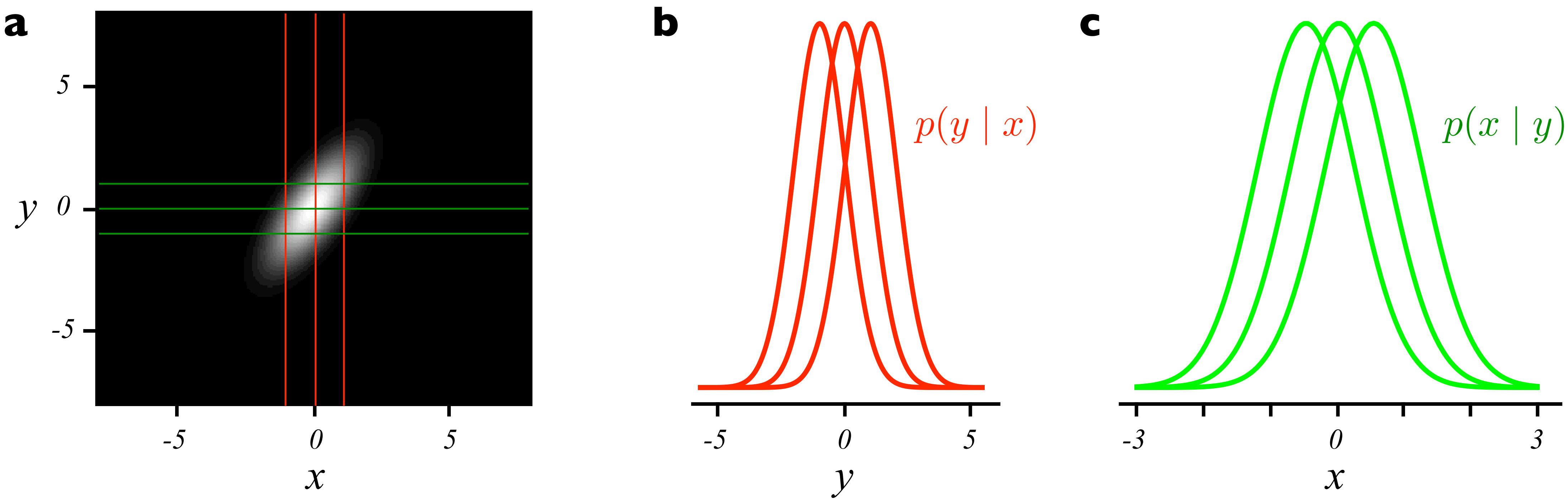

Forwards (true) model

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Continuous additive noise models

$$x_j = f_j(pa(x_j)) + \epsilon_j$$

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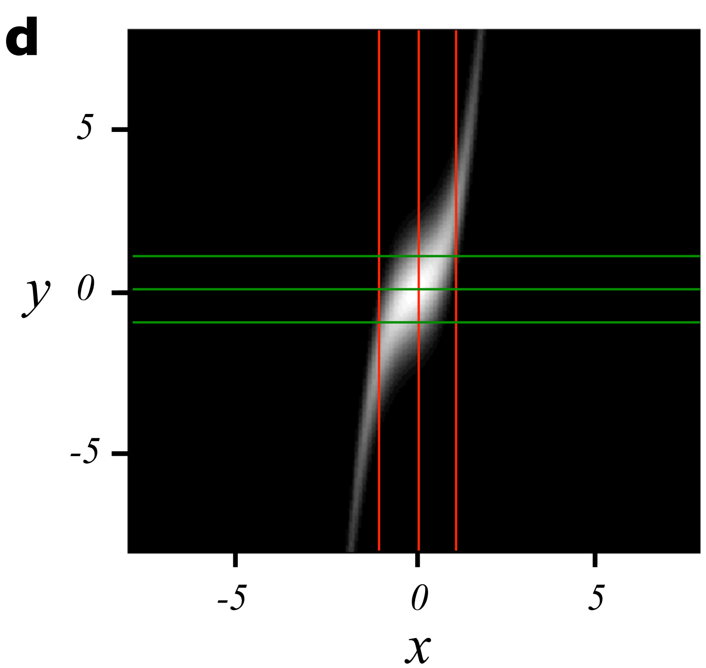
➡ More generally, under what circumstances is the causal structure represented by this class of models identifiable?

Bivariate non-linear Gaussian additive noise model

True model

$$x = \epsilon_x \qquad \epsilon_x, \epsilon_y \sim \text{indep. Gaussian}$$
$$y = x + x^3 + \epsilon_y$$



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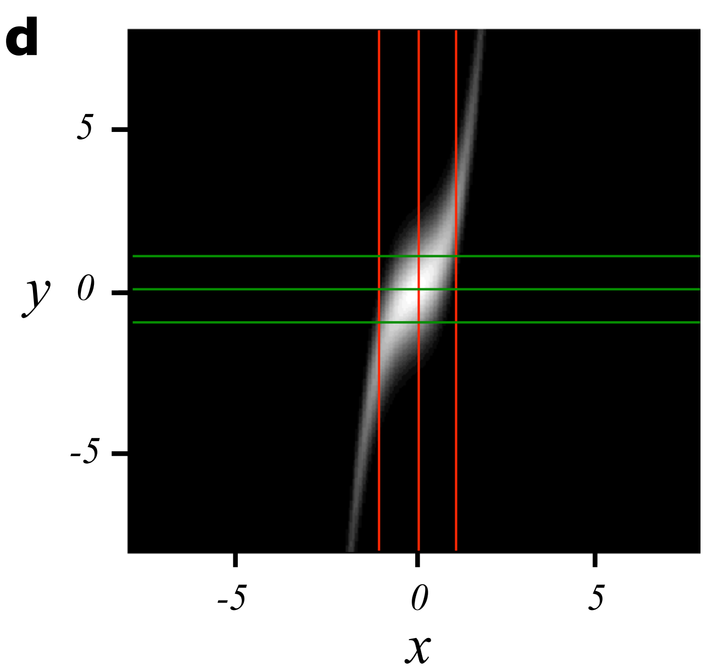

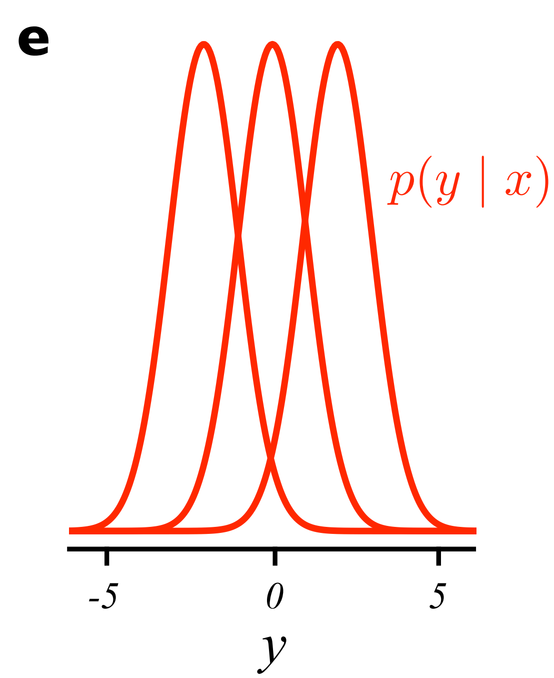

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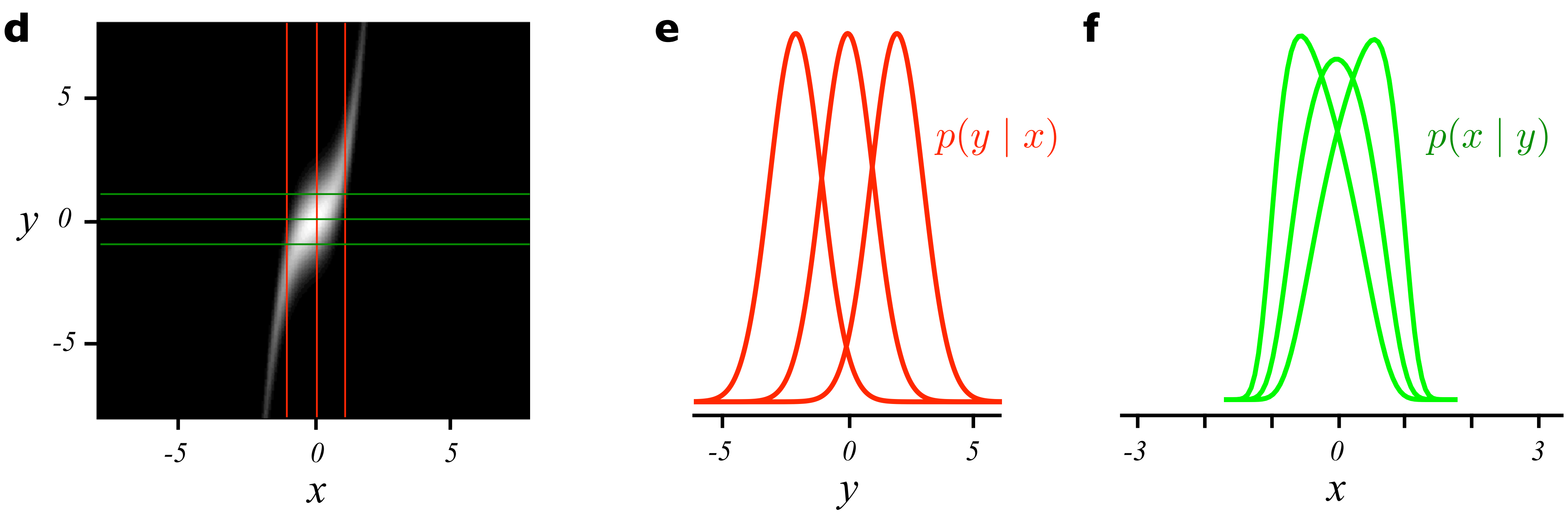

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(graphics from Hoyer et al. 2009)

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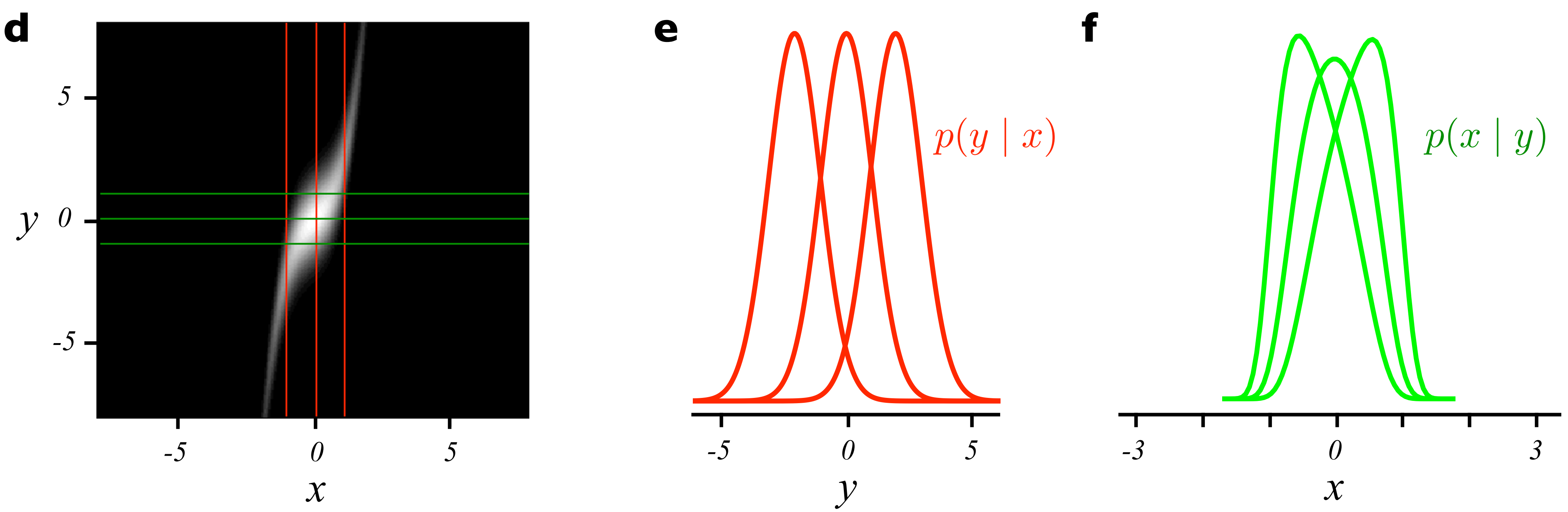

Forwards (true) model

Backwards model

$$x = g(y) + \tilde{\epsilon}_x$$
$$y \not\perp\!\!\!\perp \tilde{\epsilon}_x$$

(graphics from Hoyer et al. 2009)

General non-linear additive noise models

Hoyer Condition (HC): *Technical condition on the relation between the function, the noise distribution and the parent distribution that, if satisfied, permits a backward model.*

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  - this generalizes to multiple variables (assuming minimality*)!
  - extension to discrete additive noise models
- If the function is **linear**, but the error terms **non-Gaussian**, then one can't fit a linear backwards model (Lingam), but there are cases where **one can fit a non-linear backwards model**

algorithm/ assumptions	PC / GES	FCI	CCD	LiNGaM	lvLiNGaM	cyclic LiNGaM
Markov	✓	✓	✓	✓	✓	✓
faithfulness	✓	✓	✓	✗	✓	~
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Experiments, Background Knowledge and all the other Jazz

