Verification and search algorithms for causal DAGs

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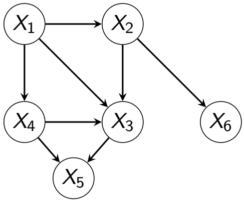
* Equal contribution

Motivation

Underlying data
generation process
(modelled as a DAG)

G^*



e.g. $X_4 = f_4(X_1, \varepsilon_4)$

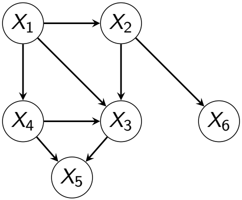
specific to node X_4

Observational data $\mathcal{D}$

	X_1	X_2	X_3	X_4	X_5	X_6
Sample 1	0.3	0.4	0.1	-0.5	0.2	-0.3
Sample 2	0.1	1.2	0.6	-0.2	-0.1	-0.4
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Motivation

G^*

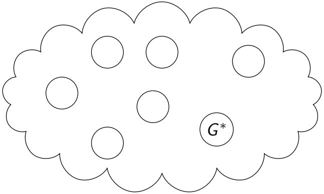


$\mathcal{D}$

	X_1	X_2	X_3	X_4	X_5	X_6
Sample 1	0.3	0.4	0.1	-0.5	0.2	-0.3
Sample 2	0.1	1.2	0.6	-0.2	-0.1	-0.4
⋮	⋮	⋮	⋮	⋮	⋮	⋮

Identify possible graphs
via conditional dependencies
(e.g. PC [SGSH00], GES [Chi02])

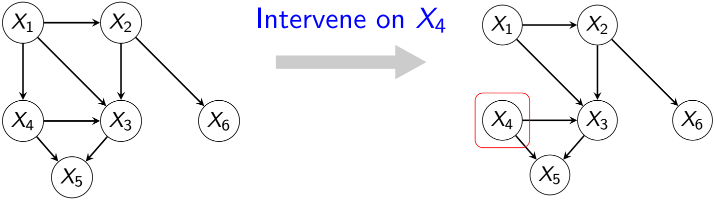
Equivalence
class of DAGs



Which is G^*?

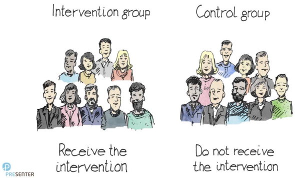
Two ways forward

1. Make model assumptions
   e.g. $X_4 = f_4(X_1, \varepsilon_4) = \alpha X_1 + \varepsilon_4$, where ε_4 is non-Gaussian
2. Perform interventions (Our focus)
   e.g. set $X_4 = 0.5$, then draw samples from the resulting intervened causal graph

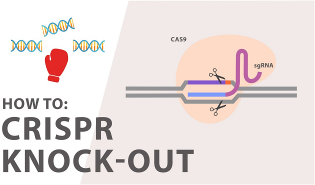


Interventions in real-life

- Randomized controlled trials



- Gene knockout experiments



Can be expensive to perform $\Rightarrow$ Minimize number of interventions!

Image credit: https://i.ytimg.com/vi/vyVyg4Bf2JY/maxresdefault.jpg
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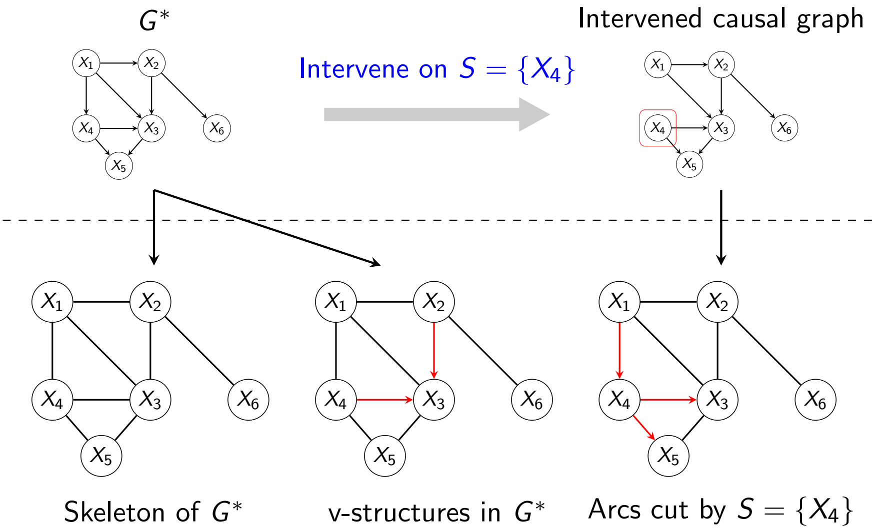
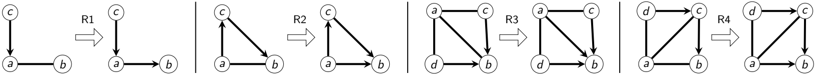
What can we learn?



