Faster algorithms for Markov equivalence

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ISI Virtual Conference, July 2021

Algorithms

This talk is largely based on Hu and Evans (2020). In the paper we give new algorithms for:

- determining Markov equivalence in **maximal ancestral graphs**;
- projecting an ADMG to a MAG.

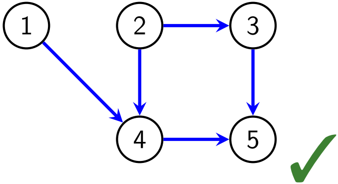
Combining these algorithms is **faster** than any previously provided method for checking Markov equivalence in ADMGs (or MAGs!).

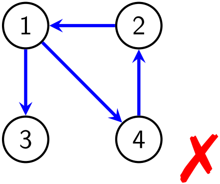
Ali et al. (2009) give an algorithm with complexity $O(ne^4)$, whereas our worst case is $O(ne^2)$.

Typically the algorithm is much faster than this.

Directed Acyclic Graph Models

A directed acyclic graph (DAG) is a directed graph that contains no (directed) cycles.





A **DAG model** imposes the factorization

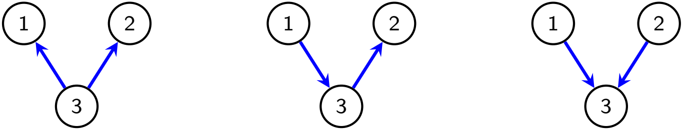
$$p(x_V) = \prod_{i \in V} p(x_i \mid x_{\mathrm{pa}(i)}).$$

where $\mathrm{pa}(i) = \{j : j \to i\}$.

Can also read off independences using **d-separation** (Verma and Pearl, 1990).

Markov Equivalence

With DAGs, sometimes two or more graphs will represent the same model:



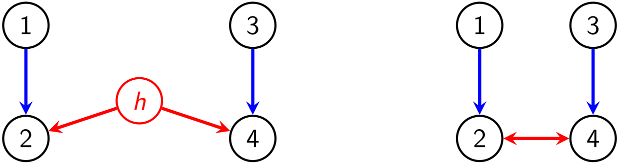
$p(x_3) \cdot p(x_1 \mid x_3) \cdot p(x_2 \mid x_3)$ $\quad$ $X_1 \perp\!\!\!\perp X_2 \mid X_3$ $\quad$ $p(x_1) \cdot p(x_2) \cdot p(x_3 \mid x_1, x_2)$

$X_1 \perp\!\!\!\perp X_2 \mid X_3$ $\quad$ $p(x_1) \cdot p(x_3 \mid x_1) \cdot p(x_2 \mid x_3)$ $\quad$ $X_1 \perp\!\!\!\perp X_2$

We can characterize this using the **skeleton** and the **unshielded colliders**.

Margins of DAG Models

DAG models are not closed under marginalization and conditioning.

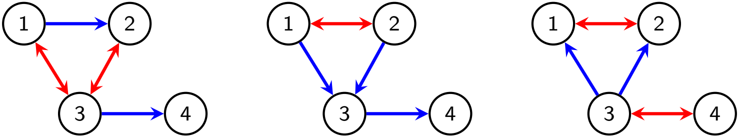


This can be solved using a **latent projection** which introduces bidirected edges ($\leftrightarrow$).

The resulting objects are called **acyclic directed mixed graphs** (ADMGs).

More Markov equivalence

All DAGs are also ADMGs, so unsurprisingly Markov equivalence is still an issue.



Maximal Ancestral Graphs (MAGs)

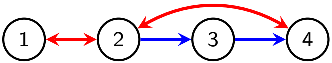
There is a subclass of ADMGs called **maximal ancestral graphs** (MAGs), introduced by Richardson and Spirtes (2002).

They are

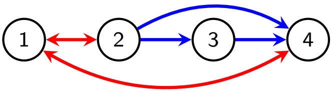
- **ancestral**: meaning no vertex is a bidirected neighbour of an ancestor; and
- **maximal**: meaning any two non-adjacent vertices have an m-separation.

Any ADMG can be 'projected' onto a **Markov equivalent** MAG.

ADMG



MAG



Main Results

We will assume that we have a MAGs with

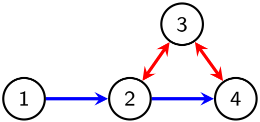
- n vertices, and
- e edges (either $\rightarrow$ or $\leftrightarrow$).