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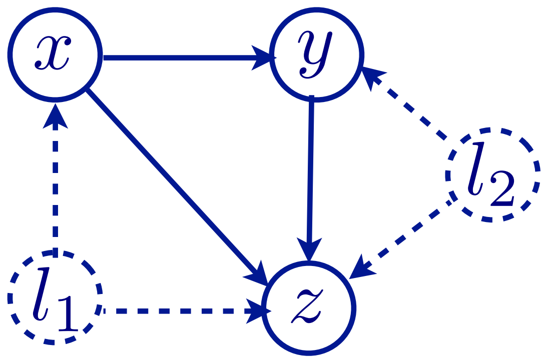

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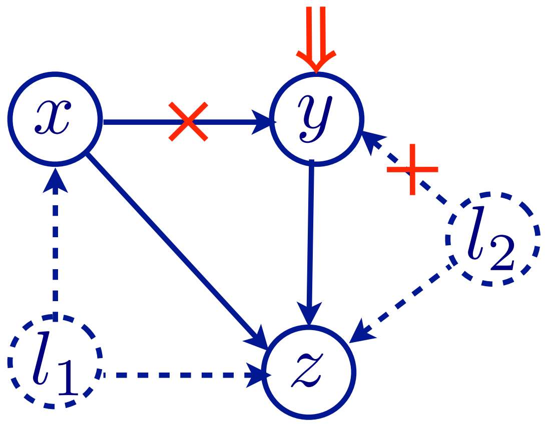

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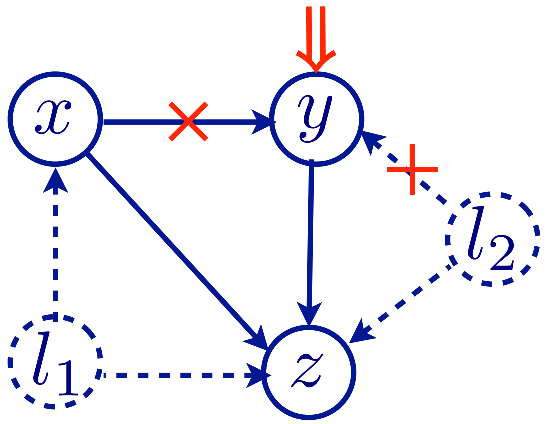

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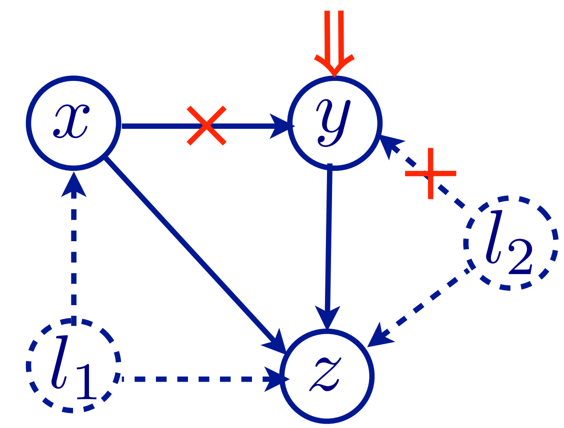

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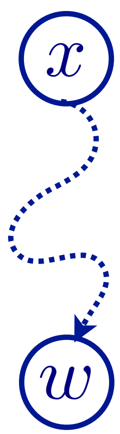
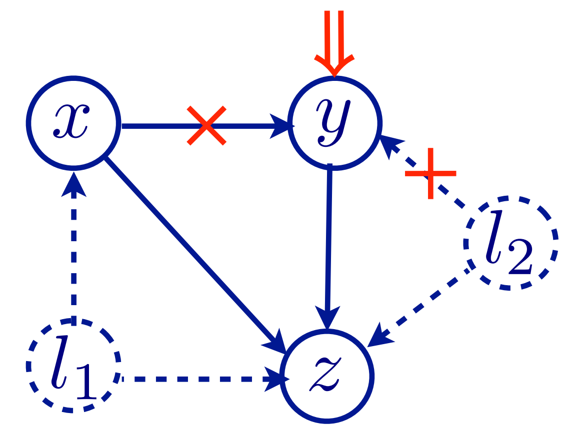


pathways

Experiments, Background Knowledge and all the other Jazz



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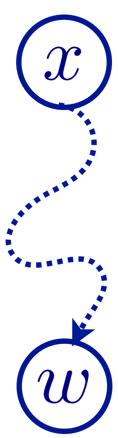

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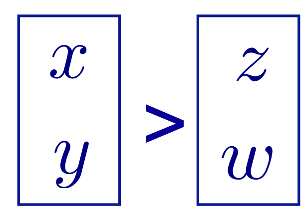

tier orderings

Experiments, Background Knowledge and all the other Jazz

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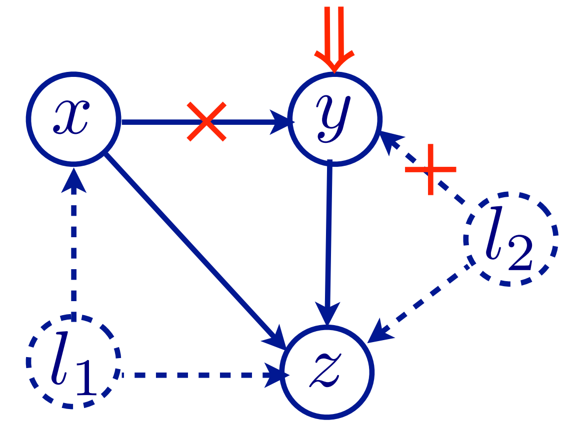

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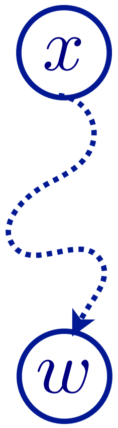

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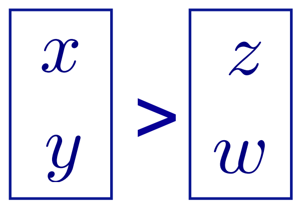

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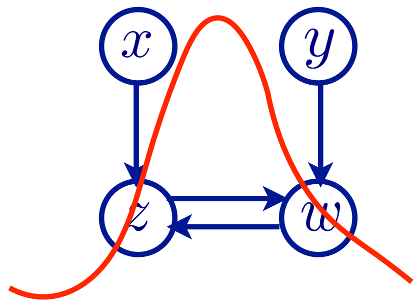

"priors"

Experiments, Background Knowledge and all the other Jazz

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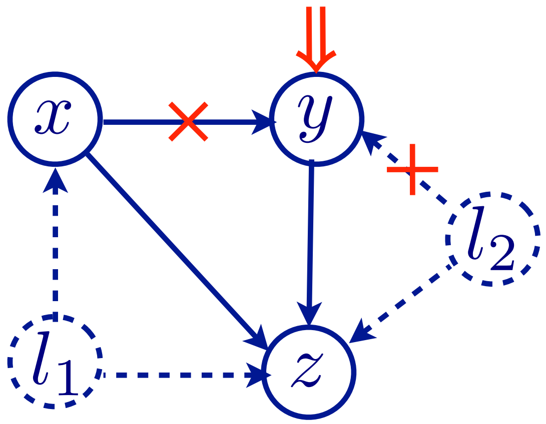

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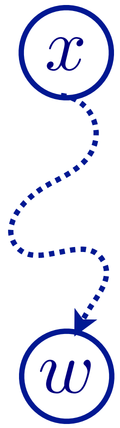

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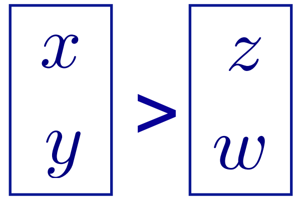

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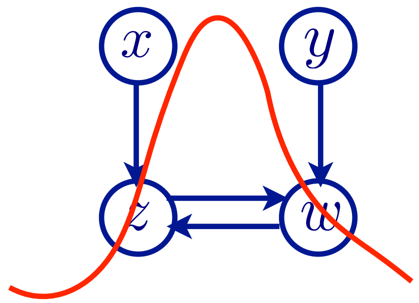

"priors"

- specific search space restrictions

Experiments, Background Knowledge and all the other Jazz

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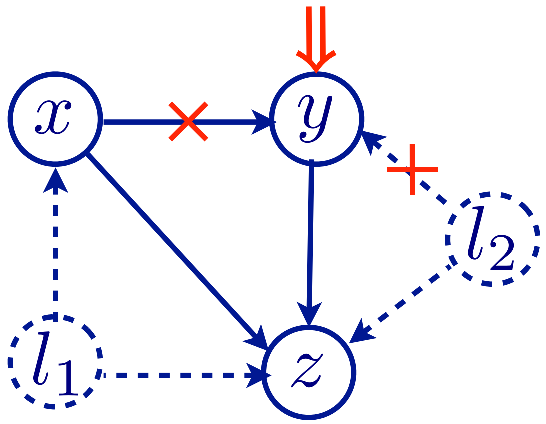

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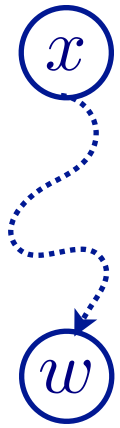

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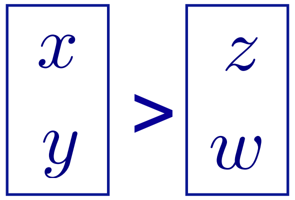

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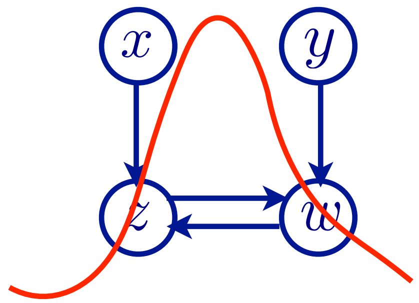

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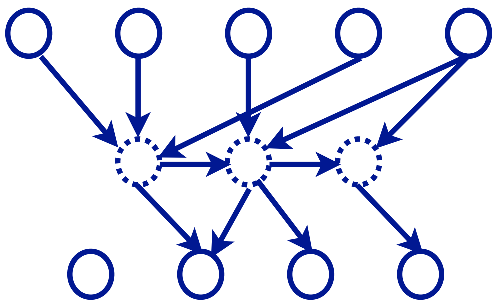
biological settings

Experiments, Background Knowledge and all the other Jazz

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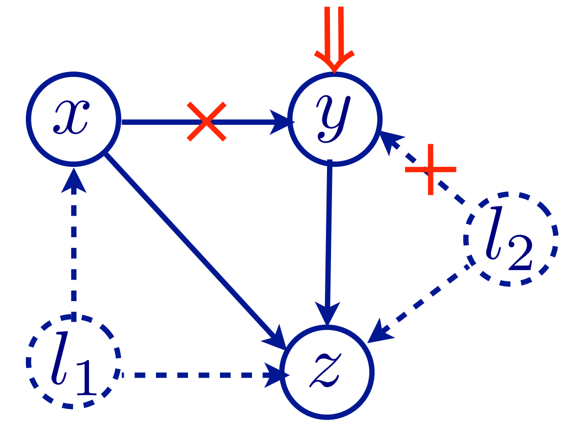

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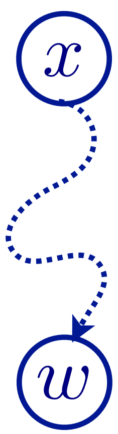

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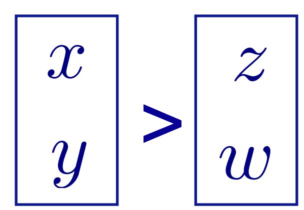

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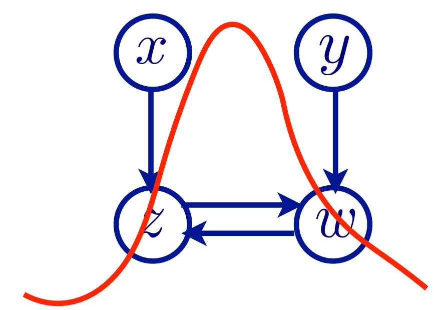

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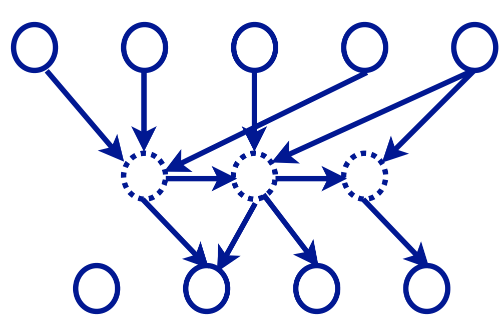

