

Minimal moralization

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Received: date / Accepted: date

1 Preliminary

In this section, we introduced the concepts that will be used throughout this paper.

Definition 1 A **graph** is a pair $G = (V, E)$ comprising a set V of vertices (or nodes) together with a set E of edges (or arcs).

Definition 2 A **directed graph** is a graph $G = (V, E)$, where E is a set of ordered pairs of distinct vertices in V .

Definition 3 A **hybrid graph** is a graph consisting of both directed and undirected edges.

Later in this section, we will introduce moral graphs, which require the direction of a directed edge to be dropped. Hence, if $G = (V, E)$ is a directed graph, we use $U(G)$ to denote the undirected version of G and $U(E)$ to denote the undirected version of G 's edges.

Definition 4 A **path** is a graph $P = (V, E)$, whose vertex set $V = \{v_1, v_2, \dots, v_{n-1}, v_n\}$ and edge set $E = \{v_1v_2, \dots, v_{n-1}v_n\}$, where $v_i \neq v_j$ for $i, j \in [1, n]$.

We use $P = v_1 \dots v_k$ to denote a path between v_1 and v_k . The path P has length k , denoted by $|P| = k$.

Definition 5 A **cycle** is a closed path $P = v_1 \dots v_{k+1}$ where $v_i \neq v_j$ for $i, j \in [1, k]$ and $v_1 = v_{k+1}$.

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A cycle of length m is called an m -cycle, denoted by C_m .

Definition 6 A graph is **connected** if every pair of vertices are connected by a path.

The vertex and edge set of G is denoted by $V(G)$ and $E(G)$ respectively. Throughout this paper, we use u, v to represent vertices in V and uv to represent an (undirected) edge in E . A graph refers to a connected undirected graph, unless it is said otherwise.

Definition 7 A directed graph $G = (V, E)$ is called a **directed acyclic graph** if it contains no directed cycles.

In a directed acyclic graph $G = (V, E)$, u is a *parent* of v , denoted by $u \in P(v)$ (or v is a *child* of u), if there is a directed edge from u to v . And u is an *ancestor* of v (or v is a *descendent* of u) if there is a directed path from u to v . Furthermore, v is a *nondescendent* of u if v is not a descendent of u .

Definition 8 Let \mathcal{P} be a joint probability distribution of the random variables in V , and $G = (V, E)$ be a directed acyclic graph. We say $\langle G, \mathcal{P} \rangle$ satisfies the **Markov condition** if for every variable $v_i \in V$, it is conditionally independent of its non-descendants given its parents set.

Definition 9 Let \mathcal{P} be a joint probability distribution of the random variables in V , and $G = (V, E)$ be a directed acyclic graph. We say $\langle G, \mathcal{P} \rangle$ forms a **Bayesian network** if it satisfies the Markov condition.

Definition 10 A Bayesian network $\langle G, \mathcal{P} \rangle$ satisfies the **faithfulness** condition if the only conditional independencies in \mathcal{P} are those entailed by the Markov condition.

Definition 11 Let $\langle G = (V, E), \mathcal{P} \rangle$ be a Bayesian network. The **Markov blanket** of u in the Bayesian network, denoted by $B(u)$, is the minimum subset of variables s.t. $u \perp\!\!\!\perp_{\mathcal{P}} v \mid B(u)$ for each $v \in V \setminus B[u]$, where $B[u] = B(u) \cup \{u\}$.

Definition 12 The **moral graph** of a directed acyclic graph $G = (V, E)$ is an undirected graph $H = (V, U(E) \cup F)$, where $F = \{uv \notin U(E) \mid u, v \in P_G(x), \forall x \in V\}$ is the set of filled edges.

The above definition implicitly states a way of obtaining a moral graph from a DAG. That is, by joining all pairs of non-adjacent parents in the DAG, then dropping all the directions. The process of obtaining a moral graph from a DAG is also known as *moralization*.

Example 1 Figure 1 shows a DAG G and its moral graph H that is obtained by joining v_3 and v_4 then dropping all the directions in the hybrid graph.

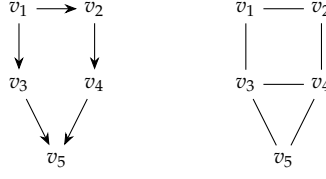


Fig. 1: A DAG $G = (V, E)$ and its moral graph $H = (V, U(E) \cup F)$, in which $v_3v_4 \in F$ is a filled edge.