Meek rules

Meek rules [Mee95]:
A set of 4 arc orientation rules that are *sound* and *complete*
(with respect to arc orientations with acyclic completion)



If $b \leftarrow a$,
then v-structure

If $b \leftarrow a$,
then cycle

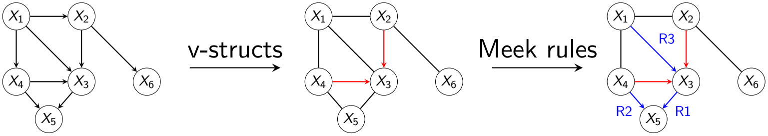
If $b \leftarrow a$, then the unoriented arcs would have been *oriented in the same way in all DAGs within the equivalence class* (via R2)
(See next slide on essential graphs)

Meek rules converge in polynomial time [WBL21, Algorithm 2].

Essential graph

We can represent an equivalence class with a partially oriented DAG called the *essential graph*

- Orient $u \to v$ if *all* DAGs agree on this direction
- An unoriented arc if there are two distinct DAGs G_1 and G_2 in the equivalence class orient it differently

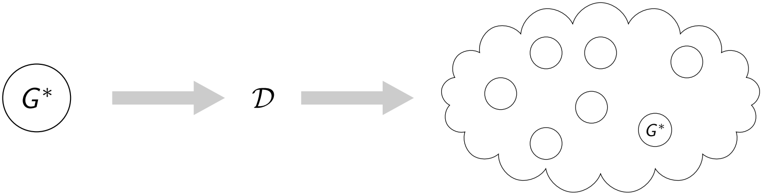


G^*

Essential graph of G^*

Problem setup

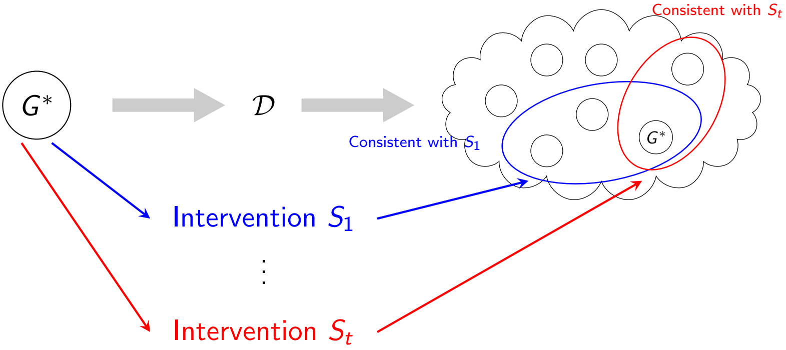
Identify G^*



Can be represented by
an essential graph
(partially oriented DAG)

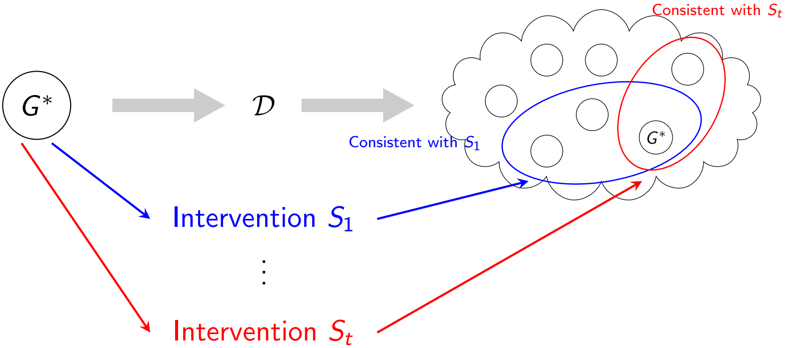
Problem setup (using interventions)

Identify G^* using as few interventions as possible (minimize t)



Problem setup (using **atomic** interventions)

Identify G^* using as few interventions as possible (minimize t)

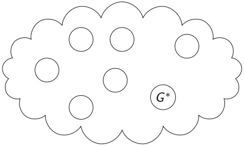


Simplifying assumption for this talk:
Each intervention is on a single node, i.e. $|S_1| = \ldots = |S_t| = 1$

Wait a minute... we have domain experts!

