A Core-Guided Approach to Learning Optimal Causal Graphs
Paper Supplement

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A Further Simulations

Figure 1 here gives a similar solver comparison to that of Figure 4 in the actual paper, here under a 7200-second per-instance time limit.

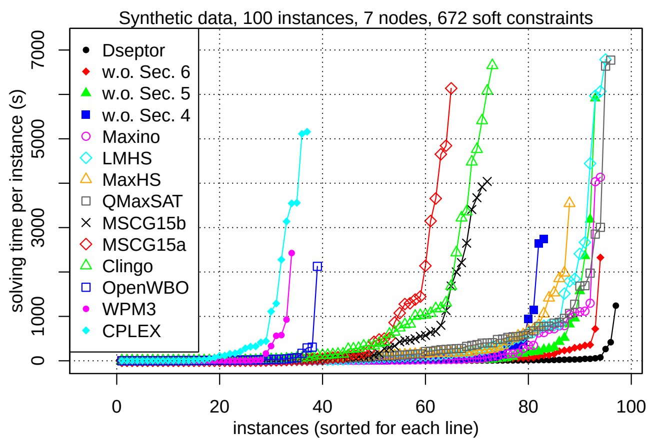

Figure 1: Solver comparison under a 7200-second per-instance time limit.

Figure 2 shows an example Dseptor run. The lower bound of plain LMHS (cyan) increases quite slowly. The domain specific cores boost the initial lower bound of Dseptor (black) already to a much higher level. Afterwards the lower bound (black) increases steadily. The upper bound of Dseptor (red) corresponding to objective values of the found solutions, reaches the optimum before 20 seconds: the optimal solution is found quite early, indicating good anytime performance here. The vertical lines (magenta, blue) show when soft constraints and edge absences are fixed using bounds based constraint hardening. The solution is proven optimal within 60 seconds here.

B Proof of Theorem 1

Here we give proofs of soundness of the problem-specific core patterns presented in Table 1 in the actual paper. We also give proofs of *minimality* of the patterns, i.e., that for all subsets of the constraints, there are causal graphs that satisfy them. Throughout we assume faithfulness, that is,

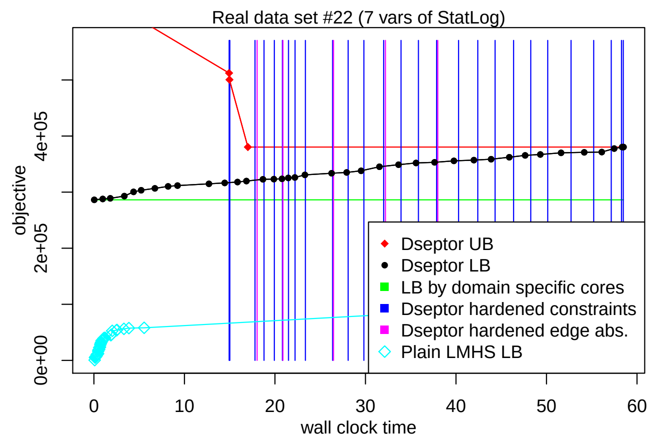

Figure 2: An example run of Dseptor. See text for details.

a d-connecting walk implies dependence. We use the d-separation definition given in the actual paper (allowing for repeated nodes and edges in a walk).

B.1 Core 1

$$\text{(i) } X \perp\!\!\!\perp Z|S, \quad \text{(ii) } X \perp\!\!\!\perp Y|S, \quad \text{(iii) } X \not\perp\!\!\!\perp Z|Y,S$$

Soundness Since there is no walk from X to Z conditional on S, and there is one conditional on S, Y, the latter d-connecting walks must be of the form $X \cdots \rightarrow Y \leftarrow \cdots Z$. Let us consider a shortest of these. The first sub-walk from X to Y violates (ii). Node Z cannot appear in this walk since we took a shortest walk.

