Exact Constraint-based Causal Discovery

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DALI 2017, Tenerife
20.4.2017

Introduction

Score-based vs. Constraint-based Causal Discovery

INPUT: Data.

TASK: Find an equivalence class of causal graph structures that may have generated the data.

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- Maximize Bayesian marginal likelihood or BIC.
- Good Accuracy, limited model space.
- **Exact**: Find the globally optimal graph(s).

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Constraint-based Methods: [Pearl, Spirtes,...]

- Deduce the graph structure from independence test results.
- General of the model space: Latent confounders, Cycles.
- Scale up by making **greedy** decision $\Rightarrow$ poor accuracy.

Exact Constraint-based Causal Discovery [Hyttinen et al. '14]

INPUT: All weighted cond. (in)dependencies K among vars.

TASK: Find G that minimizes $\sum_{k \in K \,:\, G \not\models k} w(k)$.

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- Often accurate. [Hyttinen et al. '14, Magliacane et al. '16, Borboudakis et al. '16]
- Several options for getting weighted independence constraints. [Margaritis et al. '09, Claassen et al. '12, Triantafillou et al. '15, Magliacane et al. '16]

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- Related Work: [Magliacane et al. '16, Claassen et al. '12, Triantafillou et al. '15]

Implicit Hitting Set Approach

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SAT-solver:

- Is there a graph that satisfies constraints K?
- CNF-encoding of d-separation/connection: [Hyttinen et al. '14]

$$X \not\perp\!\!\!\perp Y|C \quad \Leftrightarrow \quad X \rightarrow Y \quad \vee \quad Y \rightarrow X \quad \vee \quad X \leftrightarrow Y \quad \vee \quad \ldots$$

- Returns SAT and a solution, or UNSAT and a **core**.
- **Core** is a subset of constraints not simultaneously satisfiable.

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Integer Programming -solver:

- Finds a hitting set H that minimizes $\sum_{k \in H} w(k)$,
  s.t. $H \cap c \neq \emptyset$ for all cores c.

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Implementation:

- LMHS by [Saikko et al. '16] uses MiniSAT (backtracking depth first search) and CPLEX (simplex-based branch-and-cut).

Implicit Hitting Set Approach on a Toy Example

$Q \not\perp\!\!\!\perp X$	$Y \not\perp\!\!\!\perp Z \mid X, W$	$X \not\perp\!\!\!\perp Z \mid Y, W$	$Q \perp\!\!\!\perp Z$
$Y \not\perp\!\!\!\perp Z \mid W$	$X \perp\!\!\!\perp Y \mid Z, W$	$X \perp\!\!\!\perp Y \mid W$	$X \not\perp\!\!\!\perp Z \mid W$
$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
$W \not\perp\!\!\!\perp Z$	$Q \perp\!\!\!\perp W$	$Y \perp\!\!\!\perp Q \mid W$	$Q \perp\!\!\!\perp Z \mid W$

constraints

weights

SAT solver

IP solver

Step 1 $L = 0, U = 16$

Implicit Hitting Set Approach on a Toy Example

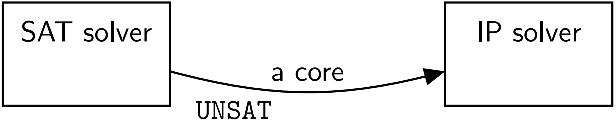
$Q \not\perp\!\!\!\perp X$	$Y \not\perp\!\!\!\perp Z \mid X, W$	$X \not\perp\!\!\!\perp Z \mid Y, W$	$Q \perp\!\!\!\perp Z$
$Y \not\perp\!\!\!\perp Z \mid W$	$X \perp\!\!\!\perp Y \mid Z, W$	$X \perp\!\!\!\perp Y \mid W$	$X \not\perp\!\!\!\perp Z \mid W$
$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
$W \not\perp\!\!\!\perp Z$	$Q \perp\!\!\!\perp W$	$Y \perp\!\!\!\perp Q \mid W$	$Q \perp\!\!\!\perp Z \mid W$