If a given Bayesian network $\langle G = (V, E), \mathcal{P} \rangle$ is faithful, the Markov blanket of a variable u consists of its parents, children and children's other parents. For any spouse v of u that is neither a parent nor child of u , the edge uv is a filled edge to make the moral graph H of G . Hence, for each node $u \in V$, there is a one-to-one correspondance between its Markov blanket in G and its neighbourhood in H . For example, in Figure 1 $B_G(v_3) = \{v_1, v_5, v_4\} = N_H(v_3)$.

Definition 13 A **collider** in a hybrid graph is a node with at least two parents.

Definition 14 A directed acyclic graph $G = (V, E)$ is a **consistent extension** of a hybrid graph $H = (V, F)$ if $U(E) = U(F)$ and G and H have the same set of colliders.

Definition 15 Let $G' = (V', E')$ and $G = (V, E)$ be two graphs. If $V' \subseteq V$ and $E' \subseteq E$, then G' is a **subgraph** of G , written as $G' \subseteq G$.

Definition 16 Let $G' = (V', E')$ and $G = (V, E)$ be two graphs. If $G' \subseteq G$ and $uv \in E$ for all $u, v \in V'$, then G' is an **induced subgraph** of G , written as $G' = G[V']$.

For simplicity, if $V' \subset V$ then we use $G - V'$ to denote $G[V \setminus V']$. If $V' = \{u\}$, then we use $G - u$. If $V' = V(H)$, then we use $G - H$. Similarly, if $E' \subset E$ then we use $G + E'$ and $G - E'$ to denote $(V, E \cup E')$ and $(V, E \setminus E')$ respectively. If $E' = \{uv\}$ then we use $G + uv$ or $G - uv$ instead.

Definition 17 Let $G = (V, E)$ be a graph. The set of **neighbours** of u in G is $N(u) = \{v \in V \mid uv \in E\}$. The closed neighbourhood of u in G is $N[u] = N(u) \cup \{u\}$.

It is also useful to define the neighbours of a subgraph $H \subset G$ as $N_G(H) = \{u \in V \setminus V(H) \mid uv \in E, \forall v \in V(H)\}$.

Definition 18 Let $G = (V, E)$ be a graph. The **maximum degree** of the graph is $\Delta(G) = \max\{d(u) \mid u \in V\}$, where $d(u) = |N(u)|$ is the degree of u .

Definition 19 A **clique** is a subset of nodes in a graph where every two distinct nodes are adjacent.

Definition 20 A **simplicial node** in a graph is a node whose neighbours form a clique.

Definition 21 Let $G = (V, E)$ be a graph. The **deficiency** of a node x in G is $D(x) = \{uv \notin E \mid u, v \in N(x)\}$.

A node u is simplicial in G if and only if $D(u) = \emptyset$. That is, no edge needs to be filled in to make the neighbours of u a clique. We write $D(G) \neq \emptyset$ if $D_G(u) \neq \emptyset, \forall u \in V$. And $D(G) = \emptyset$ if $\exists x \in V$ s.t. $D(x) = \emptyset$.

Example 2 In the moral graph H as shown in Figure 1, $D_H(v_1) = \{v_2v_3\}$ and $D_H(v_5) = \emptyset$.

Definition 22 A **chord** in a m -cycle $C_m = v_1 \dots v_m v_1$ is an edge $v_i v_j \notin E(C_m)$ for $i, j \in [1, m]$.

Definition 23 A graph is **chordal** if each m -cycle for $m \geq 4$ has a chord.

Definition 24 An **ordering** of a graph $G = (V, E)$ with n vertices is a bijection $\alpha : \{1, \dots, n\} \leftrightarrow V$.

Another equivalent property as being chordal is that G has a *perfect elimination ordering*. That is, for each $x \in V$ with $\alpha^{-1}(x) = i + 1$, we have $D_{G^i}(x) = \emptyset$, where $G^i = G - \{\alpha(1), \dots, \alpha(i)\}$ and $G^0 = G$.

Definition 25 A graph $G = (V, E)$ is **recursively simplicial** if $\exists x \in V$ with $D_G(x) = \emptyset$ s.t. the induced subgraph $G - x$ is recursively simplicial.

Being recursively simplicial is equivalent as being chordal. It makes chordality a hereditary property. The following concept is not as strong as recursively simplicial, so it requires some edges to be removed in addition to the removal of a simplicial node.

Definition 26 A graph $G = (V, E)$ is **weak recursively simplicial** if $\exists x \in V$ with $D_G(x) = \emptyset$ and $\exists E' \subseteq \{uv \in E \mid u, v \in N_G(x)\}$ s.t. the subgraph $G' = G - x - E'$ is weak recursively simplicial.

