Structure Learning for Bayesian Networks over Labeled DAGs

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Context-specific Independence [Boutilier et al. '96]

$$X \perp\!\!\!\perp Y | C, Z = 0$$

i.e. $P(X|Y, C, Z = 0) = P(X|C, Z = 0)$

but $P(X|Y, C, Z = 1) \neq P(X|C, Z = 1)$ (possibly)

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- A very natural independence restriction for any modelling task.
- For example:

$$\text{INCOME} \perp\!\!\!\perp \text{WEATHER} |\ \text{JOB} = \text{clerk}$$

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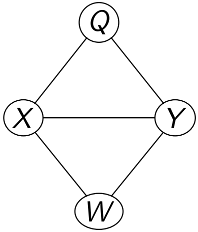
- Alarm has several of these:

$$\text{HREKG} \perp\!\!\!\perp \text{CRRCAUTER}|\ \text{HR} = \text{LOW}$$

Motivation



AND $X \perp\!\!\!\perp Y | \; Q = 0 \quad \Rightarrow \quad ?$

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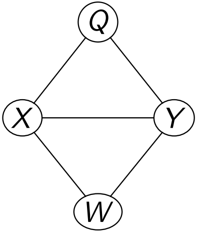

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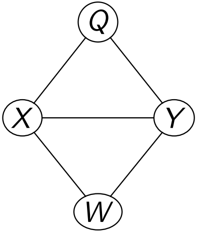
- What are good graphical models for understanding CSIs?



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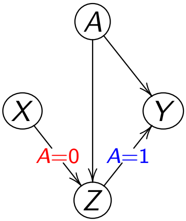
- Can we orient causal edges based on CSIs in a principled way?
- What are good graphical models for understanding CSIs?
- Can we get better causal or probabilistic models by using CSIs?

Contents

BNs over LDAGs

Bayesian Networks over Labeled DAGs [Pensar et al. 15]

$P(X)$	$X=0$	$X=1$
	0.5	0.5



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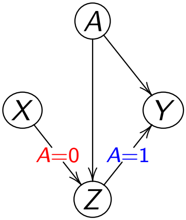

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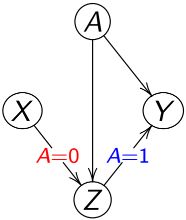

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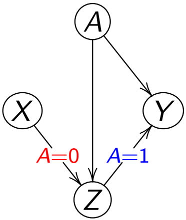

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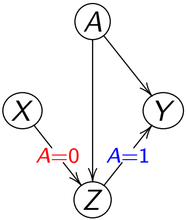

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- CPT has rows consistent with the assignment equal.

Another Bayesian Network over a Labeled DAG

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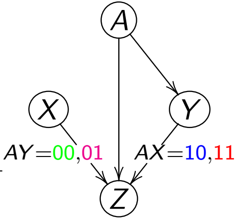

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- Local CSIs: $X \perp\!\!\!\perp Z \mid AY=00$, $X \perp\!\!\!\perp Z \mid AY=01$, $Y \perp\!\!\!\perp Z \mid AX=10$, $Y \perp\!\!\!\perp Z \mid AX=11$

Modelling local structure in BN CPTs

Alternative modelling strategies [Koller & Friedman, ch. 5]:

- Decision tree -based CPTs (subsumed in the binary case)
- Rule-CPTs
- Noisy-ORs, logistic models, etc.

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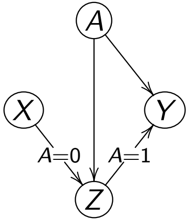
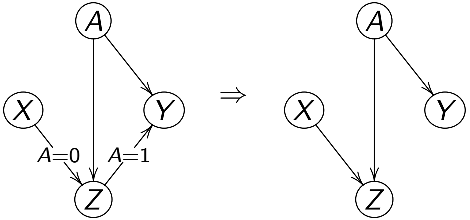
LDAGs [Pensar et al. '15]:

- Allow for developing theory using the labels.
- Markov equivalence defined based on the labels.
- Visual representation of CSIs in a single structure.



Separation Criteria

CSI-separation of [Boutilier et al. 96] for LDAGs



Original LDAG

context $A = 1$ specific DAG

- In a **context** $S = s$ **specific DAG** of an LDAG edges with labels consistent with $S = s$ are removed.