SAT solver

IP solver

Step 2 $L = 0, U = 16$

$Q \not\perp\!\!\!\perp X$	$Y \not\perp\!\!\!\perp Z \mid X, W$	$X \not\perp\!\!\!\perp Z \mid Y, W$	$Q \perp\!\!\!\perp Z$
$Y \not\perp\!\!\!\perp Z \mid W$	$X \perp\!\!\!\perp Y \mid Z, W$	$X \perp\!\!\!\perp Y \mid W$	$X \not\perp\!\!\!\perp Z \mid W$
$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
$W \not\perp\!\!\!\perp Z$	$Q \perp\!\!\!\perp W$	$Y \perp\!\!\!\perp Q \mid W$	$Q \perp\!\!\!\perp Z \mid W$



Step 3 $L = 0, U = 16$

Implicit Hitting Set Approach on a Toy Example

$Q \not\perp\!\!\!\perp X$	$Y \not\perp\!\!\!\perp Z \mid X, W$	$X \not\perp\!\!\!\perp Z \mid Y, W$	$Q \perp\!\!\!\perp Z$
$Y \not\perp\!\!\!\perp Z \mid W$	$X \perp\!\!\!\perp Y \mid Z, W$	$X \perp\!\!\!\perp Y \mid W$	$X \not\perp\!\!\!\perp Z \mid W$
$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
$W \not\perp\!\!\!\perp Z$	$Q \perp\!\!\!\perp W$	$Y \perp\!\!\!\perp Q \mid W$	$Q \perp\!\!\!\perp Z \mid W$

SAT solver

IP solver

Step 4 $L = 0, U = 16$

$Q \not\perp\!\!\!\perp X$	$Y \not\perp\!\!\!\perp Z \mid X, W$	$X \not\perp\!\!\!\perp Z \mid Y, W$	$Q \perp\!\!\!\perp Z$
$\boxed{Y \not\perp\!\!\!\perp Z \mid W}$	$X \perp\!\!\!\perp Y \mid Z, W$	$X \perp\!\!\!\perp Y \mid W$	$X \not\perp\!\!\!\perp Z \mid W$
$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
$W \not\perp\!\!\!\perp Z$	$Q \perp\!\!\!\perp W$	$Y \perp\!\!\!\perp Q \mid W$	$Q \perp\!\!\!\perp Z \mid W$

$$\boxed{\text{SAT solver}} \xleftarrow{\text{hitting set } H} \boxed{\text{IP solver}}$$

Step 5 $L = 1, U = 16$

$Q \not\perp\!\!\!\perp X$	$Y \not\perp\!\!\!\perp Z \mid X, W$	$X \not\perp\!\!\!\perp Z \mid Y, W$	$Q \perp\!\!\!\perp Z$
	$X \perp\!\!\!\perp Y \mid Z, W$	$X \perp\!\!\!\perp Y \mid W$	$X \not\perp\!\!\!\perp Z \mid W$
$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
$W \not\perp\!\!\!\perp Z$	$Q \perp\!\!\!\perp W$	$Y \perp\!\!\!\perp Q \mid W$	$Q \perp\!\!\!\perp Z \mid W$

SAT solver

IP solver

Step 6 $L = 1, U = 16$

Implicit Hitting Set Approach on a Toy Example

$Q \not\perp\!\!\!\perp X$	$Y \not\perp\!\!\!\perp Z \mid X, W$	$X \not\perp\!\!\!\perp Z \mid Y, W$	$Q \perp\!\!\!\perp Z$
	$X \perp\!\!\!\perp Y \mid Z, W$	$X \perp\!\!\!\perp Y \mid W$	$X \not\perp\!\!\!\perp Z \mid W$
$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
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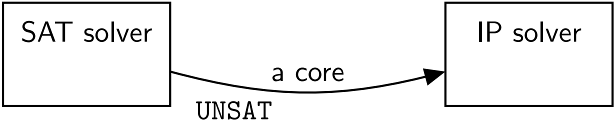

Step 7 $L = 1, U = 16$

Implicit Hitting Set Approach on a Toy Example

$Q \not\perp\!\!\!\perp X$	$Y \not\perp\!\!\!\perp Z \mid X, W$	$X \not\perp\!\!\!\perp Z \mid Y, W$	$Q \perp\!\!\!\perp Z$
$Y \not\perp\!\!\!\perp Z \mid W$	$X \perp\!\!\!\perp Y \mid Z, W$	$X \perp\!\!\!\perp Y \mid W$	$X \not\perp\!\!\!\perp Z \mid W$
$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
$W \not\perp\!\!\!\perp Z$	$Q \perp\!\!\!\perp W$	$Y \perp\!\!\!\perp Q \mid W$	$Q \perp\!\!\!\perp Z \mid W$