Minimality When $S = \emptyset$, all subsets can be satisfied.

without (i):	$Y \quad X \rightarrow Z$
without (ii):	$X \rightarrow Y \leftarrow Z$
without (iii):	$X \quad Y \quad Z$

B.2 Core 2

$$\text{(i) } X \not\perp\!\!\!\perp Z|S, \quad \text{(ii) } Y \not\perp\!\!\!\perp Z|S,$$
$$\text{(iii) } X \perp\!\!\!\perp Y|S, \quad \text{(iv) } X \perp\!\!\!\perp Y|Z,S$$

Soundness By (i) there is a shortest d-connecting walk from X to Z, and by (ii) a shortest d-connecting walk from Y to Z. Neither walk can have Z in between since these are shortest walks. Now the combination would create a d-connecting walk from X to Y, violating (iii), unless both walks have arrows into Z. But then there is a walk from X to Y additionally conditioning on Z, which violates (iv).

Minimality When $S = \emptyset$, all subsets can be satisfied.

without (i):	$X \quad Y \to Z$
without (ii):	$X \to Z \quad Y$
without (iii):	$X \leftarrow Z \to Y$
without (iv):	$X \to Z \leftarrow Y$

B.3 Core 3

$$\text{(i) } X \not\perp\!\!\!\perp Z|Y,S, \quad \text{(ii) } Y \not\perp\!\!\!\perp Z|X,S,$$
$$\text{(iii) } X \perp\!\!\!\perp Y|S, \quad \text{(iv) } X \perp\!\!\!\perp Y|Z,S$$

Soundness This core is a slight alteration of Core 2. By (i), there is a shortest walk from X to Z. This cannot go through Y due to (iii). By (ii) there must be a shortest walk from Y to Z, it cannot go through X again due to (iii). The combination of the walks is d-connecting either when conditioning or not conditioning on Z.

Minimality

without (i):	$X \quad Z \leftarrow Y$
without (ii):	$X \leftarrow Z \quad Y$
without (iii):	$X \leftarrow Z \to Y$
without (iv):	$X \to Z \leftarrow Y$

B.4 Core 4

$$\text{(i) } Y \not\perp\!\!\!\perp Z|S, \quad \text{(ii) } X \not\perp\!\!\!\perp Z|S,$$
$$\text{(iii) } Z \perp\!\!\!\perp W|X,Y,S, \ \text{(iv) } X \perp\!\!\!\perp Y|Z,S, \ \text{(v) } X \perp\!\!\!\perp Y|W,S$$

Soundness Due to (i) there is a shortest d-connecting walk from Y to Z and due to (ii) there is a shortest d-connecting walk from Z to X. Due to (iv) and the fact that the walks are shortest walks, the walks do not go through X, Y or Z. Due to (iv), at least one of the walks must be out of Z. Without sacrificing generality, assume it is the Y to Z walk (note that X and Y can be switched in the core definition). Thus we have $Y \cdots \leftarrow Z \cdots X$. Due to (v), conditioning on W should intercept this connection, hence W should be in between as a non-collider. However, then there would be a d-connecting walk between W and Z, violating (iii).

Minimality When $S = \emptyset$, all subsets can be satisfied.

without (i):	$X \leftarrow Z \quad Y \quad W$
without (ii):	$X \quad Z \to Y \quad W$
without (iii):	$X \leftarrow Z \to W \to Y$
without (iv):	$X \to Z \leftarrow Y \quad W$
without (v):	$X \leftarrow Z \to Y \quad W$

B.5 Core 5

$$\text{(i) } Y \not\perp\!\!\!\perp Z|S, \quad \text{(ii) } X \not\perp\!\!\!\perp Z|S,$$
$$\text{(iii) } Z \perp\!\!\!\perp W|Y,S, \quad \text{(iv) } X \perp\!\!\!\perp Y|Z,S, \quad \text{(v) } X \perp\!\!\!\perp Y|W,S$$

Soundness This core differs from Core 4 just by not conditioning on X in (iii). Due to (i) there is a shortest d-connecting walk from Y to Z and due to (ii) there is a shortest d-connecting walk from Z to X. Due to (iv) and the fact that the walks are shortest the walks, the walks do not go through X, Y or Z. Due to (iv), one of the walks must be out of Z. Due to (v), conditioning on W should intercept this connection, hence W should be in between as non-collider. However, then there would be a d-connecting walk between W and Z, violating (iii) (remember that X and Y cannot appear in between).