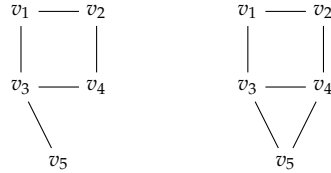


Fig. 2: An example of a non-weak recursively simplicial graph G (left) and a weak recursively simplicial graph H (right).

Example 3 H is a weak recursively simplicial (WRS) graph that can be justified by the following two criterion:

1. recursively removing $\{v_5, v_3v_4\}$, $\{v_3\}$, $\{v_4\}$, $\{v_1\}$, $\{v_2\}$ to eliminate the graph completely,
2. each node removed is a simplicial node in the current graph.

On the other hand, the graph G is not WRS, because there is no way G can be eliminated completely whilst the node removed at each step is simplicial in the current graph.

If a graph is recursively simplicial (i.e., chordal), it is also weak recursively simplicial with $E' = \emptyset$ for each simplicial node x . The converse, however, is not true. For example, the graph H in Figure 2 is WRS but not chordal.

Definition 27 A set of **excesses** of a graph $G = (V, E)$ according to an ordering α is a bijection $\epsilon_\alpha : \alpha \leftrightarrow \{\epsilon_\alpha(v_1), \dots, \epsilon_\alpha(v_n)\}$, where each $\epsilon_\alpha(v_i) \subseteq E(G[N(v_i)])$ consists of some edges between the neighbours of v_i .

The composition $\kappa = (\alpha, \epsilon_\alpha)$ of an ordering and a set of excesses is called an elimination kit of a graph G . We use $\kappa(1)$ to denote the node $\alpha(1)$ and its excess $\epsilon_\alpha(\alpha(1))$. By using the concept of elimination kit, we extend the definition of the subgraph $G^i = G - \{\kappa(1), \dots, \kappa(i)\} \subset G$ for $i \in [1, n]$, with the same convention $G^0 = G$.

Example 4 An ordering $\alpha = (v_5, v_3, v_4, v_1, v_2)$ and a set of excesses $\epsilon_\alpha = (\emptyset, \emptyset, \emptyset, \emptyset, \emptyset)$ form an elimination kit of H in Figure 1.

Definition 28 Let $G = (V, E)$ be a graph and $\kappa = (\alpha, \epsilon_\alpha)$ be an elimination kit of G . It is a **perfect elimination kit** if for each $x \in V$ with $\alpha^{-1}(x) = i + 1$, we have $D_{G^i}(x) = \emptyset$.

In general, a graph may have none, one or more than one perfect elimination kit (pek).

Example 5 The elimination kit in Example 4 is not perfect, because $D_{G^1}(v_3) \neq \emptyset$. The only pek for H is $\alpha = (v_5, v_3, v_4, v_1, v_2)$ and $\epsilon_\alpha = (\{v_3v_4\}, \emptyset, \emptyset, \emptyset, \emptyset)$.

Definition 29 Let $G = (V, E)$ be a graph and $\kappa = (\alpha, \epsilon_\alpha)$ be an elimination kit of G . It is a **partial perfect elimination kit** if there exists a non-empty subgraph $G^i \subset G$ s.t. $D(G^i) \neq \emptyset$ and $D_{G^{i-1}}(\alpha(j)) = \emptyset$ for $j \in [1, i]$.

A 4-cycle has no partial pek, because it has no simplicial node. A graph that has a pek may also have a partial pek.

Example 6 Example 4 is a partial pek, because $D(G^1) \neq \emptyset$ and $D_{G^0}(v_5) = \emptyset$.

Definition 30 A graph $H = (V, E \cup F)$ is called a **moralization** of an undirected graph $G = (V, E)$ if H is moral.

Without loss of generality, assuming $F \neq \emptyset$ and $E \cap F = \emptyset$. Every edge $e \in E \cup F$ is either an edge of the underlying graph G or a *fill edge* in F .

Definition 31 Let $G = (V, E)$ be a graph, and $H = (V, E \cup F)$ be a moral graph with $F \neq \emptyset$ and $E \cap F = \emptyset$. H is a **minimal moralization** of G if $(V, E \cup F')$ is non-moral $\forall F' \subsetneq F$. It is the **minimum moralization** if $\nexists E'$ with $|E'| < |F|$ s.t. the graph $(V, E \cup E')$ is moral.