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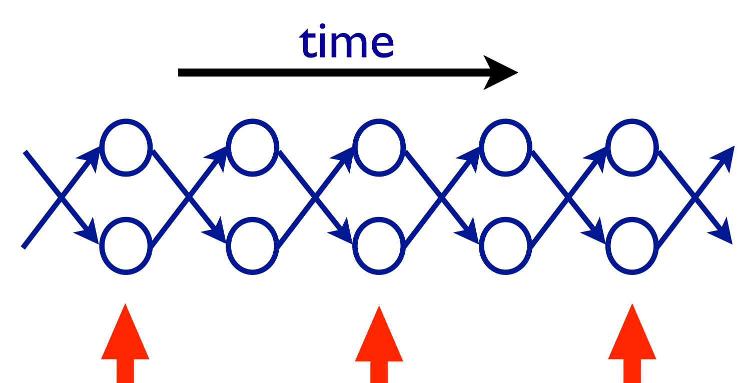

subsampled time series

Experiments, Background Knowledge and all the other Jazz

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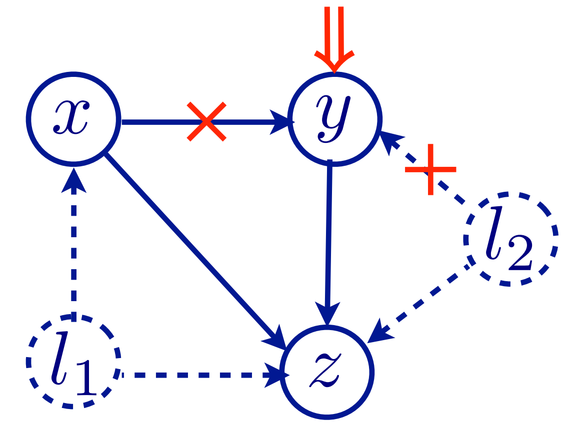

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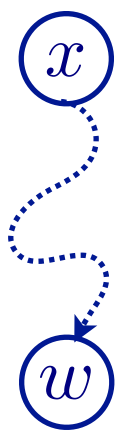
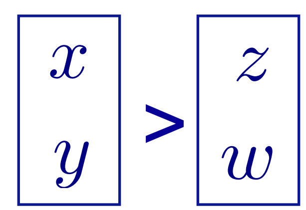
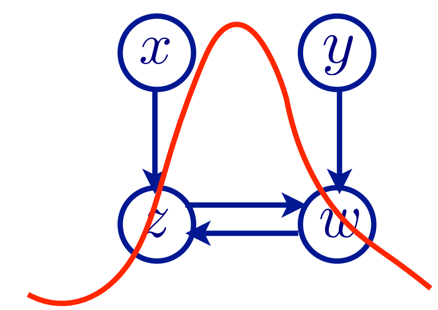


pathways

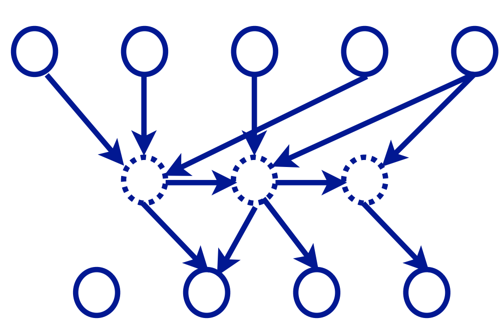


tier orderings



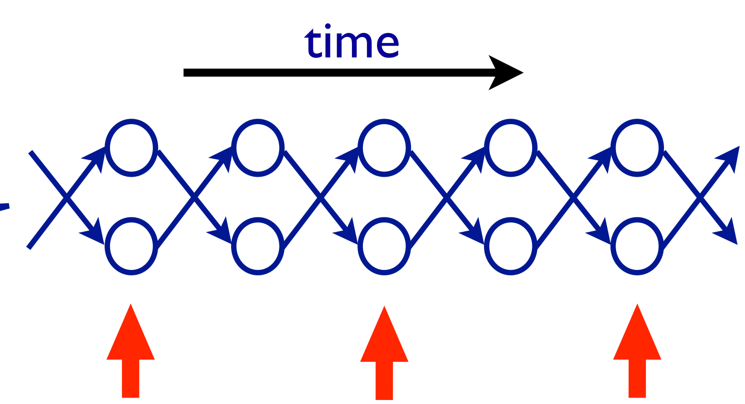
"priors"

- specific search space restrictions



biological settings

Tank talk

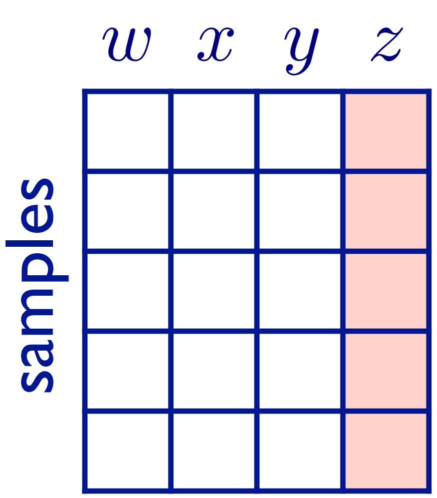


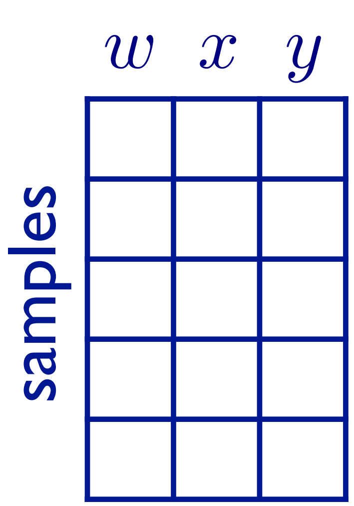
subsampled time series

High-Level

High-Level

data
sample





High-Level

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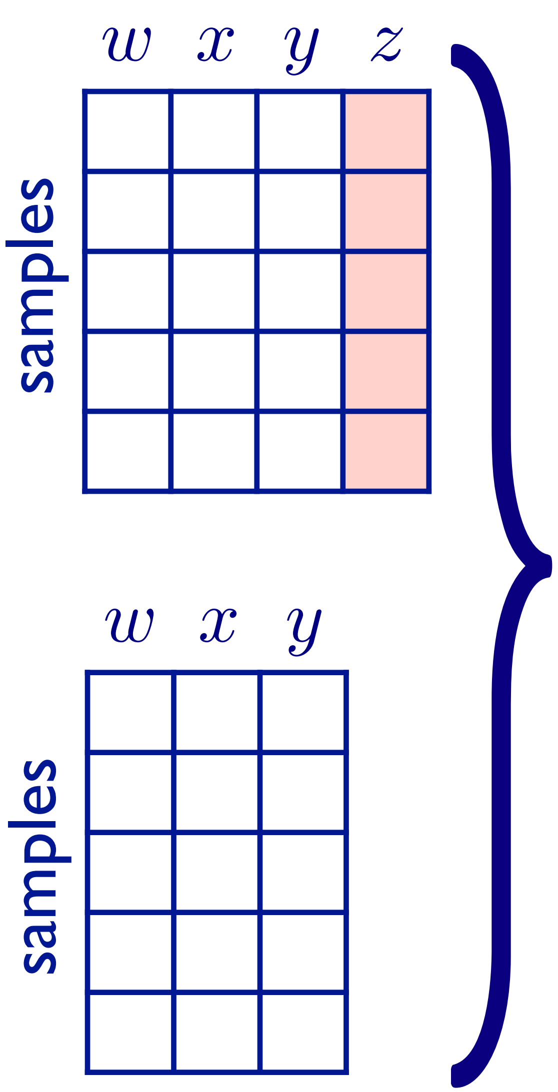


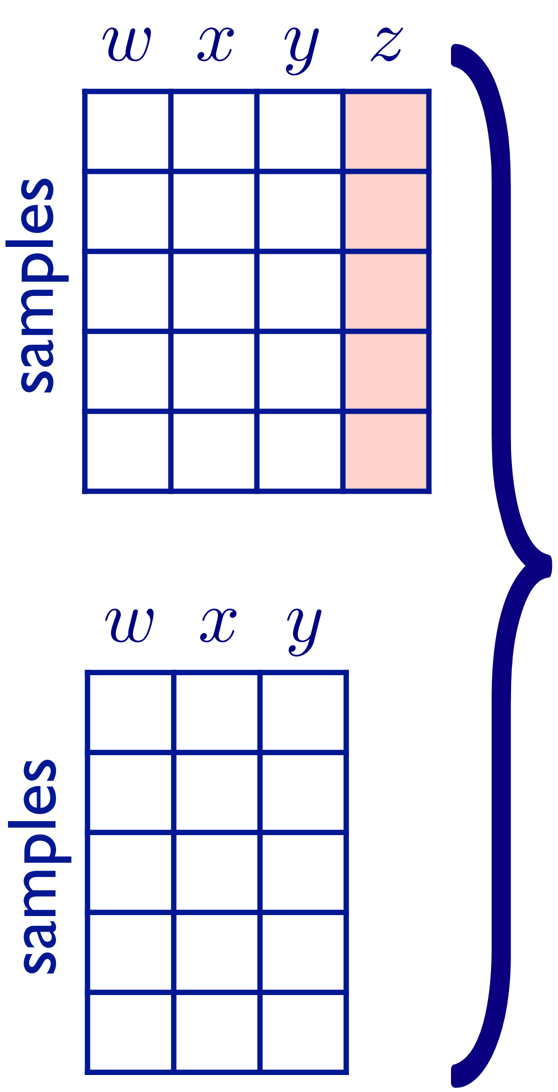
(in)dependence
constraints

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

High-Level

data
sample

assumptions, e.g.
- causal Markov
- causal faithfulness
- etc.



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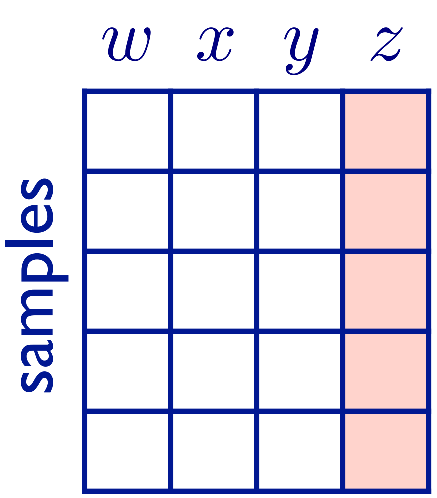
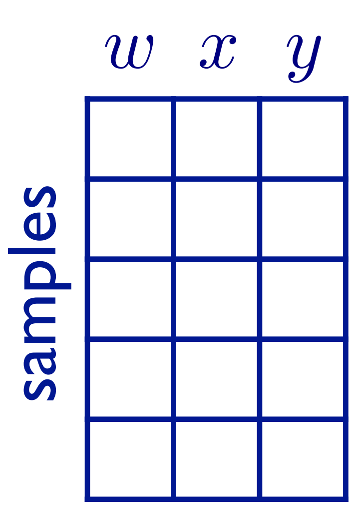
High-Level

data sample





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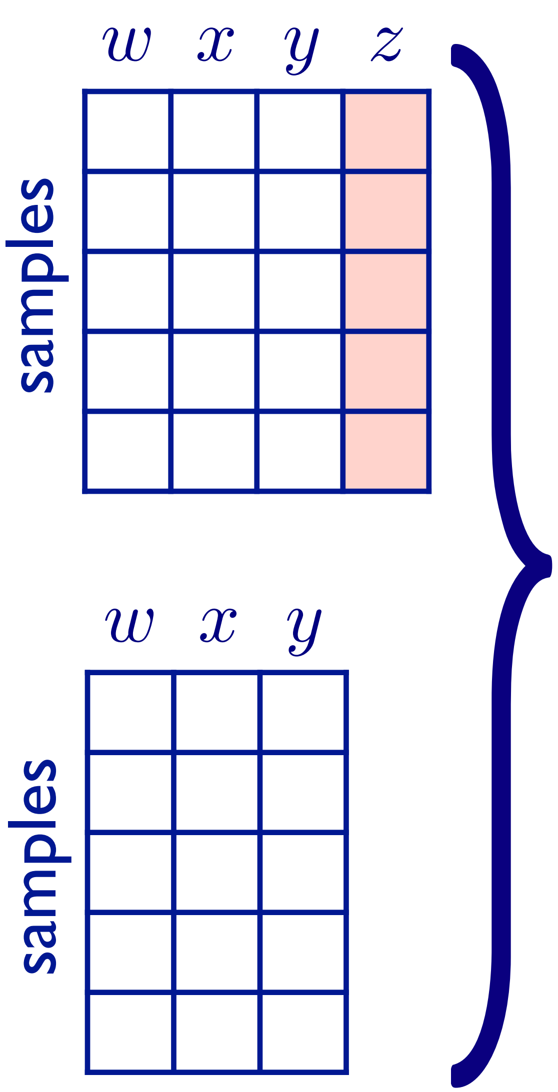