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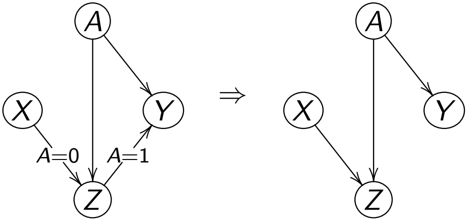

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$\Rightarrow \quad X \perp_{CSI} Y | \; A = 1$

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- X and Y are **CSI-separated** given $C, S = s$, iff X and Y are d-separated given C, S in the context $S = s$ specific DAG.

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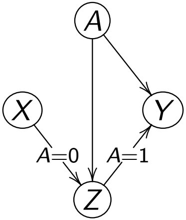

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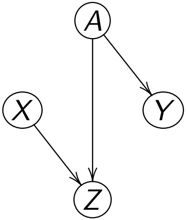

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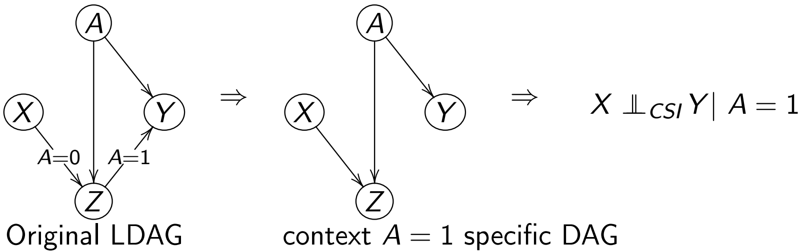

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- CSI-separation is sound and it subsumes d-separation.
- But CSI-sep. is **incomplete**: $X \perp\!\!\!\perp Y$! **NP-hard!**

New Necessary Separation Criterion for LDAGs

Theorem

For $X \perp\!\!\!\perp Y | C, S = v[S]$ to be implied by an LDAG over V
X, Y have to be a d-separated given C, S
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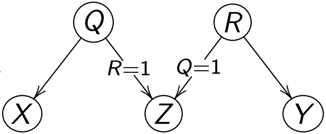

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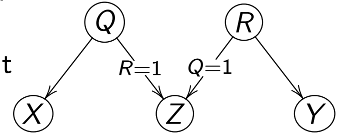

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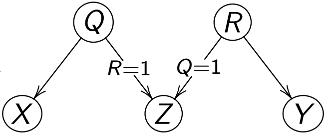

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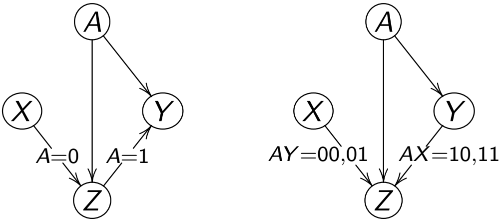
- In the following we assume faithfulness w.r.t. to the theorem.

Markov Equivalence for LDAGs



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  [Pensar et al. 15].

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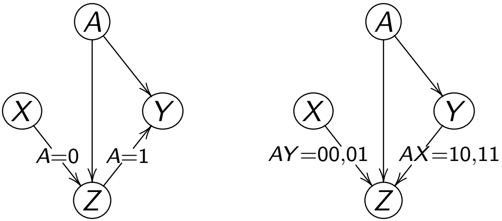

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- **LDAG-colliders**: $X \to Z \leftarrow A$ without $X - A$ in some context $V = v$ specific DAG
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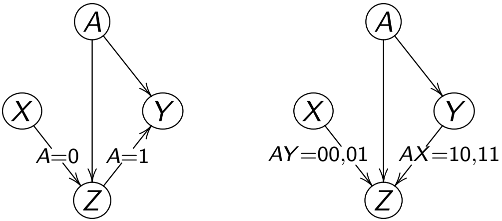

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- **LDAG-colliders**: $X \rightarrow Z \leftarrow A$ without $X - A$ in some context $V = v$ specific DAG
- **LDAG-non-colliders**: $Z - A - Y$ without $Z - Y$ in some context $V = v$ specific DAG
- Markov equivalent LDAGs share them: $X - Z - Y$ is neither.

Constraint-based learning

PC of Spirtes et al.