Minimality When $S = \emptyset$, all subsets can be satisfied.

without (i):	$X \leftarrow Z \quad Y \quad W$
without (ii):	$X \quad Z \to Y \quad W$
without (iii):	$X \leftarrow Z \to W \to Y$
without (iv):	$X \to Z \leftarrow Y \quad W$
without (v):	$X \leftarrow Z \to Y \quad W$

B.6 Core 6

$$\text{(i) } X \not\perp\!\!\!\perp Y|Z,S \quad \text{(ii) } Y \not\perp\!\!\!\perp Z|X,W,S, \quad \text{(iii) } W \not\perp\!\!\!\perp Y|Z,S,$$
$$\text{(iv) } W \perp\!\!\!\perp X|Y,Z,S, \quad \text{(v) } X \perp\!\!\!\perp Z|W,S$$

Soundness Consider a shortest d-connecting walk between Y and X given Z, S satisfying (i). Since it is a shortest walk, it does not go through Y or X. The walk does not go through W, as otherwise there would be a walk from X to first W d-connecting given Y, Z, S, violating (iv). In addition, the walk does not go through Z, as otherwise there would be a walk from X to first Z d-connecting given W, S, violating (v). Let us denote this walk with $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$.

Consider a shortest d-connecting walk between Y and Z given X, W, S, satisfying (ii). Since it is a shortest walk, it does not go through Y or Z. The walk does not go through X, as otherwise there would be a walk from Z to first X d-connecting given W, S, violating (v). Let us denote this walk with $P^{\{Y,Z,X\}}_{Y \not\perp\!\!\!\perp Z|X,W,S}$.

Consider a shortest d-connecting walk between Y and W given Z, S, satisfying (iii). Since it is a shortest walk, it does not go through Y or W. The walk does not go through X, as otherwise there would be a walk from W to first X d-connecting given Y, Z, S, violating (iv). Let us denote this walk with $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|Z,S}$.

Concatenating $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$ and $P^{\{Y,Z,X\}}_{Y \not\perp\!\!\!\perp Z|X,W,S}$ at Y would d-connect X and Z given W, S, violating (v), unless both are into Y. Thus $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$ and $P^{\{Y,Z,X\}}_{Y \not\perp\!\!\!\perp Z|X,W,S}$ are into Y. Concatenating $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$ and $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|Z,S}$ at Y would d-connect

X and W given Y, Z, S, violating (iv), unless $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|Z,S}$ is out of Y. Thus $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|Z,S}$ is out of Y.

Then, let Q be the collider node nearest to Y on $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|Z,S}$.

- If there is no Q, $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|Z,S}$ must be into W as it is out of Y, and $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|Z,S}$ cannot go through Z. From X, we can take $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$ to Y, $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|Z,S}$ to W, $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|Z,S}$ back to Y and $P^{\{Y,Z,X\}}_{Y \not\perp\!\!\!\perp Z|X,W,S}$ to Z to form a walk that is d-connecting given W, S, violating (v).
- If $Q = Z$, then from X we can take $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$ to Y and the subwalk of $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|Z,S}$ from Y to Q to form a walk that is d-connecting given W, S violating (v).
- Otherwise $Q \in S$ since $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|Z,S}$ is d-connecting. From X, we can take $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$ to Y, a subwalk of $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|Z,S}$ to Q (this is not through Z as Q is the first collider) and back to Y, and finally $P^{\{Y,Z,X\}}_{Y \not\perp\!\!\!\perp Z|X,W,S}$ to Z to form a walk that is d-connecting given W, S, violating (v).

When assuming that all constraints hold, we were able to derive contradictions in all cases. Thus the constraints form a core.