(in)dependence constraints

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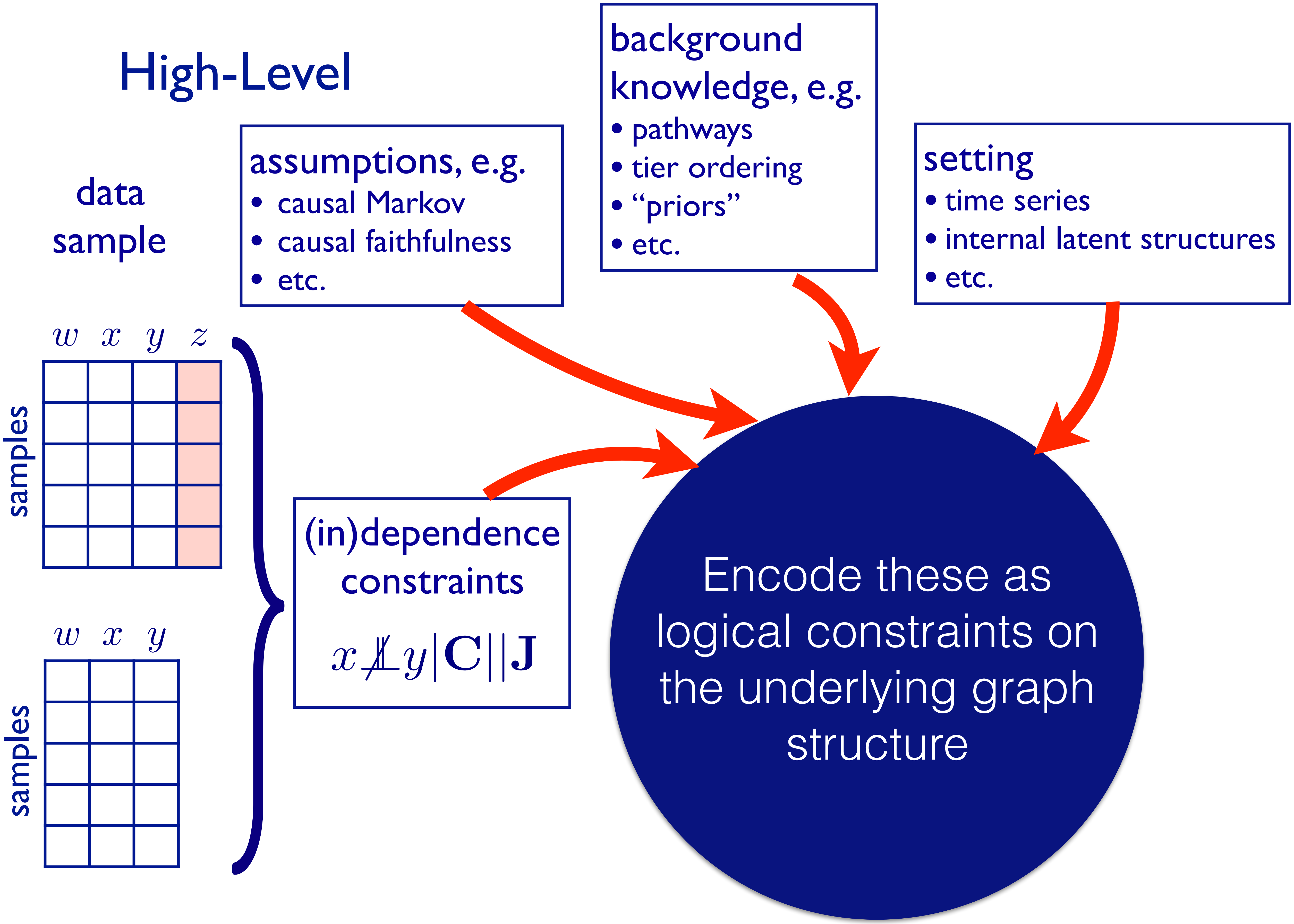
High-Level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w x y z
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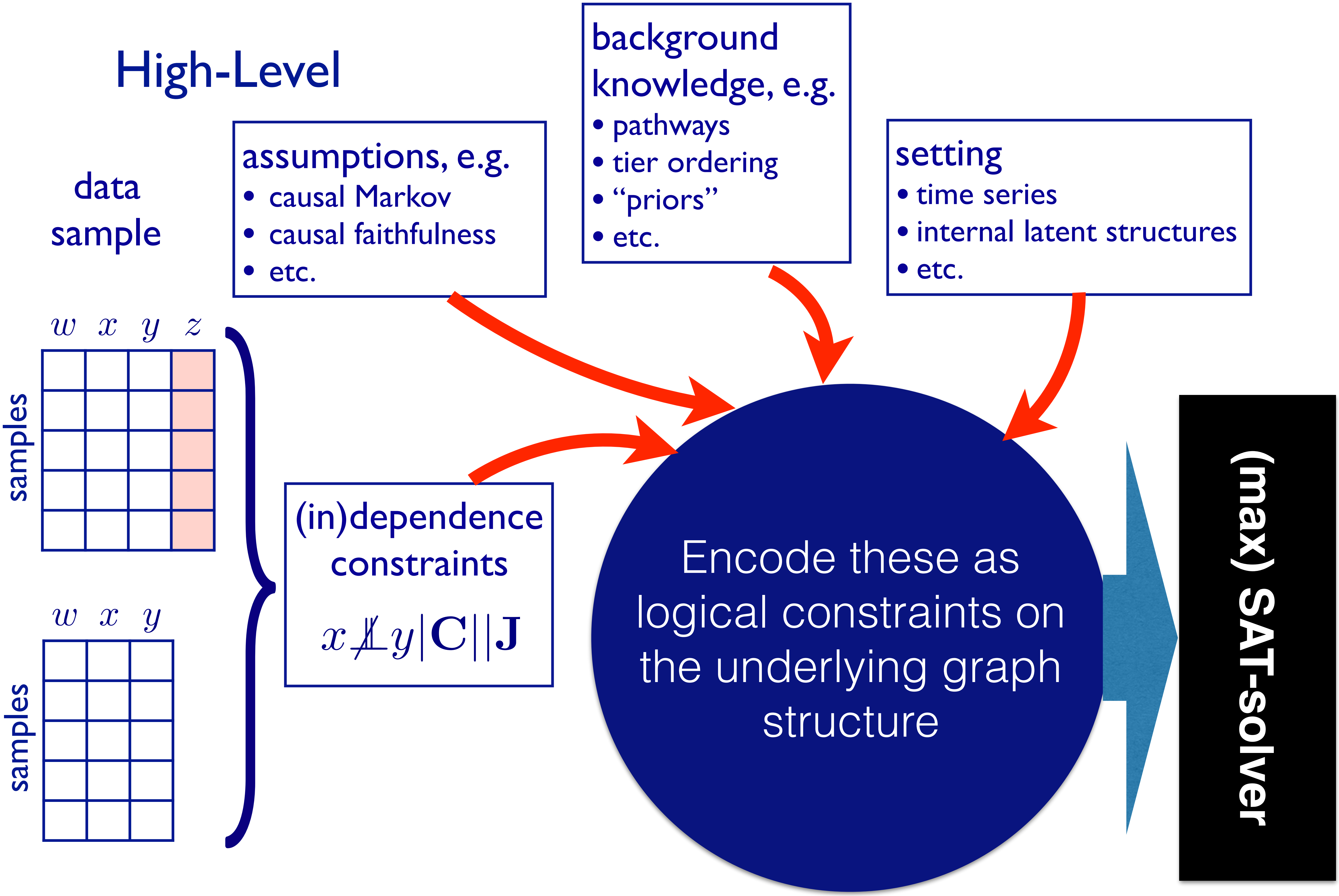
Encode these as logical constraints on the underlying graph structure

High-Level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Encode these as logical constraints on the underlying graph structure
(max) SAT-solver

SAT-based Causal Discovery

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

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

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

SAT-based Causal Discovery

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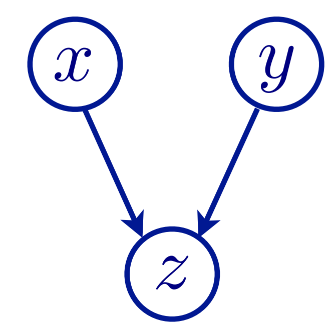
- **Find satisfying assignments using a SAT-solver**

$$A = false$$
$$B = false \iff$$
$$\ldots$$



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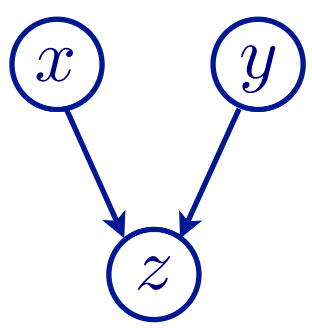

➡ very general setting (allows for cycles and latents) and trivially complete

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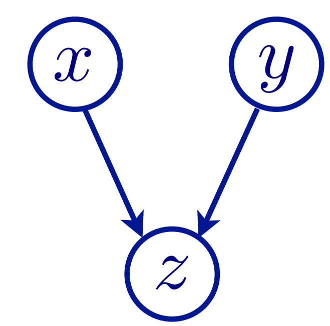


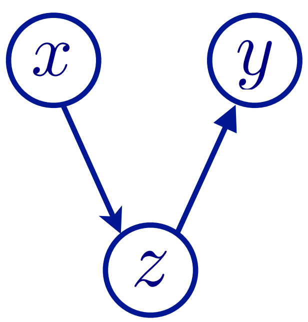
➡ very general setting (allows for cycles and latents) and trivially complete

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

Conflicts and Errors

- **Statistical independence tests produce errors**

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

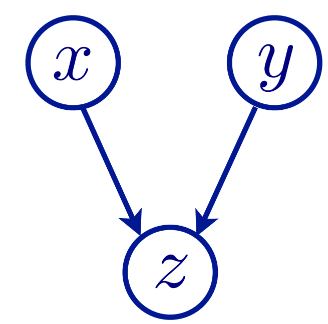


constraints

$$\Longleftarrow \boxed{x \not\perp\!\!\!\perp y}$$

$$x \perp\!\!\!\perp y$$
$$x \not\perp\!\!\!\perp z$$
$$y \not\perp\!\!\!\perp z$$
$$x \perp\!\!\!\perp y \mid z$$

$$\boxed{x \not\perp\!\!\!\perp y \mid z} \Longrightarrow$$



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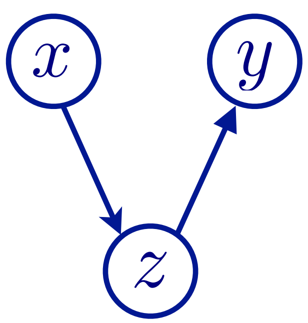
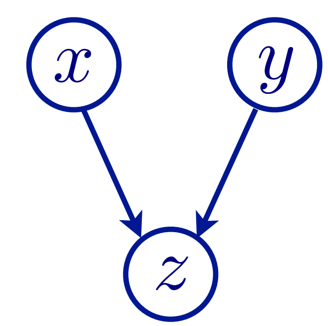


constraints	weight
$x \perp\!\!\!\perp y$	500
$x \not\perp\!\!\!\perp z$	3000
$y \not\perp\!\!\!\perp z$	2500
$x \perp\!\!\!\perp y \mid z$	250



Conflicts and Errors

Sridhar talk

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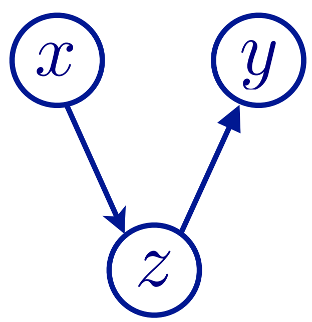

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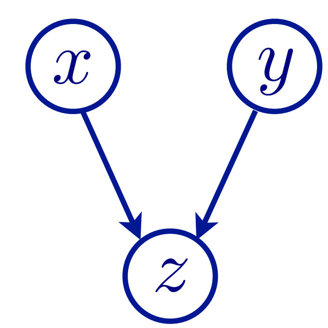

Constraint Satisfaction Approach

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

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

- **OUTPUT: a graph G that minimizes the cost**

[Hyttinen et al. 2014]

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What are suitable weights?