How do we even check if $G = G^*$?

~~Problem solved with zero interventions!~~



Experts can be wrong...

Do stuff with
discovered causal graph G

Image credit:
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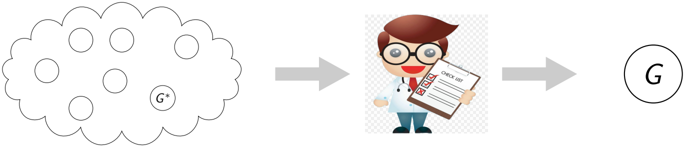
The verification problem

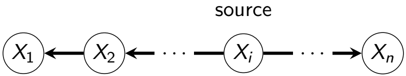
Goal: Determine if $G = G^*$
$\nu(G) =$ minimum number of interventions to answer $G \stackrel{?}{=} G^*$



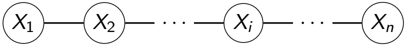
- We know: Intervening on v orients all arcs incident to v
- Trivial solution: Compute minimum vertex cover (MVC) on unoriented arcs! i.e. $\nu(G) \leq \texttt{MVC}(\text{unoriented})$

Verification: Problem with trivial solution

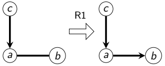
G



Essential graph



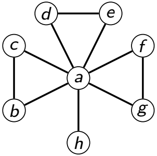
- Any line graph with a single source ($i \in \{1, \ldots, n\}$) has the same essential graph above of an unoriented line
- $\texttt{MVC}$(unoriented in essential graph) $= \left\lfloor \frac{n}{2} \right\rfloor$
- Optimal: Just 1 intervention needed!
  - Intervene on $X_i \Rightarrow$ Orient $X_{i-1} \leftarrow X_i$ and $X_i \rightarrow X_{i+1}$
  - Apply Meek R1 to orient the rest
  - If not fully oriented or $\exists$ disagreeing arcs, then $G \neq G^*$



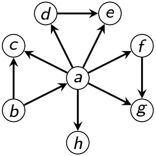
Verification: What was known

(Simplifying assumption: single undirected connected component)

1. [SMG+20]: $\nu(G) \geq \left\lfloor \frac{\omega(G)}{2} \right\rfloor$
2. [PSS22]: $\left\lceil \frac{n-r}{2} \right\rceil \leq \nu(G) \leq n - r$ (Note: 2-apx gap)



Essential graph

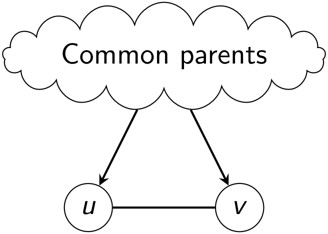


One possible DAG

- $n = 8$ nodes; $r = 4$ maximal cliques; largest clique $\omega(G) = 3$
- [SMG+20]: $\nu(G) \geq 1$; [PSS22]: $2 \leq \nu(G) \leq 4$
- Can we do better?

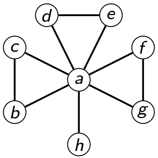
Verification: A complete characterization via covered edges

- Meek rules $\Rightarrow$ Outperform `MVC`(unoriented)
- Surprisingly, enough to compute `MVC` on a *subset of edges*
- Covered edges [Chi95]:
  $u \sim v$ is covered edge $\iff \mathrm{Pa}(u) \setminus \{v\} = \mathrm{Pa}(v) \setminus \{u\}$

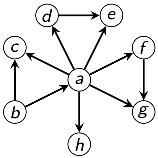


Claim: Necessary and sufficient to intervene on `MVC`(covered)
Proof: Simple (but subtle) using the notion of covered edges

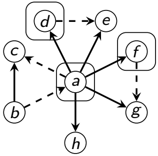
Verification: Comparing to prior work



Essential graph



DAG

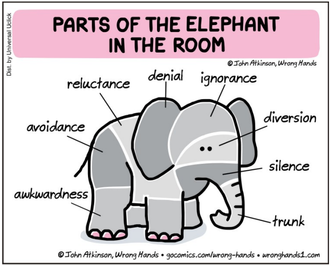


Covered edges

- $\omega(G) = 3$, $n = 8$, $r = 4 \Rightarrow \nu(G) \geq 1$; $2 \leq \nu(G) \leq 4$
- Can we do better? **Yes**
- We get *exact* $\nu(G)$ for each G in the equivalence class
- In fact, every DAG in this equivalence class needs 3 or 4 interventions, so the existing bounds on $\nu(G)$ are *not tight*.