Sometimes people also refer the set of fill edges F as a minimal moralization instead of the graph H . The following is an example of a minimal and minimum moralizations.

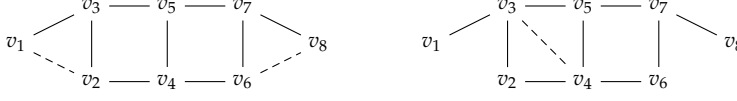


Fig. 3: An example of a minimal (left) and minimum (right) moralizations.

Definition 32 Let $\kappa = (\alpha, \epsilon_\alpha)$ be an elimination kit of a graph G . κ is **minimal** if there is no other elimination kit κ' s.t. $G_{\kappa'}^+$ is a proper subgraph of G_κ^+ . It is **perfect** if $G_\kappa^+ = G$.

Definition 33 Let $G = (V, E)$ be a connected graph. A vertex set $S \subset V$ is a **separator** if $G[V - S]$ is disconnected.

Definition 34 A graph G is called **connected** if there is a path between every pair of vertices in G .

Definition 35 Let G be a graph. A maximal connected subgraph of G is called a **component** of G .

Definition 36 Given two non-adjacent vertices u, v in a graph $G = (V, E)$. A vertex set $S \subset V$ is a u, v -**separator** if u and v belong to different components of $G[V - S]$. In particular, S is a **minimal** u, v -separator if there exists no proper subset of S that separates u and v .

2 Minimal moralization

From now on, we try to develop polynomial time algorithms for finding the maximal moral subgraph or the minimal moral supergraph of a given non-moral graph F .

Definition 37 A **simple cycle** C in a graph is a closed walk such that each node in $V(C)$ is only visited once except for the starting node.

Definition 38 An **induced simple cycle** in a graph F is a simple cycle that is an induced subgraph of F .

Remark 1 The number of induced simple cycles of length 4 or more in F gives an upper bound of the number of edges to be added/removed from F .

Remark 2 The minimal moral supergraph problem is NP-complete, because if it is polynomial then we can run an algorithm to find the minimal moral supergraph of a graph F and comparing it with F . This will identify if F is moral or not in polynomial time.

Both minimum triangulation and maximum chordal subgraph seem to be only solvable in NP-complete time complexity. But minimal triangulation and maximal subgraphs seem to be solvable in efficient time.

Minimal triangulation is related to minimal separator. A vertex $S \subset V$ is a **separator** if $F[V \setminus S]$ is disconnected. Given two vertices $u, v \in V$, S is a u, v -separator if u and v belong to different connected components of $F[V \setminus S]$. S is called a minimal u, v -separator if S has no proper subset that separates u and v . A vertex $S \subset V$ is a **minimal separator** of $F = (V, E)$ if $\exists u, v \in V$ s.t. S is a minimal u, v -separator.

- Chordality is not preserved under graph complementation, so finding the maximal chordal subgraph is not reducible to finding minimal chordal supergraphs. This is the same for morality, I've just randomly generated some graphs and their complements, they nont always have the same morality.
- Chordality is a hereditary property. That is, if a graph $F = (V, E)$ is chordal, the subgraph of F induced by $V \setminus \{x\}$ is also chordal where x is a simplicial node in F . But morality is not a hereditary property, because the induced subgraph after removing a simplicial node from F may or may not be moral.
- Since checking morality in general is NP-complete, I suspect that the finding the minimal triangulation of a graph is al NP-complete. For otherwise, we could find the minimal triangulation of a graph and compare it with the original graph. If they are identical, then the original graph is NP-complete.
- Run backtracking algorithm on a graph, if the algorithm stucks, add pick a node with the minimum degree and add its deficiency. This way will result a graph that is moral (and perhaps chordal), but won't be a minimal moral supergraph. A moral graph is a minimal supergraph of a graph F if there is no another moral graph that is a proper subgraph of it.
- Different ordering will result in different moral supergraph, hence the choice of a node to eliminate at each step is crucial.

2.1 Characterizations of minimal moralization

Firstly, we prove that for each minimal moralization H of G , there exists a mek κ s.t. $H = G_\kappa^+$. The consequence of this result is that finding a minimal moralization or a mek are equivalent problems. The result is proved by the same logic as in [?] for chordal graphs.