[Hyttinen et al. 2014]

Weighting Schemes

- Constant weights
  - unit weights for all constraint

[Hyttinen et al. 2014]

Weighting Schemes

- Constant weights
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- Hard dependencies
  - only treat rejections of the null-hypothesis as hard constraints, in line with classical statistics
  - give dependences infinite weight, maximize the independences (unit weight) in light of these dependences

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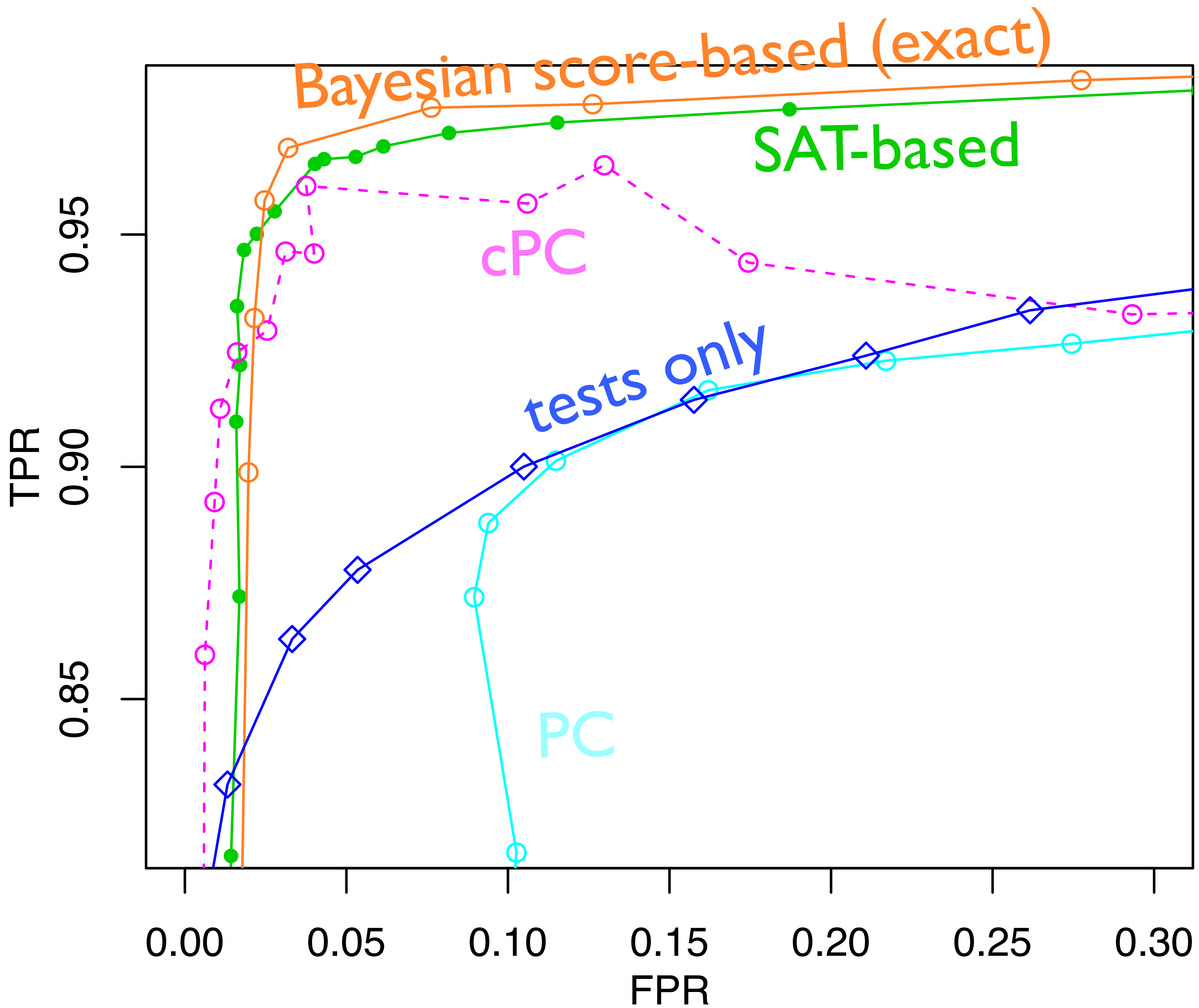
  - give dependences infinite weight, maximize the independences (unit weight) in light of these dependences
- Log weights
  - obtain the probability of an (in)dependence and weigh it according to the log of the probability
  - Model selection with Bayes rule:

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

[Hyttinen et al. 2014]

Simulation 1: no cycles, no latents, linear Gaussian

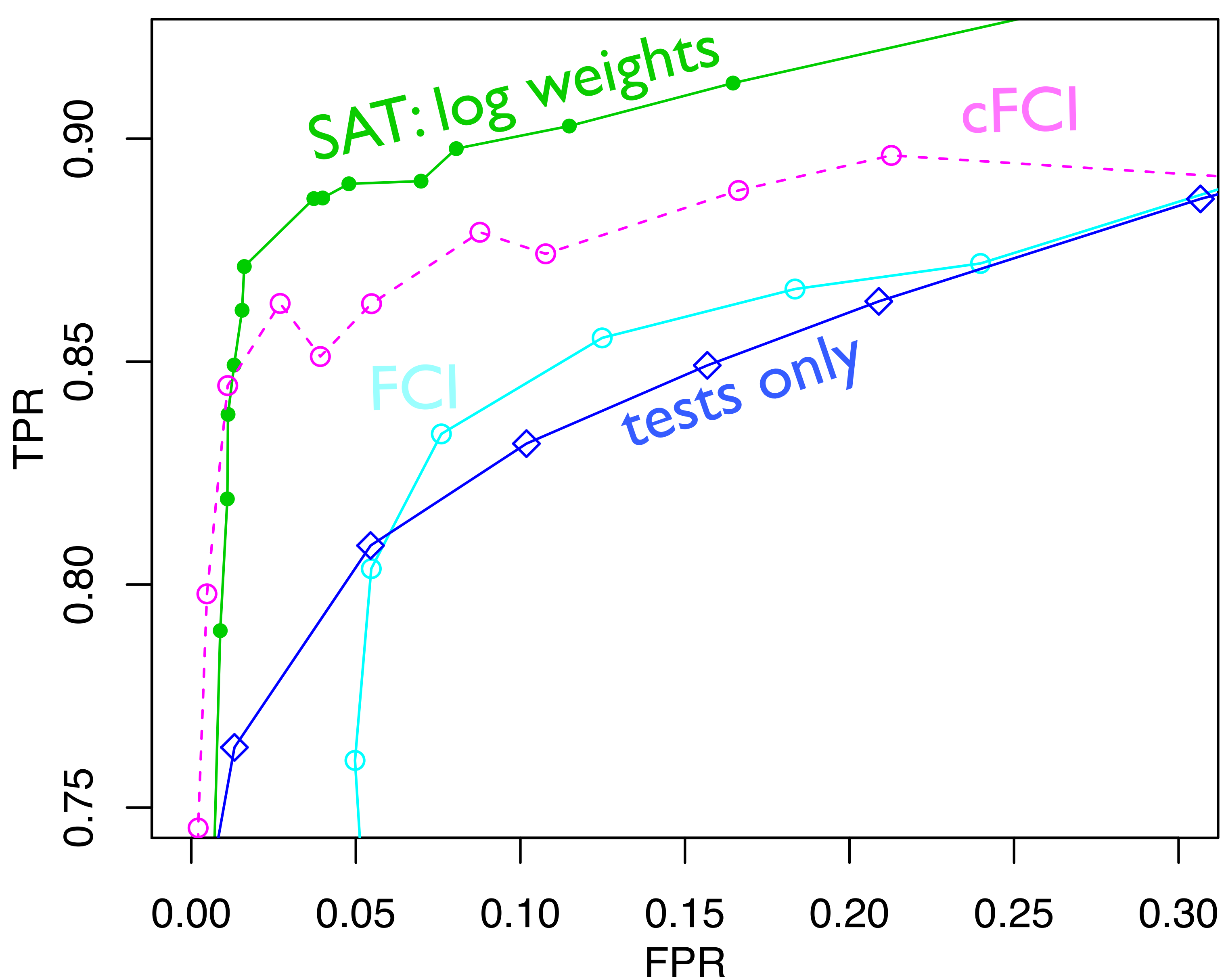


- TPR vs. FPR of all d-separation constraints of the true graph for a varying p-value cut-off
- observational data set,
  6 observed variables,
  average degree 2;
  500 samples, 200 models,
  linear Gaussian parameterization

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

[Hyttinen et al. 2014]

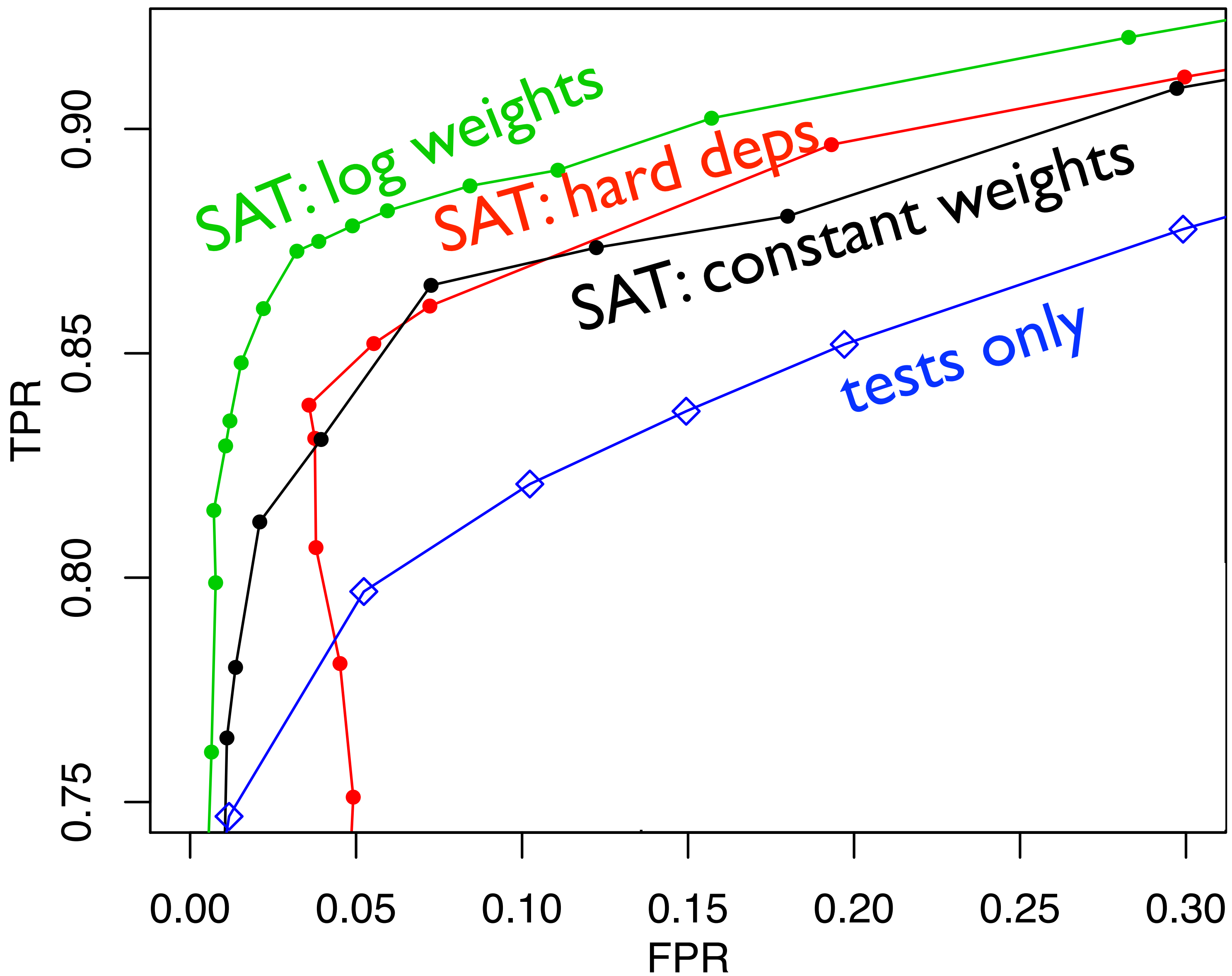
Simulation 2: no cycles, but latents



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

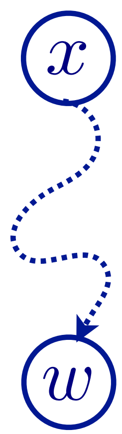
[Hyttinen et al. 2014]

Simulation 3: cycles and latents



[Hyttinen et al. 2014]

Background Knowledge



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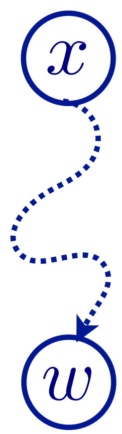
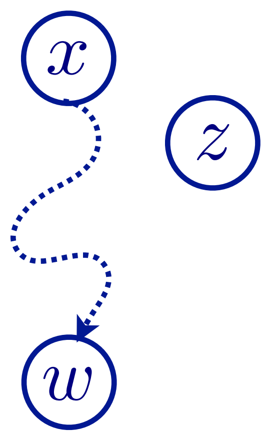


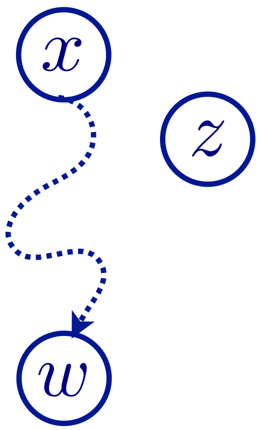
$$\iff \qquad x \not\perp\!\!\!\perp w \,||\, x$$

Background Knowledge



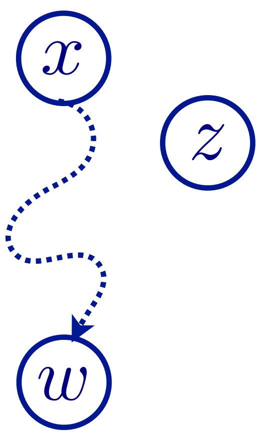
$$\Longleftrightarrow \qquad x \not\perp\!\!\!\perp w \,||\, x \; z$$

Background Knowledge



$$\Longleftrightarrow \qquad x \not\!\perp\!\!\!\perp w \,||\, x\ z \qquad weight = 0.8$$

