



# Almost Optimal Universal Lower Bound for Learning Causal DAGs with Atomic Interventions

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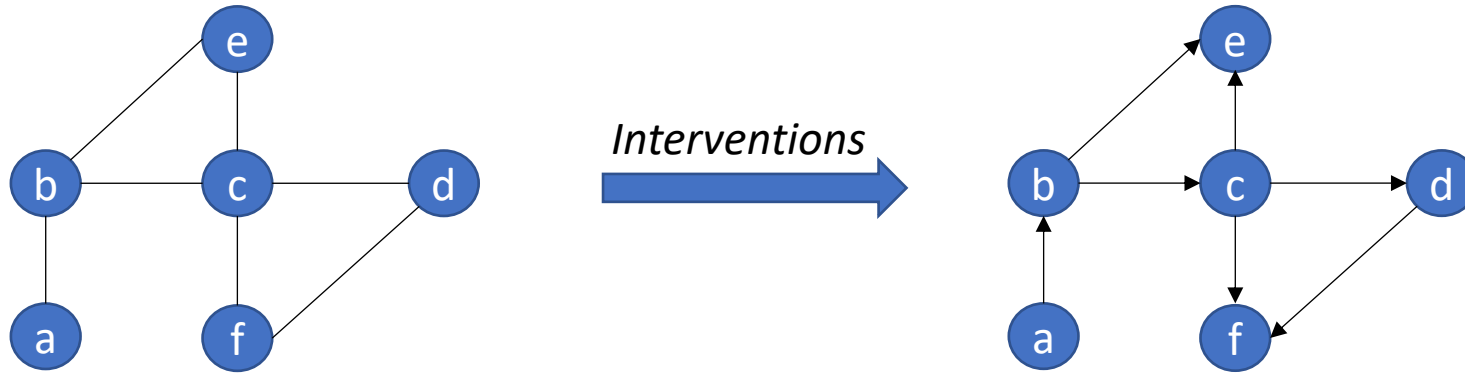


# Introduction

- Learning causal DAGs is an important problem in several fields including health science, molecular cell biology, and computational advertising.
- Using observational data, it is possible to learn a causal DAG only up to its Markov Equivalence Class (MEC).
- Interventions (or Experiments) are required to orient the remaining edges.
- An intervention on  $v$  completely randomizes the distribution of  $v$  and reveals at least the direction of all edges incident on  $v$ .

# Introduction

- Interventions are costly, and thus, a natural question is to find the *minimum number of interventions* required to learn all edges of a causal DAG.



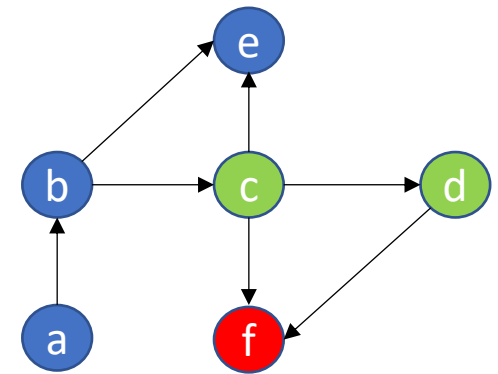
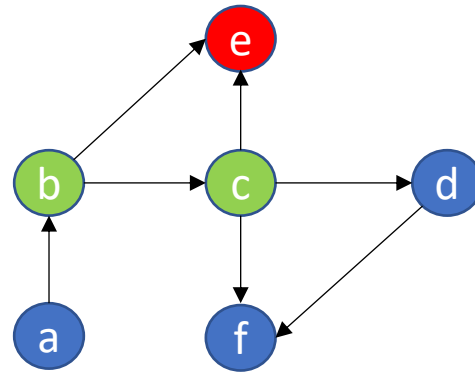
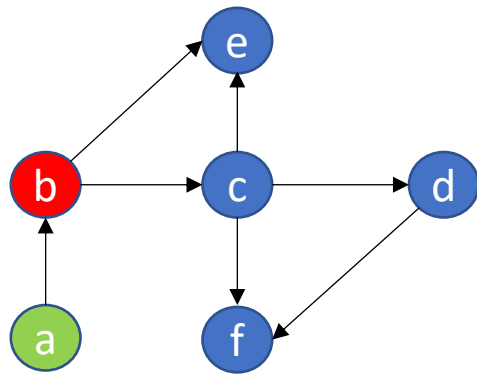
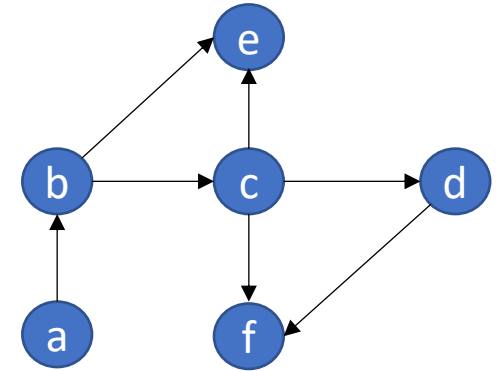
- A *v-structure* in a DAG is an induced subgraph of the form  $b \rightarrow a \leftarrow c$ .
- Lower and upper bounds on the number of interventions for learning DAGs without v-structures generalize to arbitrary DAGs (Hauser and Bühlmann, 2014).