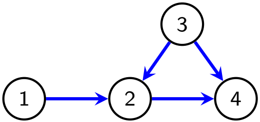
We also assume the graph is connected, so $n = O(e)$.

In this paper we present three things:

1. new non-parametric characterization of Markov equivalence class of a MAG;
2. polynomial time algorithm ($O(ne^2)$) for verifying Markov equivalence between two MAGs;
3. polynomial time algorithm ($O(n^2e)$) for transforming an ADMG into a Markov equivalent MAG.

Discriminating Paths





Both graphs have $1 \perp_m 3$.

Paths between 1 and 4 are $1 \rightarrow 2 \rightarrow 4$ and either:

$$1 \rightarrow 2 \leftrightarrow 3 \leftrightarrow 4 \qquad \text{or} \qquad 1 \rightarrow 2 \leftarrow 3 \rightarrow 4.$$

Note that for the left graph, 3 is a collider, but the right graph it is a non-collider.

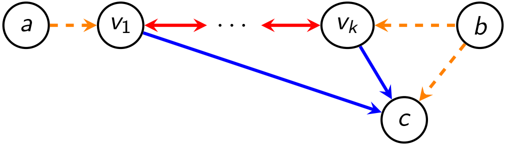
This gives us **different** m-separation sets.

$$1 \perp_m 4 \mid 2 \qquad\qquad 1 \perp_m 4 \mid 2, 3.$$

Discriminating Paths

As well as the same **skeleton** and **unshielded colliders** we need the **discriminating paths** to be the same.

A generic **discriminating path** for b is:



Note that a and c cannot be adjacent.

Since $\mathcal{G}$ is **maximal** there is (at least) one set S that m-separates a and c.

Then notice that any m-separating set S is such that

$$a \perp_m c \mid S \iff \begin{cases} b \in S \text{ and } b \text{ is a non-collider} \\ b \notin S \text{ and } b \text{ is a collider.} \end{cases}$$

Previous work

There are three graphical criteria which can be used to characterize a MAG model:

- *discriminating paths* by Spirtes and Richardson (1997);
- *minimal collider paths* (MCPs) by Zhao et al. (2005);
- *colliders with order* by Ali et al. (2009).

Using the first two approaches naïvely has exponential complexity, and the third has an $O(ne^4)$ algorithm associated with it.

Heads and Tails

Definition

A **head**, H, is a set of vertices such that:

- no vertex in H is an ancestor of any other;
- the set H is bidirected-connected within $A := \text{an}(H)$.

The corresponding **tail** is then:

$$\text{tail}_{\mathcal{G}}(H) := (\text{dis}_A(H) \setminus H) \cup \text{pa}(\text{dis}_A(H)).$$

Note that the tail is the **Markov blanket** for H within $\text{an}(H)$.

In a MAG:

- heads of size 1 are just the individual vertices;
- tails for heads of size 1 are just their parents;
- heads of size 2 just correspond to bidirected edges.

Parameterizing Sets

Define the **parametrizing sets** for a graph $\mathcal{G}$ as

$$\mathcal{S}(\mathcal{G}) := \{H \cup A : H \in \mathcal{H}(\mathcal{G}),\, A \subseteq \mathrm{tail}_{\mathcal{G}}(H)\},$$

where $\mathcal{H}(\mathcal{G})$ is the set of heads in $\mathcal{G}$.

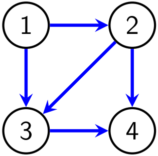
We also define:

$$\mathcal{S}_k(\mathcal{G}) := \{S \in \mathcal{S}(\mathcal{G}) : |S| \leq k\},$$

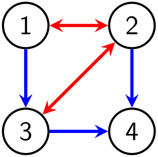
and

$$\widetilde{\mathcal{S}}_3(\mathcal{G}) = \{S \in \mathcal{S}_3(\mathcal{G}) \mid \text{1 or 2 adjacencies among vertices in } \mathcal{G}\}$$

Examples



H	T	$\mathcal{S}$
1	$\emptyset$	$\{1\}$
2	1	$\{2\}, \{1,2\}$
3	1, 2	$\{3\}, \{1,3\}$ $\{2,3\}, \{1,2,3\}$
4	2, 3	$\{4\}, \{2,4\}$ $\{3,4\}, \{2,3,4\}$



H	T	$\mathcal{S}$
1	$\emptyset$	$\{1\}$
2	$\emptyset$	$\{2\}$
1, 2	$\emptyset$	$\{1,2\}$
3	1	$\{3\}, \{1,3\}$
2, 3	1	$\{2,3\}, \{1,2,3\}$
4	2,3	$\{4\}, \{2,4\}$ $\{3,4\}, \{2,3,4\}$

Note that both these graphs have the same collection of **parametrizing sets** (i.e. all sets not containing both 1 and 4).