SAT solver

IP solver

Step 8 $L = 1, U = 16$

$Q \not\perp\!\!\!\perp X$	$Y \not\perp\!\!\!\perp Z \mid X, W$	$X \not\perp\!\!\!\perp Z \mid Y, W$	$Q \perp\!\!\!\perp Z$
$Y \not\perp\!\!\!\perp Z \mid W$	$X \perp\!\!\!\perp Y \mid Z, W$	$\boxed{X \perp\!\!\!\perp Y \mid W}$	$X \not\perp\!\!\!\perp Z \mid W$
$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
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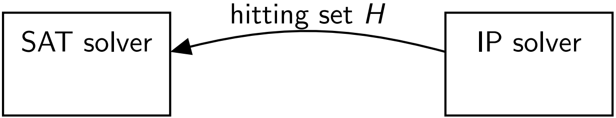

Step 9 $L = 1, U = 16$

Implicit Hitting Set Approach on a Toy Example

$Q \not\perp\!\!\!\perp X$	$Y \not\perp\!\!\!\perp Z \mid X, W$	$X \not\perp\!\!\!\perp Z \mid Y, W$	$Q \perp\!\!\!\perp Z$
$Y \not\perp\!\!\!\perp Z \mid W$	$X \perp\!\!\!\perp Y \mid Z, W$		$X \not\perp\!\!\!\perp Z \mid W$
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$W \not\perp\!\!\!\perp Z$	$Q \perp\!\!\!\perp W$	$Y \perp\!\!\!\perp Q \mid W$	$Q \perp\!\!\!\perp Z \mid W$

SAT solver

IP solver

Step 10 $L = 1, U = 16$

Implicit Hitting Set Approach on a Toy Example

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$Y \not\perp\!\!\!\perp Z \mid W$	$X \perp\!\!\!\perp Y \mid Z, W$		$X \not\perp\!\!\!\perp Z \mid W$
$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
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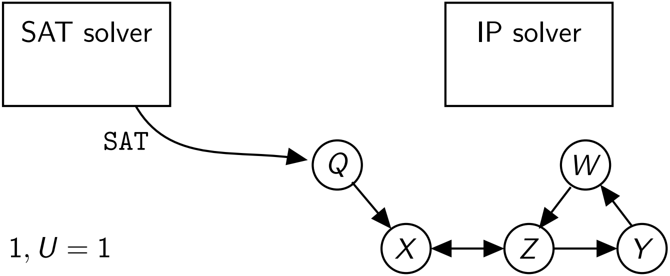

Step 11 $L = 1, U = 1$

Implicit Hitting Set Approach on a Toy Example

$Q \not\perp\!\!\!\perp X$	$Y \not\perp\!\!\!\perp Z \mid X, W$	$X \not\perp\!\!\!\perp Z \mid Y, W$	$Q \perp\!\!\!\perp Z$
$Y \not\perp\!\!\!\perp Z \mid W$	$X \perp\!\!\!\perp Y \mid Z, W$	$\boxed{X \perp\!\!\!\perp Y \mid W}$	$X \not\perp\!\!\!\perp Z \mid W$
$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
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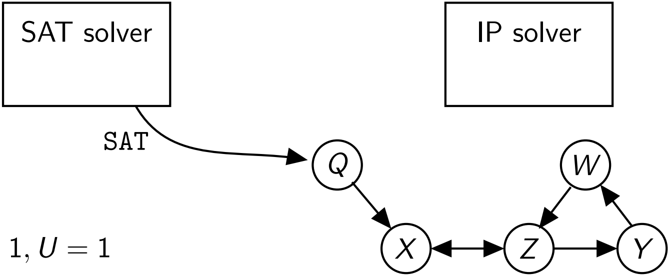

Step 12 $L = 1, U = 1$

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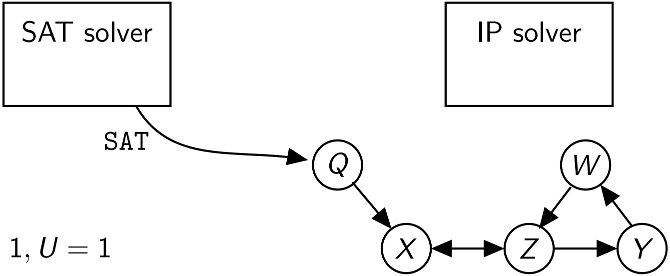

Step 13 $L = 1, U = 1$

Dseptor: Utilizing 3 Domain Specific Techniques

Technique 1: Domain Specific Cores (1)

Each extracted core call requires potentially many (NP-)SAT-solver calls. How to avoid some of these?