Background Knowledge



$$\iff$$

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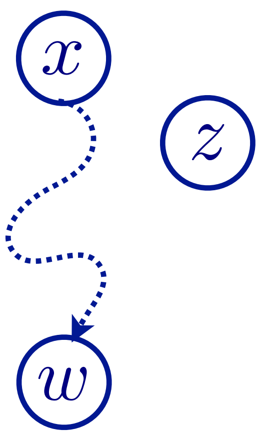
$$\boxed{\begin{array}{c} x \\ y \end{array}} > \boxed{\begin{array}{c} z \\ w \end{array}} \iff \begin{array}{l} (x > z) \wedge (x > w) \\ \wedge\ (y > z) \wedge (y > w) \end{array}$$

Background Knowledge



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“priors” $\Longleftrightarrow$

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

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

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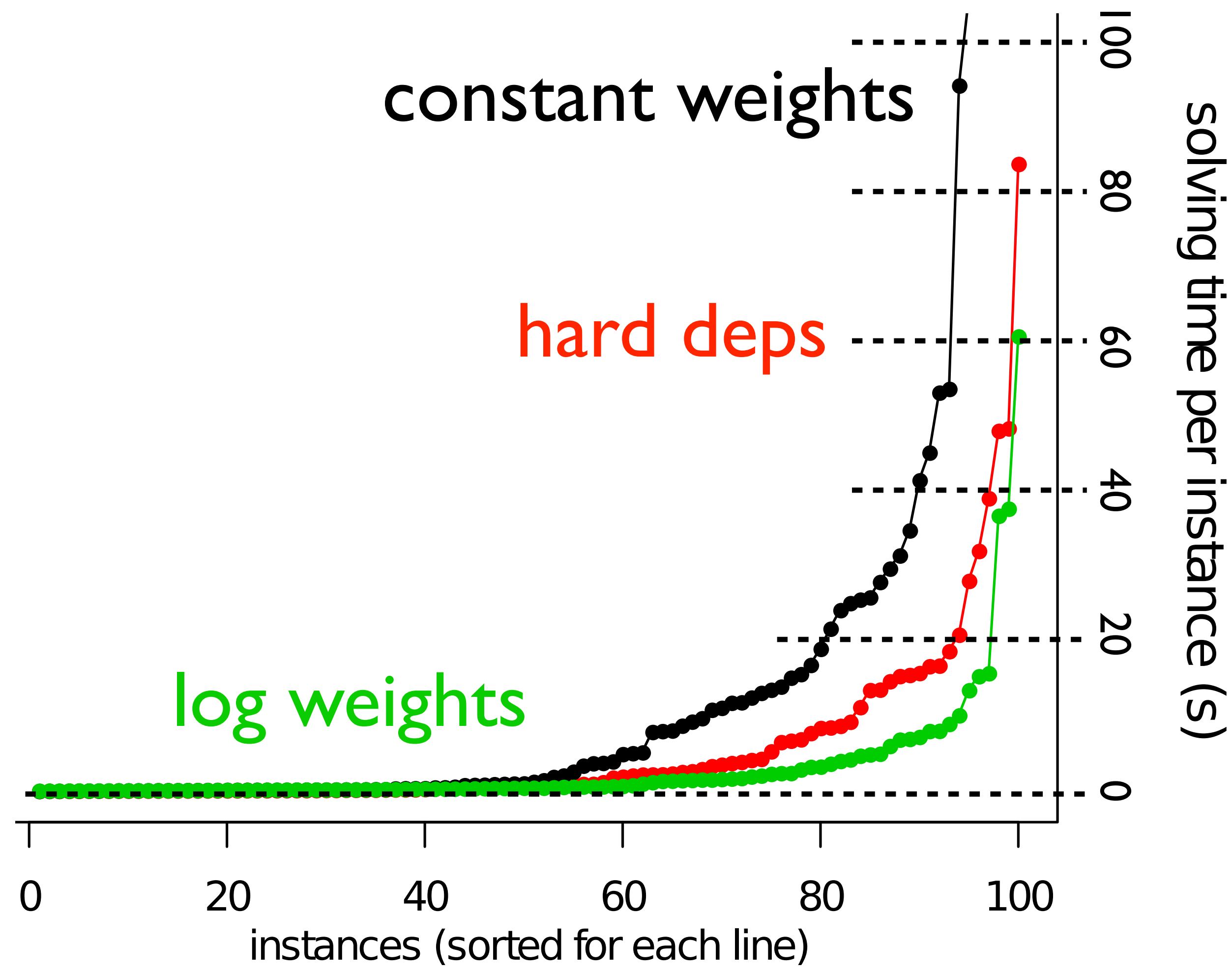
acyclicity	✓	✓	✗	✓	✓	✗	✓	✗*
parametric assumption	✗	✗	✗	linear non-Gaussian	linear non-Gaussian	linear non-Gaussian	non-linear additive noise	✗
output	Markov equivalence	PAG	PAG	unique DAG	set of DAGs	set of graphs	unique DAG	query based

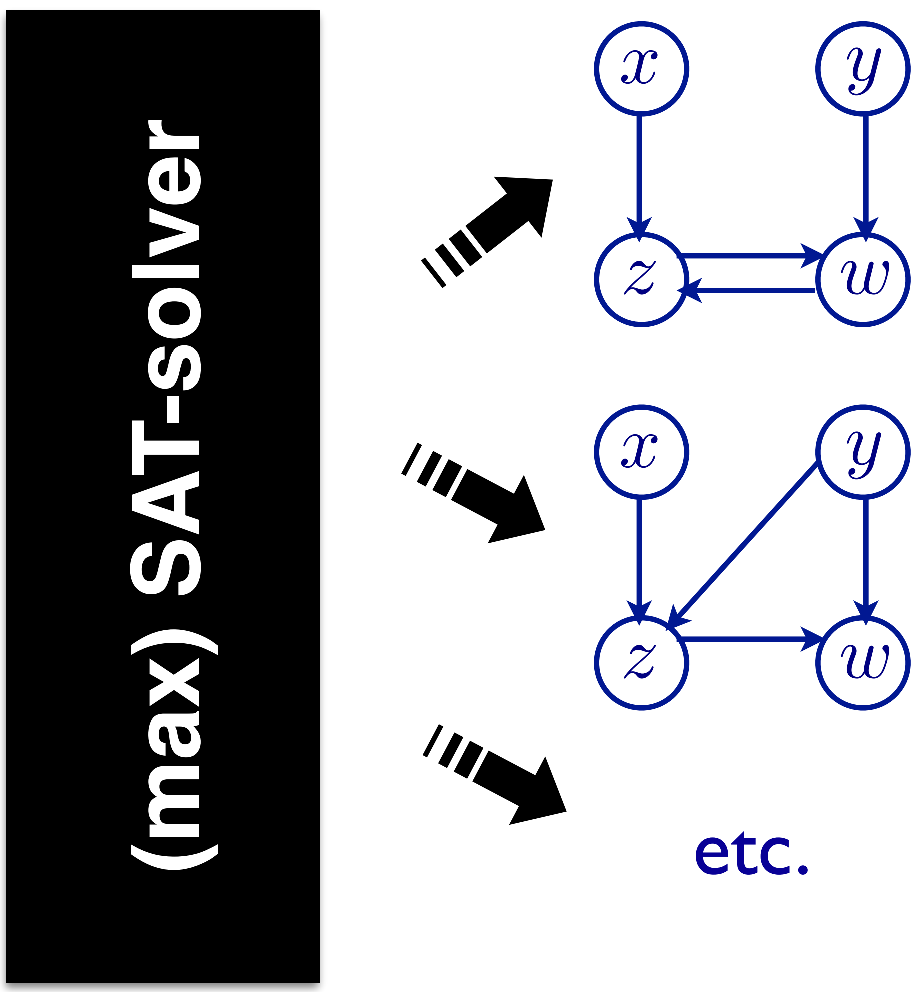
Simulation 4: Scalability



- up to 10 variables and only a few overlapping data sets for now

[Hyttinen et al. 2014]

Output of Causal Search Algorithms



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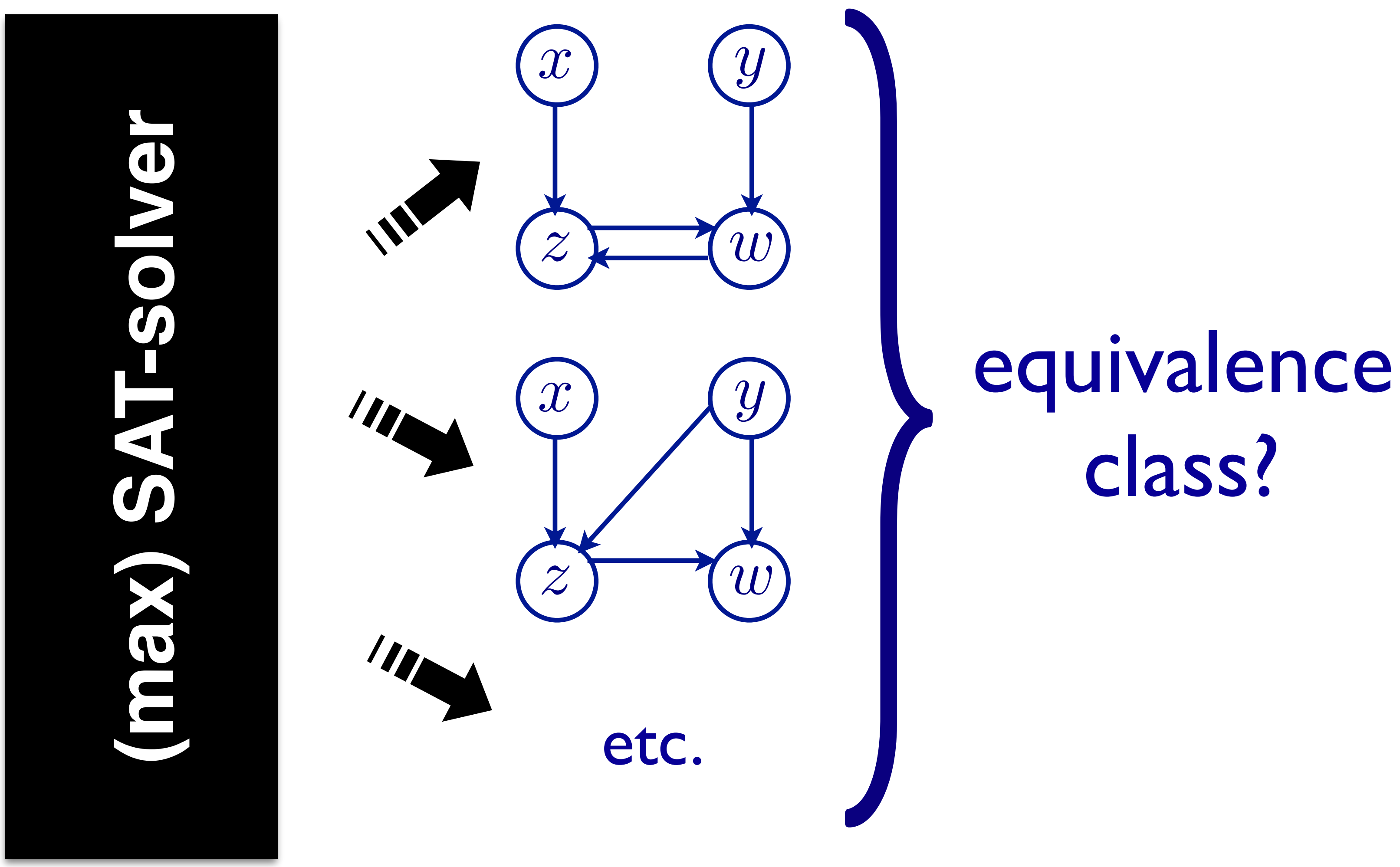


Output of Causal Search Algorithms

Query:

(max) SAT-solver

Output of Causal Search Algorithms

Query:

- list the structures in the equivalence class

(max) SAT-solver

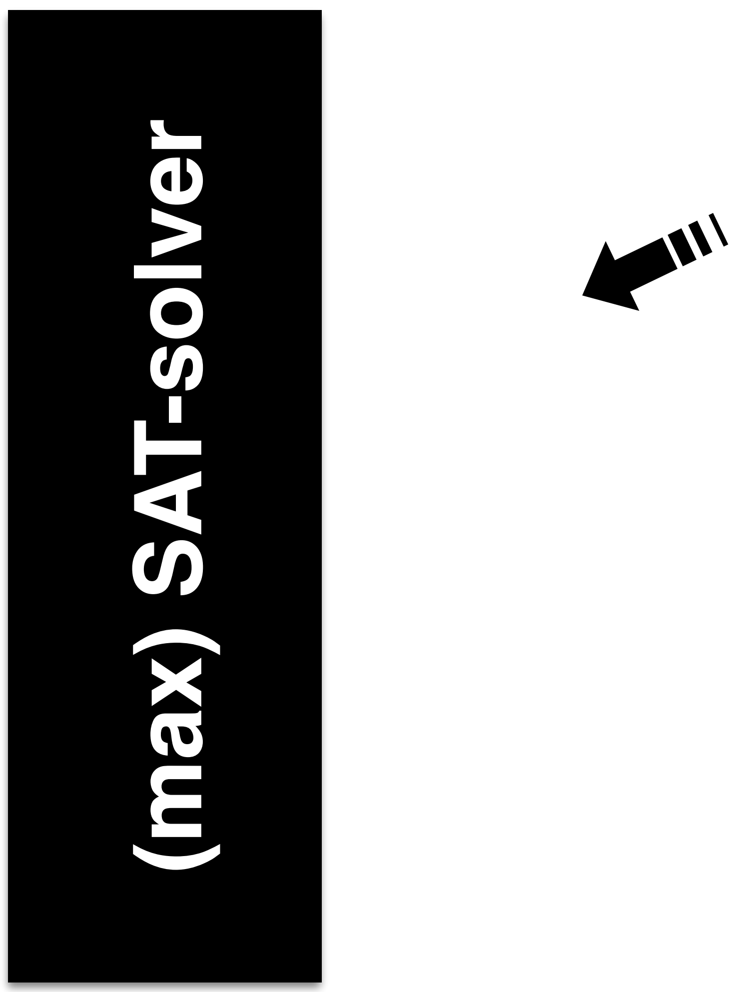
Output of Causal Search Algorithms

(max) SAT-solver

Query:

- list the structures in the equivalence class
- what structural features are determined?
  - edges, confounders
  - ancestral relations
  - pathways

Output of Causal Search Algorithms



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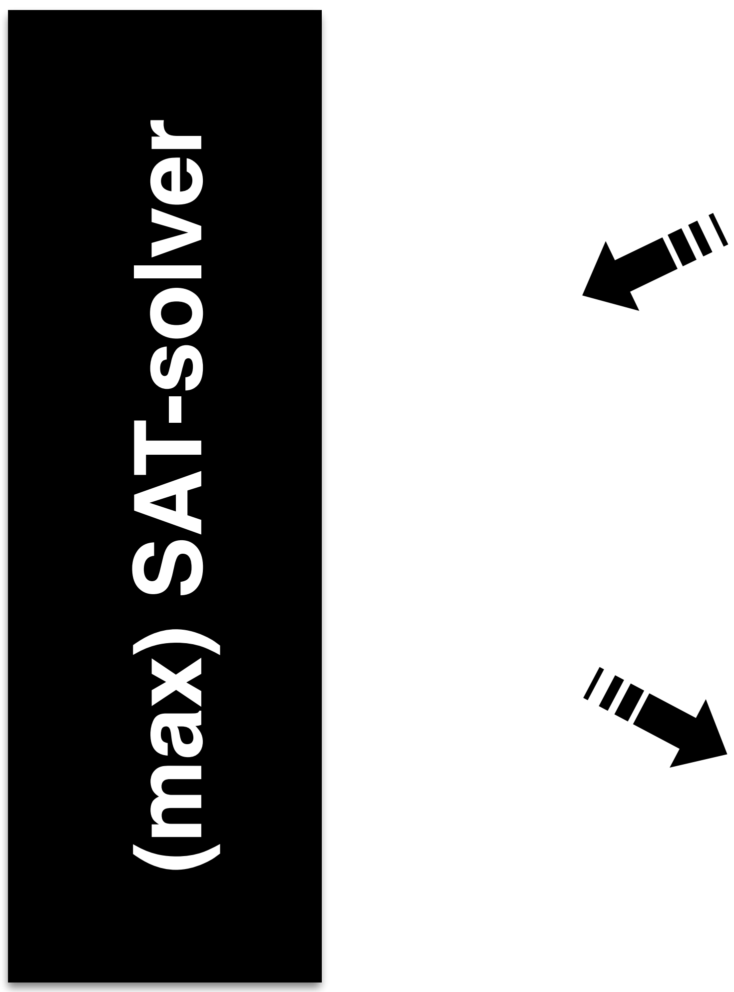
Output of Causal Search Algorithms



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- list the structures in the equivalence class
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  - ancestral relations
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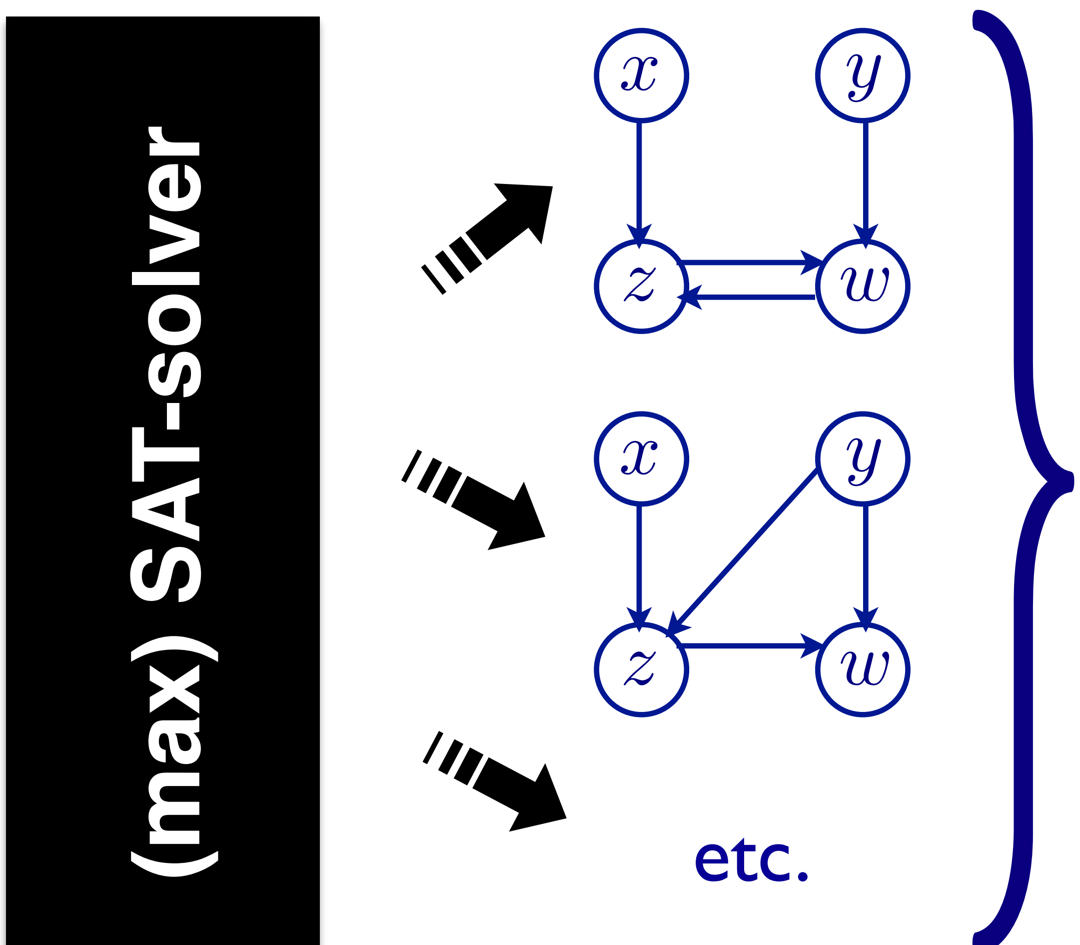
- what are the highest scoring equivalence classes?

Response:

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

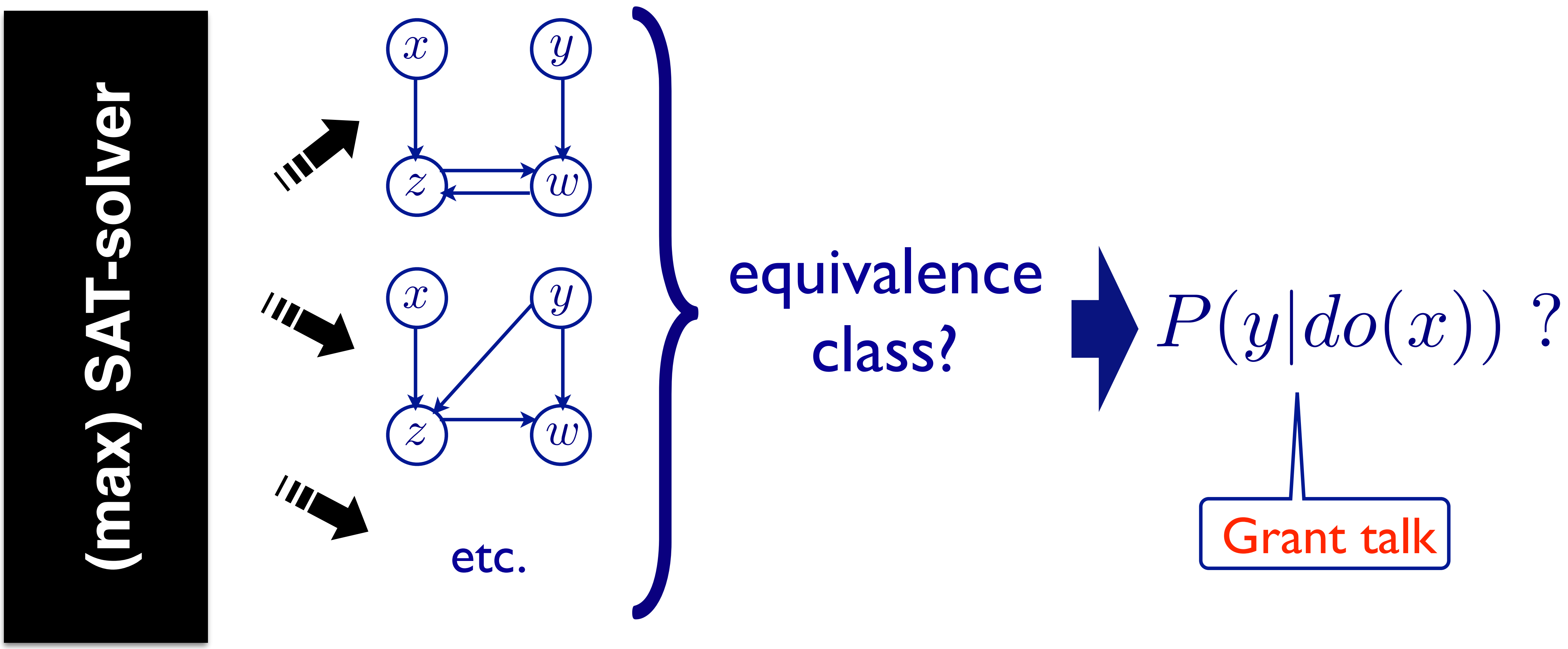
Computing Causal Effects



equivalence class?

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

Computing Causal Effects



equivalence class ➡ $P(y|do(x))$?

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

[Hyttinen et al. 2015]

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

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

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)

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

[Hyttinen et al. 2015]

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

Rule 2 (action/observation exchange)

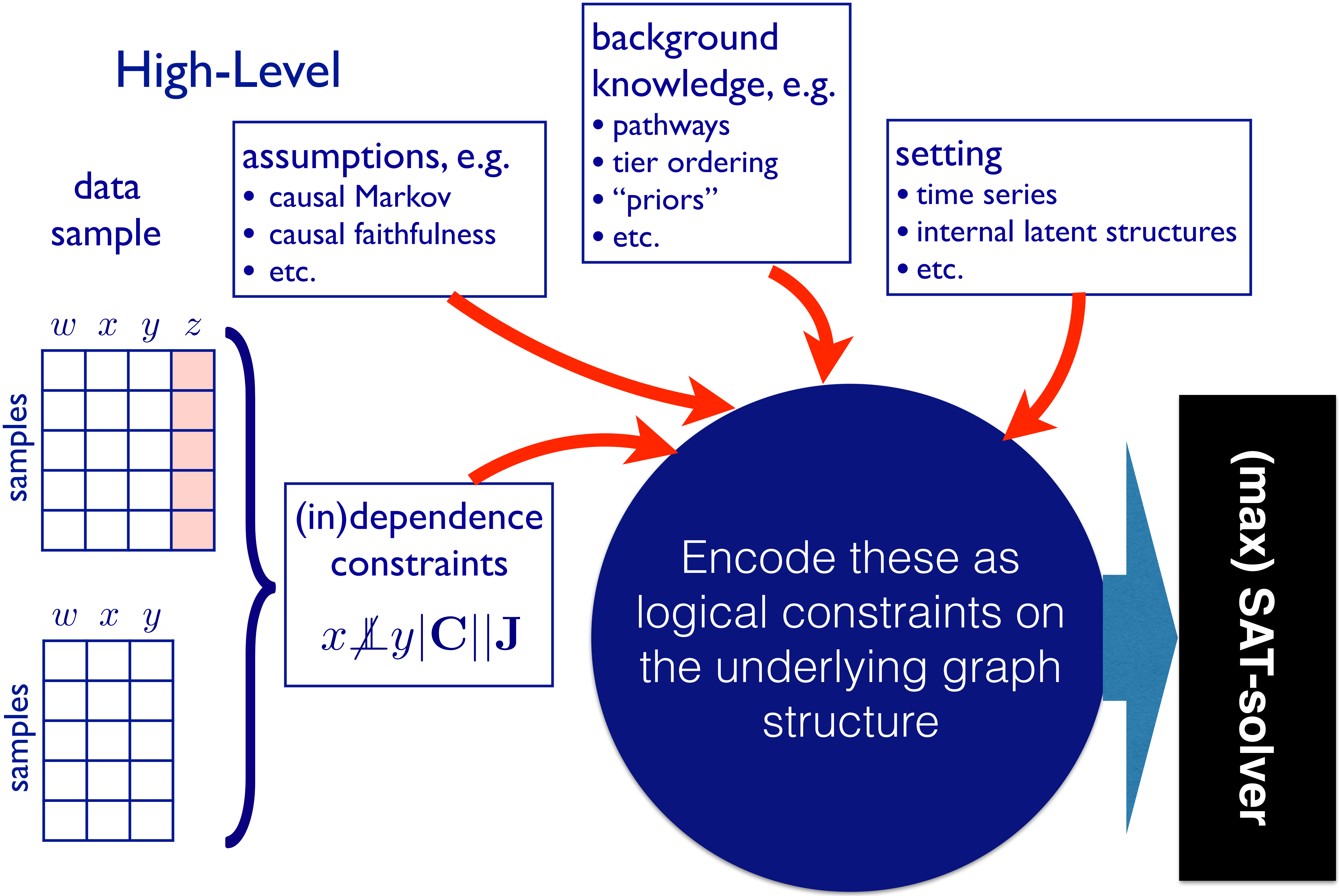
$$P(y|do(x), do(z), w) = P(y|do(x), z, w) \text{ if } Y \perp\!\!\!\perp I_Z|X, Z, W||X$$