Preliminary Results

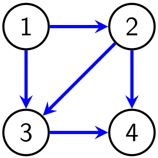
Proposition

Let $\mathcal{G}$ be a MAG and W a set of vertices. Then $W \notin \mathcal{S}(\mathcal{G})$ if and only if $\exists a, b \in W$ such that

$$a \perp_m b \mid C$$

for a set C with $W \subseteq C \cup \{a, b\}$.

Example. For the previous graphs, the sets $\{1, 4\}, \ldots, \{1, 2, 3, 4\}$ were missing, which precisely corresponds to the m-separation $1 \perp_m 4 \mid \{2, 3\}$.



Preliminary Results

Lemma

In a MAG $\mathcal{G}$, we have that there is an edge between a and b if and only if $\{a, b\} \in \mathcal{S}(\mathcal{G})$.

So we can obtain the skeleton just from $\mathcal{S}_2(\mathcal{G})$.

Lemma

If (a, b, c) is an unshielded triple, then b is a collider on this triple if and only if $\{a, b, c\} \in \mathcal{S}(\mathcal{G})$.

So we can also obtain the unshielded colliders from $\mathcal{S}_3(\mathcal{G})$.

Lemma

If π is a discriminating path from a to c for b, then b is a collider if and only if $\{a, b, c\} \in \mathcal{S}(\mathcal{G})$.

$\mathcal{S}_3(\mathcal{G})$ also gives orientations from discriminating paths!

Main Results

Theorem (Hu and Evans, 2020)

Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be two MAGs. These graphs are Markov equivalent if and only if $\mathcal{S}(\mathcal{G}_1) = \mathcal{S}(\mathcal{G}_2)$.

This is good, but the length of $\mathcal{S}(\mathcal{G})$ may be exponential in n.

Corollary

Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be two MAGs. These graphs are Markov equivalent if and only if $\mathcal{S}_3(\mathcal{G}_1) = \mathcal{S}_3(\mathcal{G}_2)$.

This is better, because now the list has length $O(n^3)$.
However, the best result we get is:

Corollary

Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be two MAGs. These graphs are Markov equivalent if and only if $\widetilde{\mathcal{S}}_3(\mathcal{G}_1) = \widetilde{\mathcal{S}}_3(\mathcal{G}_2)$.

Computing $\widetilde{\mathcal{S}}_3$

For a MAG $\mathcal{G}$, we can compute $\widetilde{\mathcal{S}}_3(\mathcal{G})$ by obtaining:

1. heads of size 2, and tails of each vertex;
2. tails of every head of size 2;
3. every head of size 3 in $\widetilde{\mathcal{S}}_3(\mathcal{G})$.

} unshielded colliders/ discriminating paths

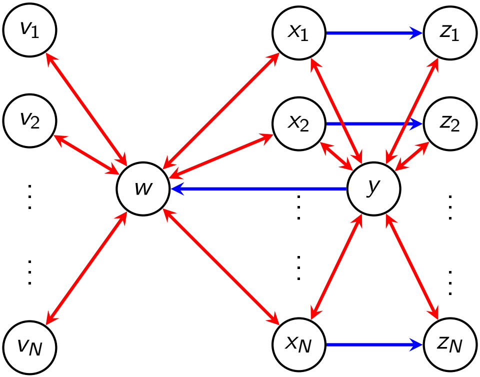
The most computationally difficult task is 3. We must:

- iterate through every bidirected edge $v \leftrightarrow w$ ($O(e)$);
- for each other vertex z ($O(n)$)...
- compute the district of v within the set of ancestors of v, w, z ($O(n + e)$) and check if z is in it.

This gives us $O(ne^2)$ complexity.

Comes from the fact that we (seem to) have to compute the ancestral district for every triple of form $v \leftrightarrow w$ and some z.

Graph achieving max complexity (Figure 5)



Consider $v_i \leftrightarrow w$ for each $i = 1, \ldots, N$, and then note that we need to consider it with each z_j for $j = 1, \ldots, N$.

These sets are all heads of size three.

There are $N^2 = O(e^2)$ such heads, which gives the required complexity.