1. Skeleton search: Try to find a separating set S such that $X \perp\!\!\!\perp Y | S$.
2. Orient colliders: $X \rightarrow Z \leftarrow Y$ if $Z \notin S$.
3. Run further orientation rules to make sure no cycles or new colliders are possible.

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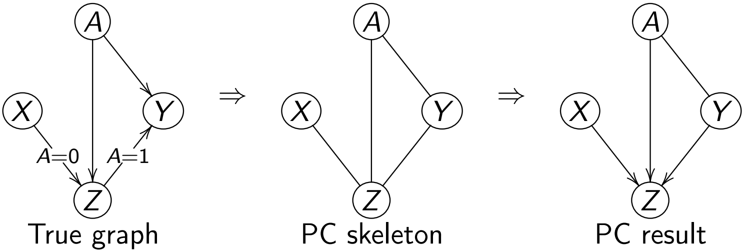

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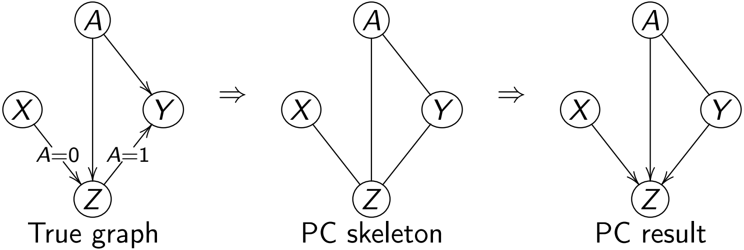

PC produces wrong orientation in the presence of CSIs!

LPC Skeleton Search

- Instead, we search for **separating contexts** $S = s$, s.t. $X \perp\!\!\!\perp Y|\, S = s$.
- Delete edges if $X \perp\!\!\!\perp Y|\, S = s$ for all s.
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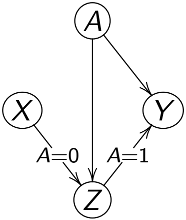


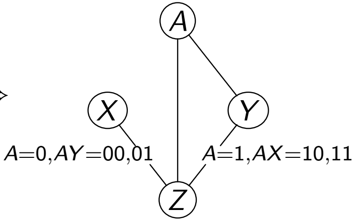
True graph

$\Rightarrow$

$$X \perp\!\!\!\perp A$$
$$X \perp\!\!\!\perp Y$$
$$X \perp\!\!\!\perp Z | \; A = 0$$
$$Z \perp\!\!\!\perp Y | \; A = 1$$
$$X \perp\!\!\!\perp Z | AY = 00$$
$$Z \perp\!\!\!\perp Y | AY = 10$$
$$X \perp\!\!\!\perp Z | AY = 01$$
$$Z \perp\!\!\!\perp Y | AY = 11$$

CSIs

$\Rightarrow$



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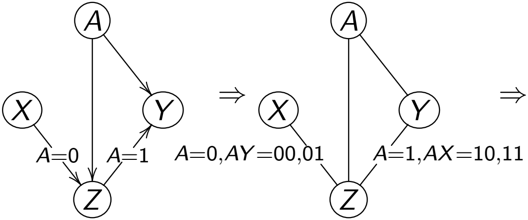
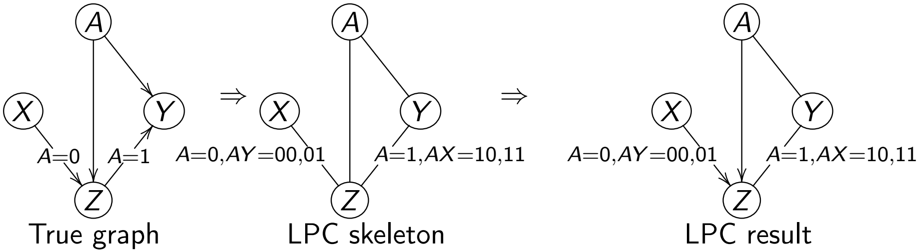


True graph LPC skeleton

- In the paper we give technical conditions for detecting LDAG-(non-)colliders from the LPC skeleton result.