Verification: Efficient computation

In general, `MVC` is NP-hard and we can only get a 2-approximation in polynomial time... [PSS22] also has a 2-approximation to $\nu(G)$.



Claim: Covered edges form a forest.

Implication: `MVC`(covered) can be computed *exactly* in *linear time*.

Image credit: https://wronghands1.com/2018/01/12/parts-of-the-elephant-in-the-room/

Easy re-interpretation of known facts via covered edges

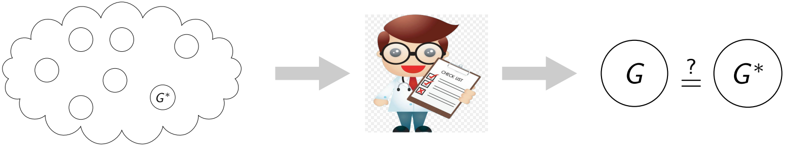
- Covered edges of clique K_n: $v_1 \to v_2, \ldots, v_{n-1} \to v_n$
- Covered edges of a tree: incident edges to root vertex
- Necessity of separating system for non-adaptive interventions
  - [Chi95]: Two graphs are equivalent $\iff$ there is a sequence of covered edge reversals to transform between them.
  - Unoriented edge $\Rightarrow$ Covered edge for *some* DAG in eq. class.
  - Conclusion: any *non-adaptive* search must cut *all* edges.
- Covered edge *cannot* have both endpoints as a sink of any maximal clique $\Rightarrow \nu(G) \leq n - r$ (result of [PSS22]).

(Slide catering to domain experts. If interested, pause to read; Else, skip)

The verification problem ✓

Can determine $G \stackrel{?}{=} G^*$

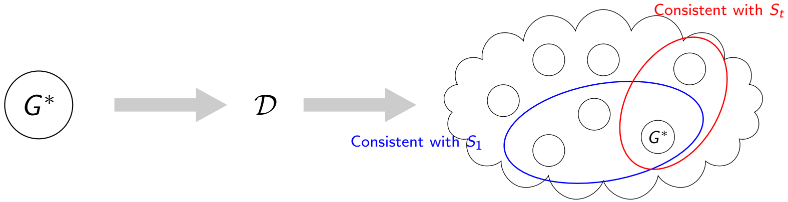
- Using $\nu(G) = \texttt{MVC}(\text{covered})$ interventions
- Computable in polynomial time



What about actually searching for G^* without the expert?

The adaptive search problem

Goal: Identify G^* using as few interventions as possible



- We know that at least $\nu(G^*)$ interventions is *necessary*
- Punchline: $\mathcal{O}(\log n \cdot \nu(G^*))$ interventions suffice

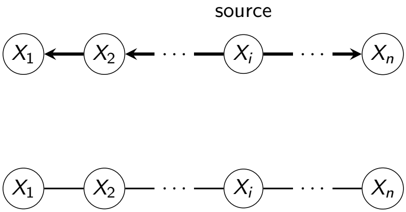
"Search is almost as easy as verification"

Adaptive search: $\mathcal{O}(\log n \cdot \nu(G^*))$ interventions suffice

- Prior works only have theoretical guarantees for special classes of graphs: cliques, trees, intersection incomparable graphs, ...
- $\Omega(\log n \cdot \nu(G^*))$ interventions are necessary in the worst case

G^*

Essential graph

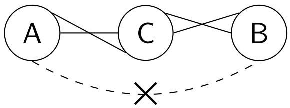


$\nu(G^*) = 1$ and identifying G^* is equivalent to binary search

- Covered edges are $X_{i-1} \leftarrow X_i \rightarrow X_{i+1} \Rightarrow$ Need to "hit" X_i
- Each intervention orients "one side" via Meek rule R1

Adaptive search: How it works

- [HB12]: Intervene and remove oriented arcs $\Rightarrow$ *Chordal* graph
- [GRE84]: For any chordal graph, there exists a clique separator C such that
  - $|A|, |B| \leq n/2$
  - C is a clique, i.e. $|C| \leq \omega(G)$
  - Computable in polynomial time