Markov equivalence for ADMGs

We also give a method for quickly ($O(n^2 e)$) turning an ADMG into a Markov equivalent MAG.

(Note: here e is the number of edges in the MAG!).

Note that length of $\widetilde{\mathcal{S}}_3(\mathcal{G})$ is at most $O(e^2)$, so we can sort the output in $O(e^2 \log e^2) = O(e^2 \log e)$ operations.

Hence we can combine our two algorithms to check equivalence of any ADMGs in at most $O(ne^2)$.

Note it is easy to add in **undirected edges** to a MAG, and we just add those pairs to the graph to obtain $\widetilde{\mathcal{S}}_3(\mathcal{G})$.

Summary

- We can identify the Markov equivalence class of any ADMG using a purely graphical approach in at most $O(ne^2)$ complexity.
- This complexity is attained by family of graphs in Figure 5.
- There is much more to do! We can deduce some conditional independences directly from the parametrizing sets.
- There is also a connection between the parameterizing sets and **imsets** (Studený, 2006).

References

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P. Spirtes and T. S. Richardson. A polynomial time algorithm for determining DAG equivalence in the presence of latent variables and selection bias, 1997.

M. Studený. *Probabilistic conditional independence structures*. Springer Science & Business Media, 2006.

T. Verma and J. Pearl. Causal networks: Semantics and expressiveness. In *Machine intelligence and pattern recognition*, volume 9, pages 69–76. Elsevier, 1990.

H. Zhao, Z. Zheng, and B. Liu. On the Markov equivalence of maximal ancestral graphs. *Science in China Series A: Mathematics*, 48(4):548–562, Apr 2005.

Thank you!

Latent Projection

Given an ADMG $\mathcal{G}$ with vertices $H \dot{\cup} O$, we define the **latent projection** of $\mathcal{G}$ onto O as the ADMG with vertices O and edges:

- $i \rightarrow j$ if there is a directed path from i to j in $\mathcal{G}$ with any intermediate vertices in H.
- $i \leftrightarrow j$ if there is a trek with arrows into both i and j and all intermediate vertices in H.

Definitions

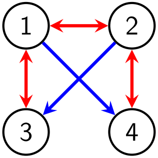
A graph $\mathcal{G}$ is called an **acyclic directed mixed graph** (ADMG) if has only directed ($\rightarrow$) and bidirected ($\leftrightarrow$) edges, and its directed edges form a DAG.

A **path** π is a sequence of distinct, adjacent vertices.

An internal vertex v on a path is called a **collider** if both adjacent edges have arrowheads at v; otherwise it is a **non-collider**.

A path from a to b is said to be **m-connecting** (or **open**) given C if:

- every non-collider is outside C;
- every collider is in $\text{an}_{\mathcal{G}}(C)$.

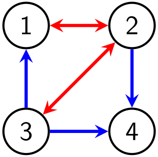


Definitions

For two vertices a, b and a disjoint set of vertices C in $\mathcal{G}$ we say that a and b are **m-separated** by C if there is no m-connecting paths given C.

Example. Consider:

- 1 and 4 given 2, 3, (m-separated);
- 1 and 4 given 2, (not m-separated).



Extension to ADMGs

Further, we show that heads and tails are preserved through the projection. Let $\mathcal{H}(\mathcal{G})$ denote the set of all heads in an ADMG $\mathcal{G}$.

Proposition

If $\mathcal{G}$ is an ADMG, $\mathcal{H}(\mathcal{G}) = \mathcal{H}(\mathcal{G}^m)$ and for every $H \in \mathcal{H}(\mathcal{G})$, $\text{tail}_{\mathcal{G}}(H) = \text{tail}_{\mathcal{G}^m}(H)$.

Independence from Parameterizing Sets

Proposition

Let $\mathcal{G}$ be a MAG and consider $W \notin \mathcal{S}(\mathcal{G})$ where $W = \{a, b\} \cup C$ such that $a, b \notin C$, if the following conditions hold:

$$(i) : \text{for any } S \supset W \text{ we have } S \in \mathcal{S}(\mathcal{G})$$
$$(ii) : \text{for any } C' \subseteq C \text{ we have } \{a, b\} \cup C' = W' \notin \mathcal{S}(\mathcal{G});$$

then $a \perp_m b \mid C$ in $\mathcal{G}$

Characteristic Imset

Note that for DAGs, the parameterizing set is the same as the **characteristic imset** (Studený, 2006).

This suggests that perhaps the parameterizing set is also the characteristic set for MAGs.