LPC Orientation



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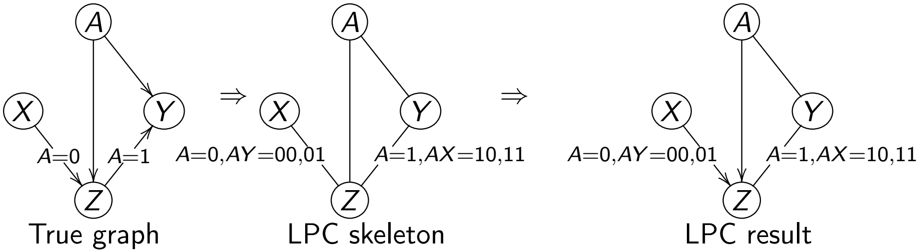

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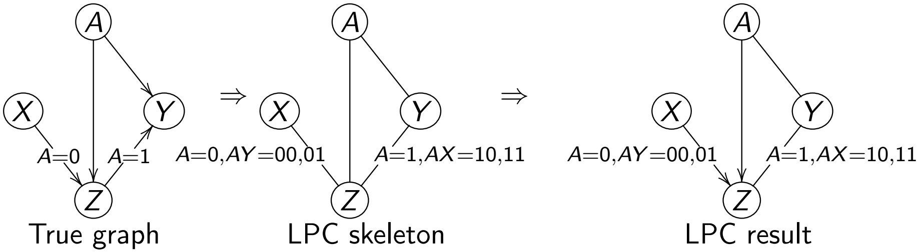

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- LPC is conjectured to be orientation complete.

Simulations: Orientation Accuracy

10-node binary LDAGs, 300 models, over the true distribution.

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algo	av. degree	label prob.	edges found	corr. oriented	reversed
PC	2.99	0 %	4481	3498	0
cPC	2.99	0 %	4481	3498	0
LPC	2.99	0 %	4481	3498	0

- Without CSIs due to labels, algorithms work similarly.

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algo	av. degree	label prob.	edges found	corr. oriented	reversed
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cPC	2.99	0 %	4481	3498	0
LPC	2.99	0 %	4481	3498	0

- Without CSIs due to labels, algorithms work similarly.

algo	av. degree	label prob.	edges found	corr. oriented	reversed
PC	2.18	50 %	3276	**2243**	**103**
cPC	2.18	50 %	3276	**2285**	**0**
LPC	2.18	50 %	3276	**2319**	**0**

- With CSIs due to labels, PC makes orientation errors.
- cPC does not but orients less.
- **LPC orients more and all orientations are correct.**

Score-based learning

BIC for LDAGs

- Maximizing BIC [Chickering '97]:

$$\max_G \sum_{X \in V} s(X, \mathrm{pa}_G(X)),$$

$$s(X, \mathrm{pa}_G(X)) = \max_{\mathsf{LABELS}} s(X, \mathrm{pa}_G(X), \mathsf{LABELS})$$

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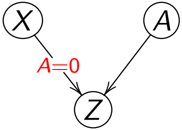
- LABELS imply a partition of rows:



$\Leftrightarrow$

$P(Z \mid A, X)$	$Z = 0$	$Z = 1$
$AX = 00$	θ_1	$1 - \theta_1$
$AX = 01$	θ_1	$1 - \theta_1$
$AX = 10$	θ_2	$1 - \theta_2$
$AX = 11$	θ_3	$1 - \theta_3$

$\Leftrightarrow \{ \{1, 2\}, \{3\}, \{4\} \}$

$$s(X, \mathrm{pa}_G(X), \text{LABELS}) = \mathrm{L} - R \cdot \log N/2$$

L is max. likelihood, R number of parts, both w.r.t. LABELS.

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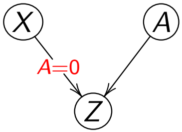