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- Instead, we can find general patterns of cores:
  - **Observe** which cores the solver uses, e.g.

$$\{X \perp\!\!\!\perp Z; \quad X \not\perp\!\!\!\perp Z|Y; \quad X \perp\!\!\!\perp Y\}$$

  - **Generalize** a core to a pattern, e.g.

$$\{X \perp\!\!\!\perp Z|C; \quad X \not\perp\!\!\!\perp Z|Y, C; \quad X \perp\!\!\!\perp Y|C\}, \quad \forall X, Y, Z, C$$

  - **Prove** that the pattern generally gives a (minimal) core.

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- We identified 7 cores patterns among 3-4 nodes and 3-5 constraints, each including independencies and dependencies.

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  - **Prove** that the pattern generally gives a (minimal) core.
- We identified 7 cores patterns among 3-4 nodes and 3-5 constraints, each including independencies and dependencies.

Benefit: Thousands of small cores can be found in a fraction of the total solving time.

Technique 1: Domain Specific Cores (2)

For all instantiations of nodes X, Y, Z, W and set C:

(i) $\{X \perp\!\!\!\perp Z|C; \quad X \perp\!\!\!\perp Y|C; \quad X \not\perp\!\!\!\perp Z|Y, C\}$

(ii) $\{X \not\perp\!\!\!\perp Z|C; \quad Y \not\perp\!\!\!\perp Z|C; \quad X \perp\!\!\!\perp Y|C; \quad X \perp\!\!\!\perp Y|Z, C\}$

(iii) $\{X \not\perp\!\!\!\perp Z|Y, C; \quad Y \not\perp\!\!\!\perp Z|X, C; \quad X \perp\!\!\!\perp Y|C; \quad X \perp\!\!\!\perp Y|Z, C\}$

(iv) $\{Y \not\perp\!\!\!\perp Z|C; \quad X \not\perp\!\!\!\perp Z|C; \quad Z \perp\!\!\!\perp W|X, Y, C;$
$X \perp\!\!\!\perp Y|Z, C; \quad X \perp\!\!\!\perp Y|W, C\}$

(v) $\{Y \not\perp\!\!\!\perp Z|C; \quad X \not\perp\!\!\!\perp Z|C; \quad Z \perp\!\!\!\perp W|Y, C;$
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(vi) $\{X \not\perp\!\!\!\perp Y|Z, C; \quad Y \not\perp\!\!\!\perp Z|X, W, C; \quad W \not\perp\!\!\!\perp Y|Z, C;$
$W \perp\!\!\!\perp X|Y, Z, C; \quad X \perp\!\!\!\perp Z|W, C\}$

(vii) $\{X \not\perp\!\!\!\perp Y|Z, C; \quad Y \not\perp\!\!\!\perp Z|X, W, C; \quad W \not\perp\!\!\!\perp Y|C;$
$W \perp\!\!\!\perp X|Y, C; \quad X \perp\!\!\!\perp Z|W, C\}$

are minimal cores.

Technique 2: Incremental Core Extraction

Plain IHS-approach tends to produce large cores. How find diverse and disjoint cores for exact causal discovery?

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$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
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$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
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- Instead, we can input constraints one by one, and check satisfiability. [See Triantafillou et al. '15]
- Which order?

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$W \not\perp\!\!\!\perp Z$	$Q \perp\!\!\!\perp W$	$Y \perp\!\!\!\perp Q \mid W$	$Q \perp\!\!\!\perp Z \mid W$

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- Which order? — random order (currently).

Technique 2: Incremental Core Extraction

Plain IHS-approach tends to produce large cores. How find diverse and disjoint cores for exact causal discovery?