Lemma 1 *Let $G = (V, E)$ be a graph and $H = (V, E \cup F)$ be a minimal moralization of G . Then there exists a minimal elimination kit κ s.t. $G_\kappa^+ = H$.*

Proof H is moral implies it has a pek κ . $G \subset H$ implies $G_\kappa^+ = (V, E \cup F') \subset H$. Since H is minimal, $F' = F$ and consequently $G_\kappa^+ = H$. Assuming H has another pek κ' with $G_{\kappa'}^+ = (V, E \cup E') \subsetneq G_\kappa^+$. It entails that $E' \subsetneq F$, which contradicts H being minimal. \square

Lemma 2 *Let κ be a minimal elimination kit of a graph $G = (V, E)$. Then G_κ^+ is a minimal moralization of G .*

Proof Assuming $G_\kappa^+ = (V, E \cup E')$ is not minimal. That is, there exists another set of fill edges $F \subsetneq E'$ with $H = (V, E \cup F)$ being moral. Without loss of generality, assuming H is a minimal. Lemma 1 implies that $\exists \kappa'$ s.t. $G_{\kappa'}^+ = H \subsetneq G_\kappa^+$. It contradicts with κ being a mek. \square

Theorem 1 *A graph H is a minimal moralization of G if and only if there exists a minimal elimination kit κ s.t. $H = G_\kappa^+$.*

Proof The theorem follow from Lemma 1 and Lemma 2. \square

Theorem 2 *A graph is moral if and only if it has a perfect elimination kit.*

Proof The proof is trivial. \square

If there exists a perfect elimination kit (pek) κ with $\epsilon_\alpha = \emptyset$, then G is chordal and the outputs $G_\kappa^+ = G_\alpha^+$.

The EA algorithm outputs a moralized graph that possibly contains more edges than needed for moralization. To pursue a smaller moralized graph, the *minimal moralization sandwich problem* looks for a minimal moralization H of G s.t. $G \subseteq H \subseteq G_\kappa^+$ for a given elimination kit.

The following lemmas and theorems are stated and proved in similar ways as those for triangulated graphs in [?].

Lemma 3 *Let $G = (V, E)$ be a moral graph with a pek $\kappa = (\alpha, \epsilon_\alpha)$. For any node $x \in V$, the graph $G' = (V, E \cup D_G(x))$ has a pek $\kappa' = (\alpha, \epsilon'_\alpha)$.*

Proof We want to show that for any two distinct edges $\{v_i v_j, v_i v_k\} \subset E \cup D_G(x) - E'$ with $\alpha^{-1}(v_i) < \min\{\alpha^{-1}(v_j), \alpha^{-1}(v_k)\}$, the edge $v_j v_k \in E \cup D_G(x) - E'$ where $E' = \{\epsilon'_\alpha(v_1), \dots, \epsilon'_\alpha(v_{i-1})\}$ is the set of removed edges up to v_i according to κ' .

Case 1: If $\{v_i v_j, v_i v_k\} \subset E - E'$, since v_i comes before v_j and v_k in α , the edge $v_j v_k \in E - E'$ because κ' is perfect.

Case 2: If $\{v_i v_j, v_i v_k\} \subset D_G(x) - E'$, then $\{v_i, v_j, v_k\} \subset N_G(x)$ so $v_j v_k \in D_G(x)$. It remains to show that $v_j v_k \notin E'$. If there is a node v_l with $\alpha^{-1}(v_l) < \alpha^{-1}(v_i)$ and $v_j v_k \in \epsilon_\alpha(v_l)$ because it is in a cycle, then it is possible for $v_j v_k \in \epsilon'_\alpha(v_i)$ to break the same cycle.

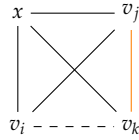


Fig. 4: An example of case 3. The solid lines are in E . The dashed is in $D(x)$. The orange is the edge we want to prove to belong to $E \cup D(x)$.

Case 3: If $v_i v_j \in E - E'$ and $v_i v_k \in D_G(x) - E'$, then $\{v_i, v_k\} \subset N_G(x)$. If $x = v_j$ then $v_j v_k \in E$. Otherwise (Figure 4), we have $\alpha^{-1}(v_i) < \alpha^{-1}(x)$ because $v_i v_k \in D_G(x)$. If so, $x v_j \in E$ because $\{x, v_j\} \subset N_G(v_i)$. It then follows that $v_j v_k \in E \cup D_G(x)$ because $\{v_j, v_k\} \subset N_G(x)$. For the same argument in case 2, $v_j v_k \notin E'$. \square

Corollary 1 Let $G = (V, E)$ be a moral graph and x be any node with $D_G(x) = \emptyset$. Then there is a pek $\kappa = (\alpha, \epsilon_\alpha)$ of G with $\alpha(1) = x$.