Rule 3 (insertion/deletion of actions)

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

[Hyttinen et al. 2015]

High-Level



data sample
assumptions, e.g.
• causal Markov
• causal faithfulness
• etc.
background knowledge, e.g.
• pathways
• tier ordering
• “priors”
• etc.
setting
• time series
• internal latent structures
• etc.
w x y z
samples
w x y
samples
(in)dependence constraints
$x \not\perp\!\!\!\perp y \,|\, \mathbf{C} \,||\, \mathbf{J}$
Encode these as logical constraints on the underlying graph structure
(max) SAT-solver

High-Level

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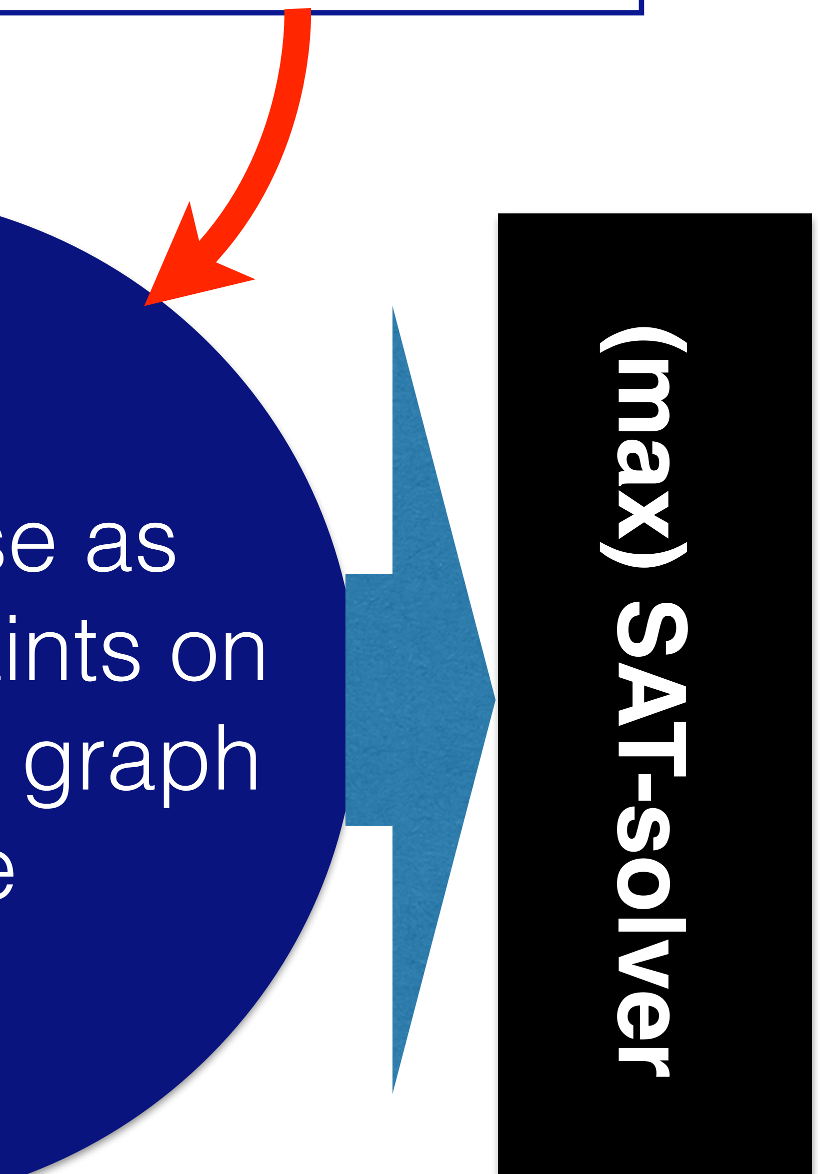
tc.



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(max) SAT-solver

High-Level

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tc.

QUERY?

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ints on
graph
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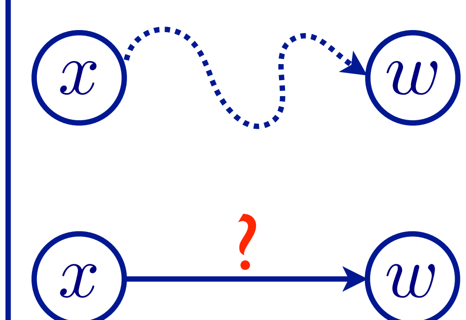
(max) SAT-solver

$$P(y \,|\, do(x))$$



Just getting started…

Just getting started…

- application

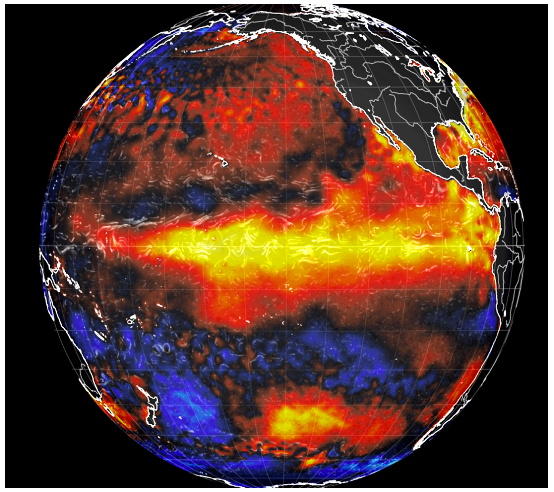
[Stekhoven et al. 2012]

Just getting started…

- application

[Stekhoven et al. 2012]

- multi-scale causal analysis: micro- to macro-variables



[Chalupka et al. 2016]

Just getting started…

- application

[Stekhoven et al. 2012]

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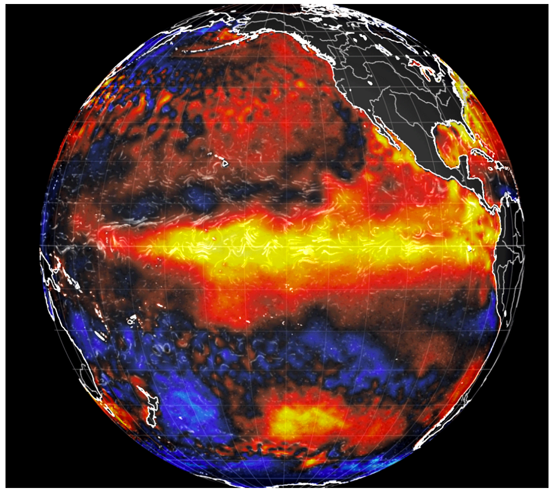
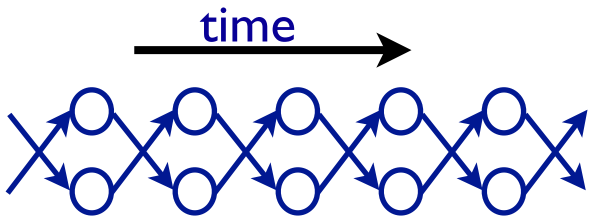


[Chalupka et al. 2016]

- time-series and dynamics

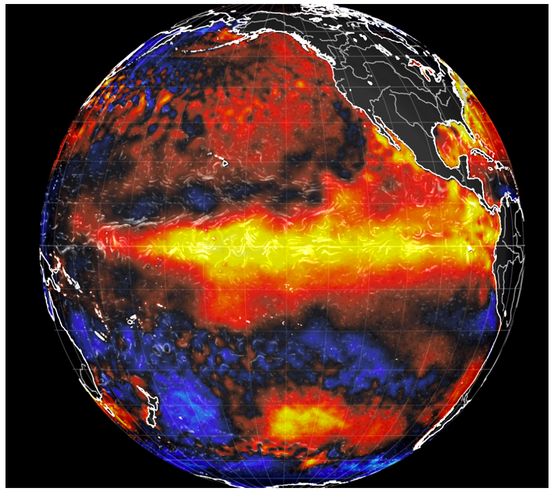


Just getting started…

- application

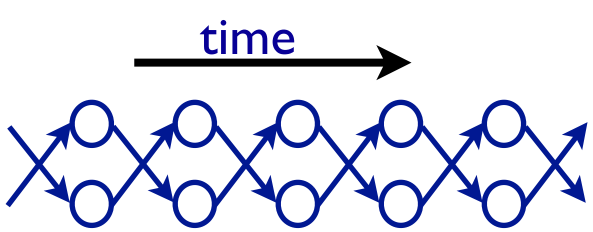
[Stekhoven et al. 2012]

- multi-scale causal analysis: micro- to macro-variables

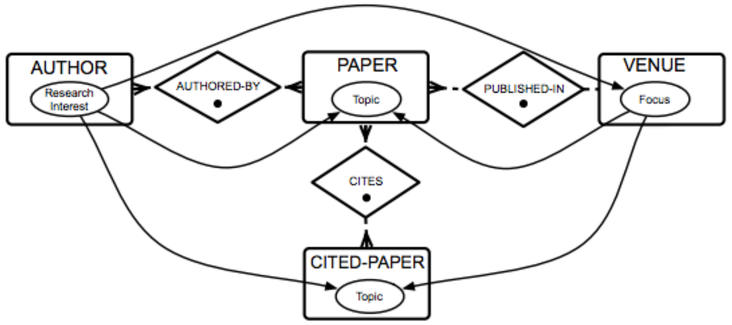


[Chalupka et al. 2016]

- time-series and dynamics



- violations of the Markov property: non-causal relations



[Maier et al. 2013]

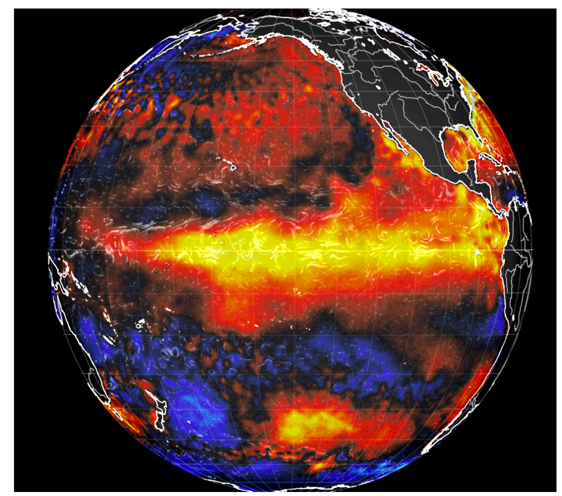
Just getting started…

Sokolova talk

- application

[Stekhoven et al. 2012]

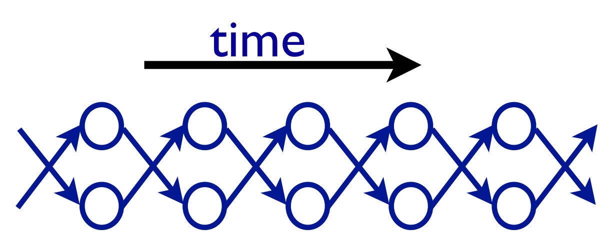
- multi-scale causal analysis: micro- to macro-variables



[Chalupka et al. 2016]

Blondel talk

- time-series and dynamics



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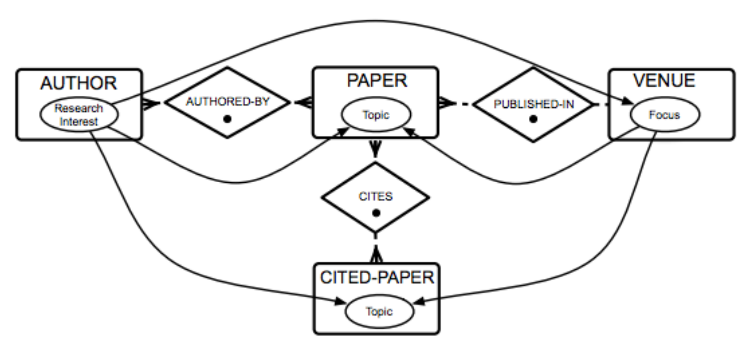

[Maier et al. 2013]

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Thank you!