$Q \not\perp\!\!\!\perp X$	$Y \not\perp\!\!\!\perp Z \mid X, W$	$X \not\perp\!\!\!\perp Z \mid Y, W$	$Q \perp\!\!\!\perp Z$
$\boxed{Y \not\perp\!\!\!\perp Z \mid W}$	$X \perp\!\!\!\perp Y \mid Z, W$	$X \perp\!\!\!\perp Y \mid W$	$X \not\perp\!\!\!\perp Z \mid W$
$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
$W \not\perp\!\!\!\perp Z$	$Q \perp\!\!\!\perp W$	$Y \perp\!\!\!\perp Q \mid W$	$Q \perp\!\!\!\perp Z \mid W$

- Plain IHS-approach enforces all constraints, except H.
- Instead, we can input constraints one by one, and check satisfiability. [See Triantafillou et al. '15]
- Which order? — random order (currently).

Benefits: Smaller diverse cores, good upper bounds.

Technique 3: Bounds-based Constraint Hardening

How can we exploit sparseness without losing exactness?

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$X \not\perp\!\!\!\perp W$	$X \not\perp\!\!\!\perp W \mid Z$	$X \not\perp\!\!\!\perp Y \mid W, Q$	$Q \not\perp\!\!\!\perp Y \mid X$
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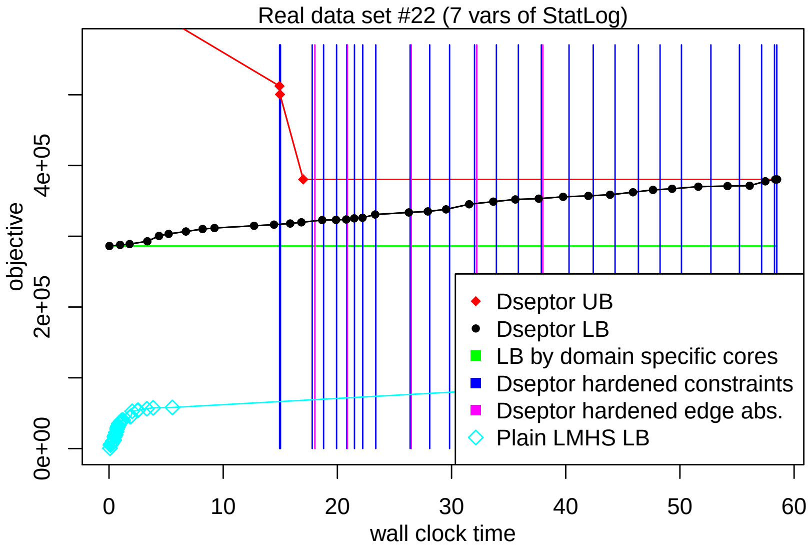
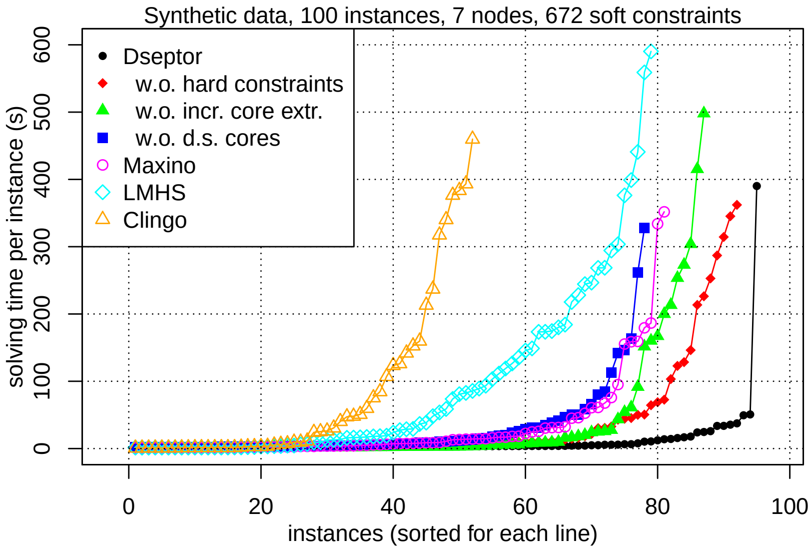
Benefits: Less soft constraints, SAT-instances are tighter.