Minimality When $S = \emptyset$, all subsets can be satisfied.

$$\begin{array}{rl}
\text{without (i):} & X \quad Z \leftarrow Y \rightarrow W \\
\text{without (ii):} & Z \quad X \leftarrow Y \rightarrow W \\
\text{without (iii):} & W \quad X \rightarrow Y \leftarrow Z \\
\text{without (iv):} & X \rightarrow Y \leftarrow Z, W \rightarrow Y \\
\text{without (v):} & Z \leftarrow Y, X \leftarrow Y \rightarrow W
\end{array}$$

B.7 Core 7

(i) $X \not\perp\!\!\!\perp Y|Z, S$, (ii) $Y \not\perp\!\!\!\perp Z|X, W, S$, (iii) $W \not\perp\!\!\!\perp Y|S$, (iv) $W \perp\!\!\!\perp X|Y, S$, (v) $X \perp\!\!\!\perp Z|W, S$

Soundness This is a slight alteration of Core 6, without having Z in the conditioning sets for (iii) and (iv). Consider a shortest d-connecting walk between Y and X given Z, S satisfying (i). Since it is a shortest walk, it does not go through Y or X. The walk does not go through W or Z, as otherwise there would be a walk from X to first W or Z violating either (iv) or (v). Let us denote this walk with $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$.

Consider a shortest d-connecting walk between Y and Z given X, W, S, satisfying (ii). Since it is a shortest walk, it does not go through Y or Z. The walk does not go through X, as otherwise there would be a walk from Z to first X d-connecting given W, S, violating (v). Let us denote this walk with $P^{\{Y,Z,X\}}_{Y \not\perp\!\!\!\perp Z|X,W,S}$.

Consider a shortest d-connecting walk between Y and W given S, satisfying (iii). Since it is a shortest walk, it does not go through Y or W. The walk does not go through X, as otherwise there would be a walk from W to first X d-connecting given Y, S, violating (iv). Let us denote this walk with $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$.

Concatenating $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$ and $P^{\{Y,Z,X\}}_{Y \not\perp\!\!\!\perp Z|X,W,S}$ at Y would d-connect X and Z given W, S, violating (v), unless both are into Y. Thus $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$ and $P^{\{Y,Z,X\}}_{Y \not\perp\!\!\!\perp Z|X,W,S}$ are into Y. Concatenating $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$ and $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$ at Y would d-connect X and W given Y, S, violating (iv), unless $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$ is out of Y. Thus $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$ is out of Y.

Then, let Q be the collider node nearest to Y on $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$ or node Z, whichever is nearest to Y on $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$.

- If there is no Q, $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$ must be into W as it is out of Y, and $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$ cannot go through Z. From X, we can take $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$ to Y, $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$ to W, $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$ back to Y and $P^{\{Y,Z,X\}}_{Y \not\perp\!\!\!\perp Z|X,W,S}$ to Z to form a walk that is d-connecting given W, S, violating (v).
- If $Q = Z$, from X we can take $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$ to Y and the subwalk of $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$ from Y to Q forming a d-connecting walk given W, S violating (v).
- Otherwise $Q \in S$ since $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$ is d-connecting. From X, we can take $P^{\{X,Y,Z,W\}}_{X \not\perp\!\!\!\perp Y|Z,S}$ to Y, a subwalk of $P^{\{W,Y,X\}}_{W \not\perp\!\!\!\perp Y|S}$ to Q and back to Y (this is not through Z), and finally $P^{\{Y,Z,X\}}_{Y \not\perp\!\!\!\perp Z|X,W,S}$ to Z to form a walk that is d-connecting given W, S, violating (v).

When assuming that all constraints hold, we were able to derive contradictions in all cases. Thus the constraints form a core.

Minimality When $S = \emptyset$, all subsets can be satisfied.

$$\begin{array}{rl}
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\text{without (ii):} & Z \quad X \leftarrow Y \rightarrow W \\
\text{without (iii):} & W \quad X \rightarrow Y \leftarrow Z \\
\text{without (iv):} & X \rightarrow Y \leftarrow Z, W \rightarrow Y \\
\text{without (v):} & Z \leftarrow Y, X \leftarrow Y \rightarrow W
\end{array}$$