Proof Let $R = \{x \mid D_G(x) = \emptyset\}$. Morality implies that $|R| \geq 1$. If $|R| = 1$, it is certain that $\alpha(1) = x$. Otherwise, for any $x \in R$, there is a different pek $\kappa = (\alpha, \epsilon_\alpha)$ for G with $\alpha(1) = x$. **Not quite a proof!** \square

Corollary 2 Let $G = (V, E)$ be a moral graph with a pek $(\alpha, \epsilon_\alpha)$ and x is any node in G . Then there exists a pek $\kappa' = (\alpha, \epsilon'_\alpha)$ for the graph $G' = (V, E \cup D_G(x))$ s.t. the subgraph $G'_x = (V - \{x\}, E(G[V \setminus \{x\}]) \cup D_G(x) - \epsilon'_\alpha(x))$ is also moral.

Proof Lemma 3 implies that $G' = (V, E \cup D_G(x))$ is moral. Corollary 1 suggests that G' has a pek $\kappa' = (\alpha, \epsilon'_\alpha)$ with $\alpha(1) = x$. Hence, $G'_x = (V - \{x\}, E(G[V \setminus \{x\}]) \cup D_G(x) - \epsilon'_\alpha(x))$ is also moral because of the hereditary property of morality. \square

Lemma 4 Let $G = (V, E)$ and $H = (V, E \cup F)$ be moral graphs with peks $(\alpha, \epsilon_\alpha)$ and (β, ϵ_β) respectively and $F \neq \emptyset$, $E \cap F = \emptyset$. Then there exists at least one edge $f = uv \in F$ with $\beta^{-1}(u) < \beta^{-1}(v)$ s.t. $H - f - E' = (V, E \cup F - \{f\} - E')$ is moral, where $E' = \{vw \in F \mid vw \in \epsilon_\beta(u)\}$.

Proof We prove the lemma by induction on the number of nodes. When $|V| \leq 3$, all graphs are moral so the lemma is true. Assuming it is true for $|V| = n - 1 \geq 4$, we want to show that the lemma is also true for n nodes. Let $R = \{x \mid D_G(x) = \emptyset\}$ and $S = \{x \mid D_H(x) = \emptyset\}$. Since both graphs are moral, none of these sets is empty. The proof is divided into two cases, depending on whether or not there exists a node $u \in S$ with $f = uv \in F$.

Case 1: $\exists u \in S$ with $f = uv \in F$. Since $u \in S$, Corollary 1 suggests H has a pek (β, ϵ_β) with $\beta(1) = u$. Furthermore, $N_H(u) - \{v\}$ still forms a clique after removing f and E' that contains the edges between v and the other neighbours of u . Therefore, $H - f - E'$ is moral with a pek $(\beta, \epsilon_\beta - E')$.

Case 2: $\nexists u \in S$ with $f = uv \in F$. In this case, we want to show that $\exists x \in S$ with $F \not\subseteq D_G(x)$. (an exmaple is sufficient?) Assuming $\nexists x \in S$. That is, $\forall x \in S$ satisfy $F \subseteq D_G(x)$. Being in S implies $D_G(x) \subseteq F$, so $F = D_G(x)$. For any node $x \in R$, Corollary 1 suggests there is a pek $(\alpha, \epsilon_\alpha)$ for G with $\alpha(1) = x$. Lemma 3 implies $(\alpha, \epsilon'_\alpha)$ is a pek for $(V, E \cup D(x)) = (V, E \cup F) = H$, hence $x \in S$. Therefore, for any node in R , it is also in S . But $x \in R$ implies $D_G(x) = \emptyset$. In conjunction with $F \neq \emptyset$, it entails that $F \not\subseteq D_G(x)$ that is a contradiction. Therefore, if case 2 is true $\exists x \in S$ with $F \not\subseteq D_G(x)$ (Figure 5).

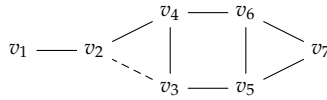


Fig. 5: An example of case 2, where $F = \{v_2v_3\}$, $R = S = \{v_1, v_7\}$. Each node $x \in S$ satisfies that $F \not\subseteq D_G(x)$.