$\Leftrightarrow$

$P(Z\|A,X)$	$Z=0$	$Z=1$
$AX=00$	θ_1	$1-\theta_1$
$AX=01$	θ_1	$1-\theta_1$
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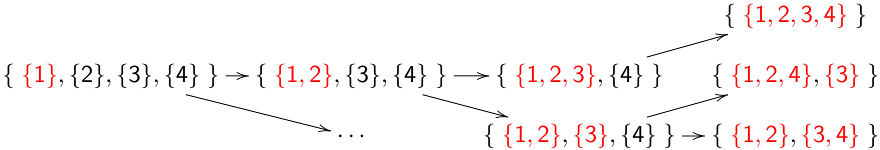
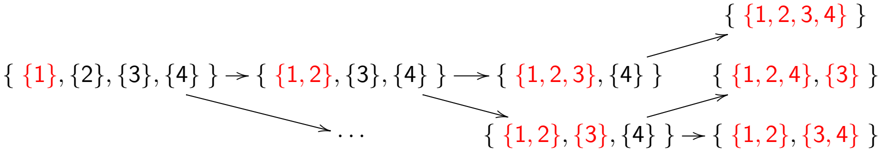
- For 4 binary parents, 27 million different label structures.

Branching . . .

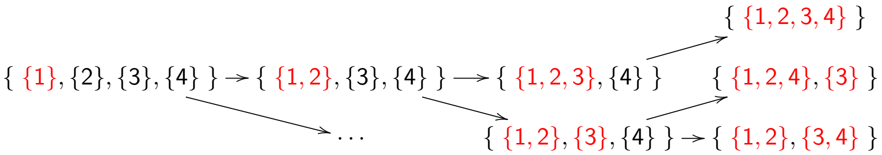


- Search over partitions of rows from complex towards simpler.



- Search over partitions of rows from complex towards simpler.
- Keep a set of parts fixed (in red).
- Combine the first unfixed part to the fixed parts to avoid visiting the same partitions more than once (symmetry breaking).

... and Bounding

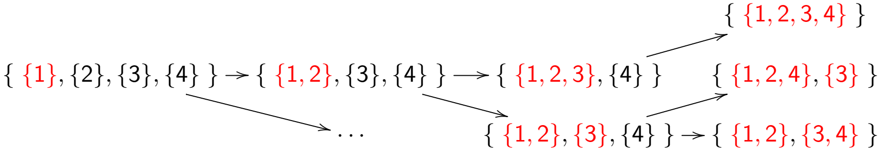


- **Upper bound** for partitions further in the branch:

$$\mathrm{L} - f \cdot \log N/2$$

Here L is the current likelihood, f is the number of fixed parts.

. . . and Bounding



- **Upper bound** for partitions further in the branch:

$$\mathrm{L} - f \cdot \log N/2$$

  Here L is the current likelihood, f is the number of fixed parts.
- **Initial best:** best solution to the subsets of parents.

. . . and Bounding

$\{ \{1\}, \{2\}, \{3\}, \{4\} \} \to \{ \{1,2\}, \{3\}, \{4\} \} \longrightarrow \{ \{1,2,3\}, \{4\} \} \to \{ \{1,2,3,4\} \}$

$\{ \{1\}, \{2\}, \{3\}, \{4\} \} \to \dots$

$\{ \{1,2\}, \{3\}, \{4\} \} \to \{ \{1,2\}, \{3\}, \{4\} \} \to \{ \{1,2,4\}, \{3\} \}$

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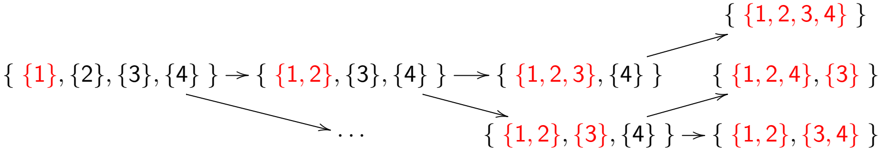

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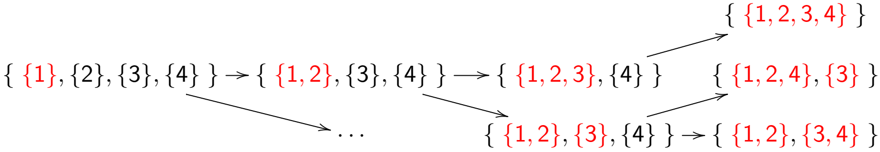

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- **Initial best:** best solution to the subsets of parents.
- **LDAG consistency check** whenever a new best found.
- Scales up to 4 parents.
- Finally: maximization over the local scores by **Gobnilp**.