# Universal Lower Bounds

- Squires et al. (2020) introduced the concept of universal lower bounds.
- A universal lower bound of  $L$  interventions for a MEC means that if a set of interventions  $I$  is of size less than  $L$ , then for any ground-truth DAG in the MEC,  $I$  will fail to fully orient the MEC.
- Universality properties:
  - The lower bound applies to all DAGs in the MEC.
  - The lower bound applies to every set of interventions regardless of the method by which the intervention set was obtained.
- We address the problem of obtaining *tight* universal lower bounds.

# Maximal-Clique-Sink Nodes

- Let  $D$  be a DAG without v-structures having  $n$  nodes.
- Let  $r$  denote the number of maximal cliques in  $D$ .
- The node with no outgoing edges in  $D[C]$  is called the *maximal-clique-sink* node corresponding to the maximal clique  $C$ .

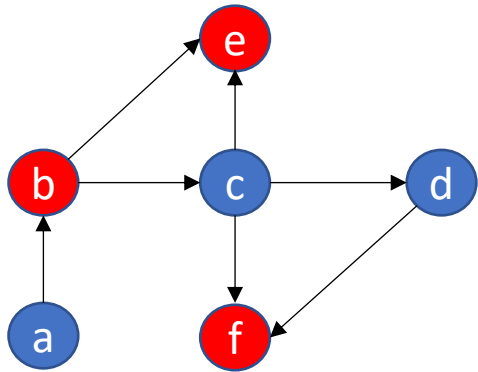


# Clique-Block Shared-Parents (CBSP) orderings

- Let  $\sigma$  be a topological ordering of  $D$  and let  $s_1, s_2, \dots, s_r$  be its maximal-clique-sink nodes indexed so that  $\sigma(s_i) < \sigma(s_j)$  when  $i < j$ .
- Let  $L_1(\sigma)$  be the set of nodes that occur before or at the same position as  $s_1$  in  $\sigma$ .
- For  $2 \leq i \leq r$ , define  $L_i(\sigma)$  to be the set of nodes that occur in  $\sigma$  before or at the same position as  $s_i$ , but strictly after  $s_{i-1}$ .
- $\sigma$  is said to be a CBSP ordering if it satisfies the following two properties:
  - (P1) *Clique block property*: For each  $i \in [r]$  the subgraph induced by  $L_i(\sigma)$  in  $D$  is a clique.
  - (P2) *Shared parents property*: If  $a$  and  $b$  are consecutive in  $\sigma$ , and also lie in the same  $L_i(\sigma)$  for some  $i \in [r]$ , then all parents of  $a$  are also parents of  $b$  in  $D$ .

# CBSP orderings: Example

- Consider the following topological orderings.



$$\sigma' = a b c d e f$$

$$\sigma = a b c d f e$$

$$\tau = a b c e d f$$

- Here,  $\sigma'$  does not satisfy P1 or P2,  $\sigma$  satisfies only P1,  $\tau$  satisfies both P1 and P2 and therefore,  $\tau$  is a CBSP ordering.