For such a node $x \in S$, Lemma 3 and Corollary 2 imply the following moral graphs and peks

$$\begin{aligned} G &= (V, E) \text{ with } (\alpha, \epsilon_\alpha) \\ G' &= (V, E \cup D_G(x)) \text{ with } (\alpha, \epsilon'_\alpha) \\ G'_x &= (V - \{x\}, E(G[V - \{x\}]) \cup D_G(x) - \epsilon'_\alpha(x)) \\ H &= (V, E \cup F) \text{ with } (\beta, \epsilon_\beta) \\ H' &= (V, E \cup F \cup D_G(x)) \text{ with } (\beta, \epsilon'_\beta) \\ H'_x &= (V - \{x\}, E(G[V - \{x\}]) \cup F \cup D_G(x) - \epsilon'_\beta(x)). \end{aligned}$$

$F \not\subseteq D(x)$ entails $G' \subsetneq H'$. Since $\alpha(1) = \beta(1) = x$, there exist excesses s.t. $\epsilon'_\beta(x) \subseteq \epsilon'_\alpha(x)$. Let $F' = E(H'_x) - E(G'_x) = (F - D(x)) \cup (\epsilon'_\alpha(x) - \epsilon'_\beta(x))$. It follows that $F' \neq \emptyset$ and $F' \cap E(G'_x) = \emptyset$. By the inductive hypothesis, there exists an edge $f = uv \in F'$ with $\beta^{-1}(u) < \beta^{-1}(v)$ s.t. $H'_x - f - E'$ is moral where $E' = \{vw \in F' \mid vw \in \epsilon'_\beta(u)\}$. Neither of $\{f\}$ or E' is in $D(x)$, so adding $\{x\}$ and $\epsilon'_\beta(x)$ back to H'_x does not change the morality of $H' - f - E'$. \square

The following theorem is one of the main results for this section.

Theorem 3 *Let $G = (V, E)$ be a graph, and $G' = (V, E \cup F)$ be a moralization of G with $E \cap F = \emptyset$. Then F is a minimal moralization if and only if there exists a pek (β, ϵ_β) s.t. for each $f = uv \in F$ with $\beta^{-1}(u) < \beta^{-1}(v)$, $G' - f - E' = (V, E \cup F - \{f\} - E')$ is not moral, where $E' = \{vw \in F \mid vw \in \epsilon_\beta(u)\}$.*

Proof The theorem is proved by the definition of minimal moralization and Lemma 4. \square

A consequence of the theorem is that if both F and H are moralizations of G and $F \subsetneq H$, then there is a sequence of subsets of edges $\{f\} \cup E'$ that can be removed from H one by one, such that the resulting graph after each removal is moral.

Every minimal separator of a chordal graph is a clique [?]. This result, however, is not true for moral graphs which are more general than chordal graphs. The following theorem states the relation between minimal separator and moral graphs.

Theorem 4 *A graph $G = (V, E)$ is moral if and only if there exists an elimination kit $\kappa = (\alpha, \epsilon_\alpha)$ s.t. for every pair of non-adjacent vertices $u, v \in V$ with $i = \min\{\alpha^{-1}(u), \alpha^{-1}(v)\}$, the minimal u, v -separator is a clique in $G^i = G - \{\alpha(1), \dots, \alpha(i-1)\} - \{\epsilon_\alpha(\alpha(1)), \dots, \epsilon_\alpha(\alpha(i-1))\}$.*

Proof If G is moral with n nodes, there exists a pek $\kappa = (\alpha, \epsilon_\alpha)$. Without loss of generality, assuming $i = \alpha^{-1}(u) < \alpha^{-1}(v)$ for any two nodes $u, v \in V$. In addition, $uv \notin E$ implies that v is separated from u by $S \subseteq N_G(u)$. Since κ is a pek, u must be a simplicial node in the subgraph G^i . Therefore, $N_G(u)$ forms a clique and consequently any subset of it is also a clique.

To prove the sufficient condition, assume G is not moral. That is, $\exists H \subset G$ a mpe subgraph s.t. $D(H) \neq \emptyset$. Hence, $\exists C_m \subset H$ an atomic cycle for $m \geq 4$ s.t. $\exists u, v \in V(C_m)$ with $uv \notin E(C_m)$. Therefore, the minimal u, v -separator is not a clique, which is a contradiction. \square

2.2 Minimal moralization algorithms

We have defined $G^i = G - \{\alpha(1), \dots, \alpha(i-1)\} - \{\epsilon_\alpha(\alpha(1)), \dots, \epsilon_\alpha(\alpha(i-1))\}$, which can be interpreted as the resulting graph in step i of the EG algorithm.