Experiments

Example Run of Dseptor



Running Time Performance (1)



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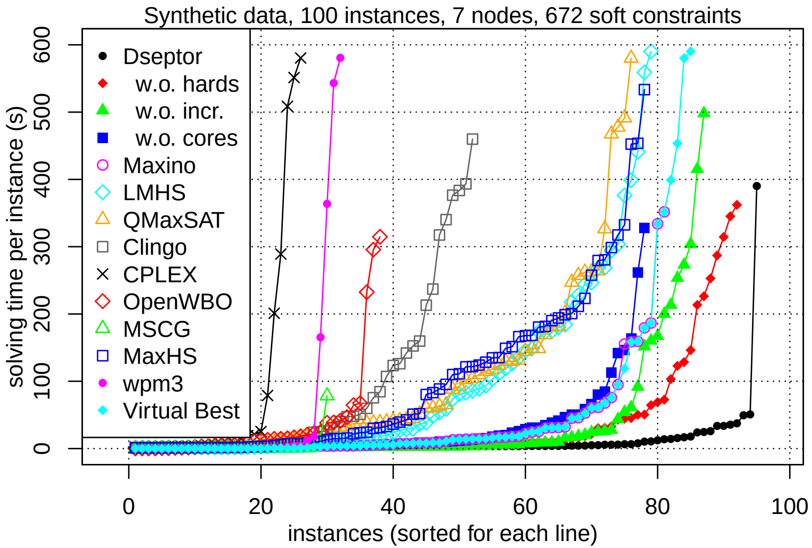
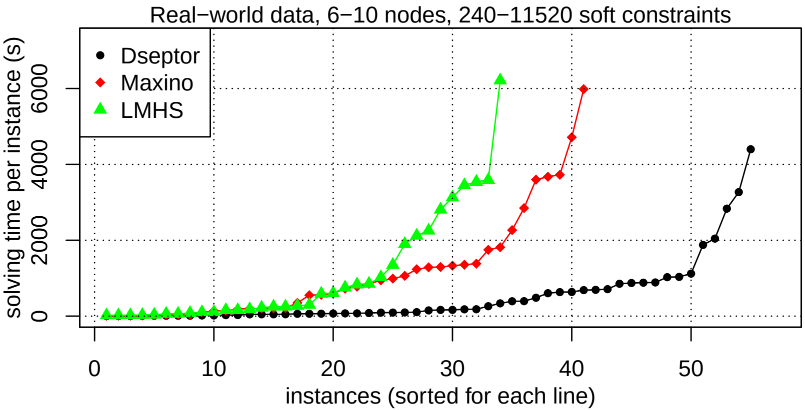


Running Time Performance (2)



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- A new approach for solving the optimization problem
- Exploiting a general MaxSAT solver and
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  2. Incremental core extraction
  3. Bounds-based constraint hardening
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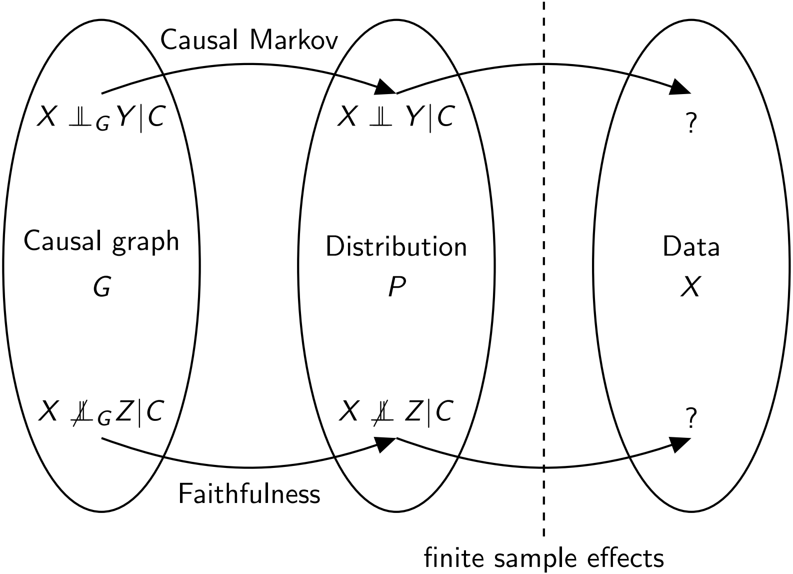
Thanks!


Causal Markov
$X \perp\!\!\!\perp_G Y|C$
$X \perp\!\!\!\perp Y|C$
?
Causal graph
G
Distribution
P
Data
X
$X \not\!\perp\!\!\!\perp_G Z|C$
$X \not\!\perp\!\!\!\perp Z|C$
?
Faithfulness
finite sample effects