# Overview of our Results

- Lower bound: Let  $D$  be a DAG without v-structures. Then, any set of atomic interventions that learns all edges of  $D$  must be of size at least  $\left\lceil \frac{n-r}{2} \right\rceil$ .
- Upper bound: There exists an intervention set  $I$  of size  $n - r$  that can learn all edges of  $D$ , showing that our lower bound is tight up to a factor of 2.
- We show that  $n - r \geq \omega - 1$  in chordal graphs, proving that our lower bound is at least as good as the one by Squires et al. (2020).
- Through simulations and by constructing examples of graphs, we show that our lower bound is often significantly better.



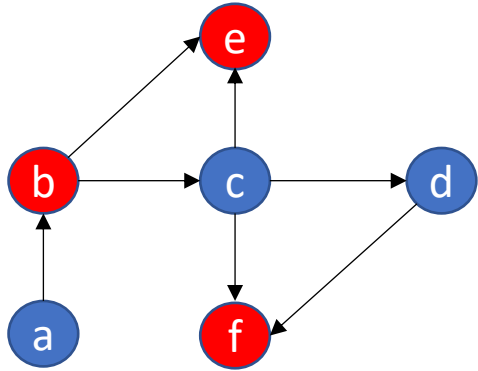
# Proof Sketch for our Lower Bound

- Step 1: Prove that any DAG without v-structures has a CBSP ordering.
- Step 2: Take a CBSP ordering  $\sigma$  of  $D$ . Let  $a, b$  be two consecutive nodes of  $\sigma$  and  $a, b \in L_i(\sigma)$  for some  $i \in [r]$ .
- Step 3: Show that if  $I$  is such that  $I \cap \{a, b\} = \emptyset$ , then  $I$  cannot orient the edge  $a - b$ .
- Step 4: Thus, if  $I$  learns all edges of  $D$  then,

$$\begin{aligned} |I| &\geq \sum_{i=1}^r \left\lceil \frac{|L_i(\sigma)| - 1}{2} \right\rceil \geq \left\lceil \sum_{i=1}^r \frac{|L_i(\sigma)| - 1}{2} \right\rceil \\ &= \left\lceil \frac{\sum_{i=1}^r |L_i(\sigma)|}{2} - \frac{r}{2} \right\rceil = \left\lceil \frac{n - r}{2} \right\rceil \end{aligned}$$

# Example

- Let  $D$  be the following DAG and  $\tau$  be a CBSP ordering of  $D$ .



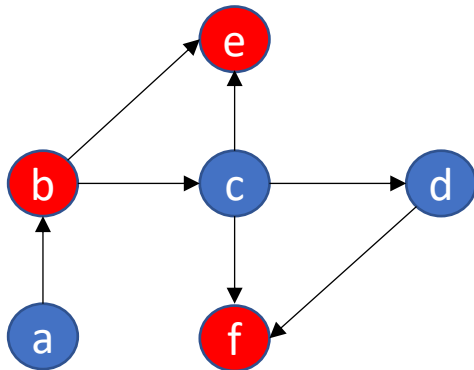
$$\tau = a b c e d f$$

- Let  $I$  be an intervention set that can learn all edges of  $D$ .

- $I$  must be of size at least  $\left\lceil \frac{|\{a,b\}|-1}{2} \right\rceil + \left\lceil \frac{|\{c,e\}|-1}{2} \right\rceil + \left\lceil \frac{|\{d,f\}|-1}{2} \right\rceil = 3$ .

# Tightness of Universal Lower Bound

- Let the set of maximal-clique-sink nodes of  $D$  be  $S = \{s_1, s_2, \dots, s_r\}$ .
- We can show that  $I^* = V \setminus S$  is a set of interventions that can orient the MEC of  $D$  if the underlying DAG was  $D$ .
- Note that,  $|I^*| = n - r$ , showing that our universal lower bound is tight up to a factor of 2.



$$I^* = \{a, c, d\}$$

$$\left\lceil \frac{n - r}{2} \right\rceil = 2$$

# References

- Hauser, A. and Bühlmann, P. (2014). Two Optimal Strategies for Active Learning of Causal Models from Interventional Data. *International Journal of Approximate Reasoning*, 55(4):926-939.
- Squires, C., Magliacane, S., Greenewald, K. H., Katz, D., Kocaoglu, M., and Shanmugam, K. (2020). Active Structure Learning of Causal DAGs via Directed Clique Trees. *Proceedings of 34th Annual Conference on Neural Information Processing Systems (NeurIPS 2020)*. [arXiv:2011.00641](https://arxiv.org/abs/2011.00641).

Thanks!