- An extra edge does not always increase the BIC penalty:

$P(Z\|X)$	$Z=0$	$Z=1$
$X=0$	0.4	0.6
$X=1$	0.6	0.4

$\Rightarrow$

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Remedies for Overfitting

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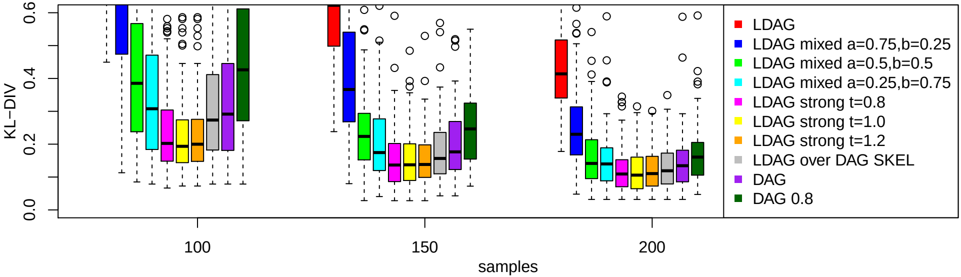
- **Strong Score Pruning** Delete a local score if it is not better than for a subset by a margin controlled by t.
- **Mixed BIC Penalty** Penalize by

  $a \cdot$ LDAG-based BIC $+\, b \cdot$ DAG-based BIC.
- **LDAG over Optimal DAG Skeleton** Only orient with the LDAG-based BIC score.

10-node binary LDAGs, 0.5 label probability. At most 3 parents.



- LDAG-based BIC overfits considerably (red).

Simulations: Probabilistic Model Accuracy

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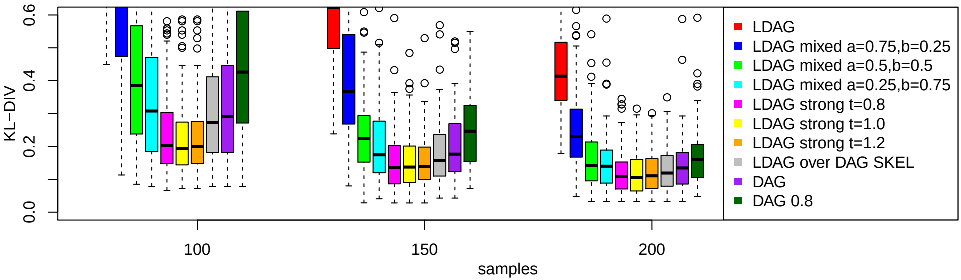

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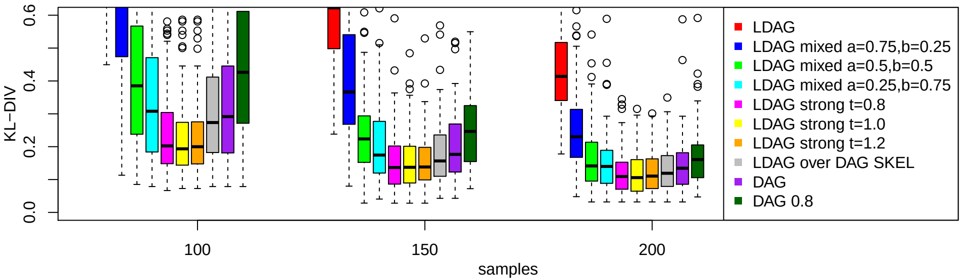
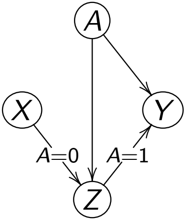


- LDAG-based BIC overfits considerably (red).
- With strong score pruning LDAG is better than a DAG (yellow vs. purple).
- With more samples DAGs catch up but still keep CSIs hidden.

Conclusion



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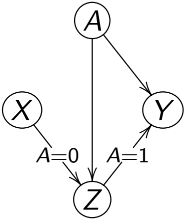

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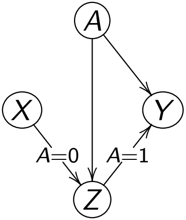

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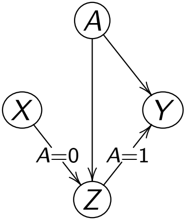

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  - A Branch and Bound for local score calculation.
  - Strong score pruning to avoid overfitting.
- CSIs are common and powerful but discovering them in sample data can be quite challenging!