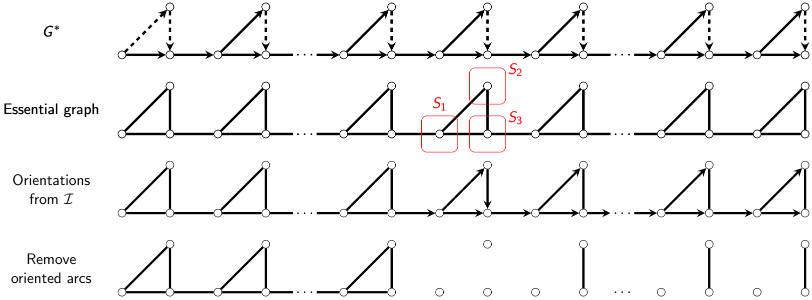
- Algorithm: Find clique separator in *each component*; Intervene on each node in all clique separators; Recurse
- Analysis:
  - $\mathcal{O}(\log n)$ rounds suffice $\leftarrow$ [GRE84]
  - $\mathcal{O}(\nu(G^*))$ per round $\leftarrow$ We prove new lower bound on $\nu(G^*)$

A stronger (but not computable) lower bound

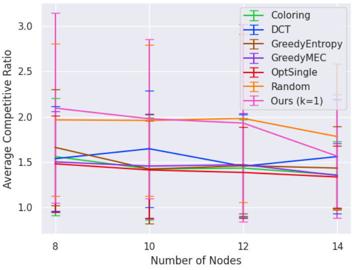
Intuition [HB14]: In any interventional essential graph, interventions across different "connected components" *do not* help.

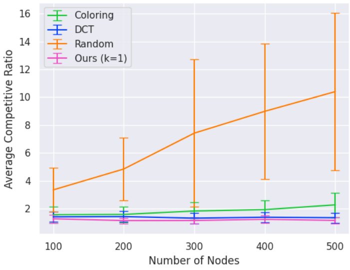
Claim: Fix an essential graph and some DAG G in it. Then,

$$\nu(G) \geq \max_{\substack{\text{atomic} \\ \text{interventions} \\ S_1,\ldots,S_t}} \sum_{\substack{\text{connected components} \\ H \in \text{ after removing oriented arcs} \\ \text{after interventions } S_1, \ldots, S_t}} \left\lfloor \frac{\omega(H)}{2} \right\rfloor$$



Experiments (Atomic search comparision)



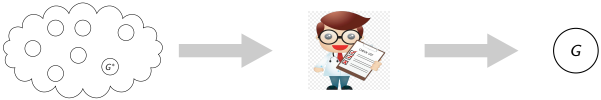


Qualitatively, our algorithm is competitive with the state-of-the-art search algorithms while being ∼10x faster in some experiments.

Implementation: https://github.com/cxjdavin/verification-and-search-algorithms-for-causal-DAGs

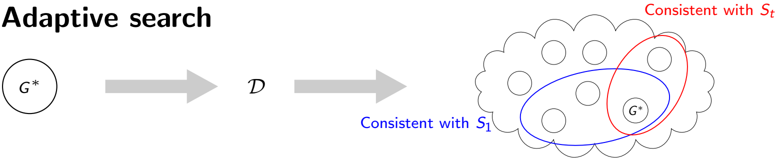
Summary

1. Verification



- Polynomial time *exact characterization* of $\nu(G)$
- $\nu(G) = \texttt{MVC}(\text{covered})$ to determine if $G \stackrel{?}{=} G^*$

2. Adaptive search



- Polynomial time adaptive search algorithm using interventions
- $\mathcal{O}(\log n \cdot \nu(G^*))$ suffice for *any general graph*
- $\Omega(\log n \cdot \nu(G^*))$ worst case necessary

Natural follow up questions

- In this work, we studied *verification* and *search* under an idealized setting with hard interventions and infinite samples.
- Soft interventions may be more realistic in certain real-life scenarios (e.g. effects from parental vertices are not completely removed but only altered); see [KJSB19]
- Sample complexities also play a crucial role when one has limited experimental budget; see [ABDK18]
- We also make standard assumptions such as the Markov assumption, the faithfulness assumption, and causal sufficiency [SGSH00]. Can we remove/weaken these assumptions?

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