We have shown that the associated standard imset defines the model for **some** MAGs... but not all!

Indeed, the bidirected 5-cycle is a counterexample to our conjecture.

Algorithm 2: Projection from ADMG to MAGs

Algorithm 2: Obtain a MAG $\mathcal{G}^m$ from an ADMG $\mathcal{G}$

Input: ADMG $\mathcal{G}$ (list of parents and siblings of each vertex)
Output: Markov equivalent MAG $\mathcal{G}^m$

for $v \in V$ **do**
  compute $\mathrm{an}_{\mathcal{G}}(v) = \{v\} \cup \mathrm{an}_{\mathcal{G}}(\mathrm{pa}_{\mathcal{G}}(v))$;
  compute $\mathrm{tail}_{\mathcal{G}}(v) = (\mathrm{dis}_{\mathrm{an}(v)}(v) \setminus \{v\}) \cup \mathrm{pa}_{\mathcal{G}}(\mathrm{dis}_{\mathrm{an}(v)}(v))$;
  add in $p \to v$ for each $p \in \mathrm{tail}_{\mathcal{G}}(v)$;
end
for v, w *same district* **do**
  if $w \in \mathrm{dis}_{\mathrm{an}(\{v,w\})}(v)$ then add $v \leftrightarrow w$;
end

Notice first loop is $O(n(n+e))$ and second is $O(n^2(n+e))$.

Hence overall complexity is $O(n^2 e)$.

Algorithm 2: convert an ADMG to a Markov equivalent MAG

A projection from Richardson and Spirtes (2002) convert an ADMG $\mathcal{G}$ to a Markov equivalent MAG $\mathcal{G}^m$.

Lemma

Suppose $\mathcal{G}$ is an ADMG, let v, w be two vertices then (i) $v \rightarrow w$ in $\mathcal{G}^m$ if and only if $v \in \text{tail}_{\mathcal{G}}(w)$ and (ii) $v \leftrightarrow w$ in $\mathcal{G}^m$ if and only if $\{v, w\} \in \mathcal{H}(\mathcal{G})$.

For the complexity :

- upper bounded by $O(n^2 e)$;
- the average complexity is at $O(n^2)$ if each edge has an *i.i.d* Bernoulli distribution.

Definitions

Two ADMGs $\mathcal{G}_1$ and $\mathcal{G}_2$ with the same vertex sets, are said to be *Markov equivalent* if any m-separation holds in $\mathcal{G}_1$ if and only if it holds in $\mathcal{G}_2$.

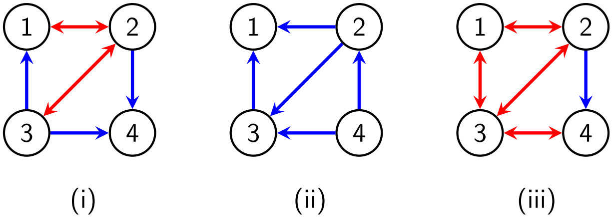


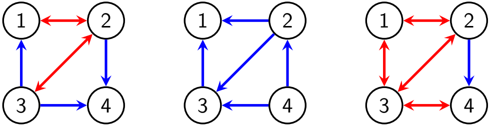
Figure: Three ADMGs where (i) and (ii) are Markov equivalent but (iii) is not.

Projection from ADMGs to Markov equivalent MAGs

Richardson and Spirtes (2002) :

- every pair of vertices $a, b \in \mathcal{V}$ in $\mathcal{G}$ that are connected by an *inducing path* becomes adjacent in $\mathcal{G}^m$;
- an edge connecting a, b in $\mathcal{G}^m$ is oriented as follows: if $a \in \text{an}_{\mathcal{G}}(b)$ then $a \to b$; if $b \in \text{an}_{\mathcal{G}}(a)$ then $b \to a$; if neither is the case, then $a \leftrightarrow b$.
- An *inducing path* between a, b is a collider path such that every collider is in $\text{an}(\{a, b\})$.
- Ancestral relations are preserved.

Examples



(i) (ii) (iii)

Figure	heads	tails	Figure	heads	tails
(i)	1	3	(iii)	1	∅
	2	∅		2	∅
	3	∅		3	∅
	4	2,3		4	2
	1,2	3		1,2	∅
	2,3	∅		1,3	∅
(ii)	1	2,3		2,3	∅
	2	4		3,4	2
	3	2,4		1,2,3	∅
	4	∅		1,3,4	2