Definition 39 Let $G = (V, E)$ be a graph and $\kappa = (\alpha, \epsilon_\alpha)$ be an elimination kit of G . If $D_{G^i}(\alpha(i)) = \emptyset$ for $i \in [1, p]$ and $\nexists \kappa' = (\beta, \epsilon_\beta)$ s.t. $D_{G^i}(\beta(i)) = \emptyset$ for $i \in [1, q]$ and $\{\alpha(1), \dots, \alpha(p)\} \subsetneq \{\beta(1), \dots, \beta(q)\}$ where $p, q \leq |V|$, then κ is called a **maximal perfect elimination kit** of G .

If κ is a maximal perfect elimination kit of G with $D_{G^i}(\alpha(i)) = \emptyset$ for $i \in [1, p]$, then $H = G - \{\alpha(1), \dots, \alpha(p)\} - \{\epsilon_\alpha(\alpha(1)), \dots, \epsilon_\alpha(\alpha(p))\}$ is called a *minimal perfect eliminated (mpe) subgraph* of G . If κ is a pek, then the mpe subgraph of G is empty. If $D(G) \neq \emptyset$, then G is the mpe subgraph of itself.

Conjecture: If $H \subset G$ is a mpe subgraph of G , then a minimal moralization of H is also a minimal moralization of G . If G has many mpe subgraphs and none of them is overlapped, then this seems trivial. But if $\exists H_1, H_2 \subset G$ are both mpe of G and $H_1 \cap H_2 \neq \emptyset$ then ?

3 Some random notes

Proposition 1 *Let F be a moral*

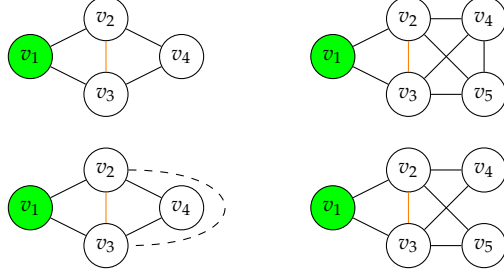


Fig. 6: A simplicial K_3 over $\{v_1, v_2, v_3\}$ shares an edge with a K_3 (top left), K_4 (top right), $\{K_3, C_m\}$ (bottom left) or $\{K_3, K_3\}$ (bottom right).

Lloyd's conjecture: knowing a graph is WRS, adding an edge to obtain a supergraph, perhaps it is efficient to check if the supergraph is wrs.

Proof because remove the added edge, then we obtain the original graph which we know is wrs. however, we don't remove a random edge when checking wrs unless the edge connects to a simplicial node. what if the edge is not connected with a sim node? if we know the original graph is wrs and we know the set of sim nodes in the recursion and the set of edges to delete, then we could easily check if the new edge is connected with any one of the sim node, if it is then good. if not, then we could check if the new edge is connected with two neighbours of a sim node, if it is then good. if a graph is wrs, then it eventually will diminish, so the new edge must appear somewhere in the recursion to either stop the recursion or don't stop it.

Corollary 3 *DAGs in the same Markov equivalent class produce the same Markov blanket sets B_X .*

Proof If two DAGs G_1 and G_2 are Markov equivalent, they have the same skeleton and the same set of colliders. This implies $B_i^{G_1} = B_i^{G_2}, \forall X_i \in X$. \square

Notice that two Markov equivalent classes could entail the same B_X . For example...

Corollary 4 $|\{\text{chordal graphs}\}| \leq |B_X| \leq |\{\text{Markov equivalent classes}\}|$.

Counting labelled chordal graphs [?], counting Markov equivalent classes (asymptotic ratio of around 0.27 to DAGs) [?].

Proposition 2 *Let G be a DAG and F be the moral graph of G . If a node x is a leaf in G , then it must be a simplicial node in F .*

Proof If x is a leaf in G , it has only parents, which form a clique after moralization. By definition, x is a simplicial node in F . \square

Table 1: Comparison between the number of labelled connected chordal graphs, the number of weak recursively simplicial graphs, the number of undirected graphs and the number of Markov equivalent classes.

# nodes	# con-C.G.	# C.G.	# WRS	# U.G.	# MEC
1	1	1	1	1	1
2	1	2	2	2	2
3	4	8	8	8	11
4	35	61	61	64	185
5	541	822	882	1024	8782
6	13302	18154		32768	1067825
7	489287	617675		2097152	312510571
8	25864897	30888596		268435456	212133402500
9	1910753782	2192816760		68719476736	326266056291213
10	1.93×10^{11}	2.15×10^{11}		3.52×10^{13}	1.19×10^{17}

Corollary 5 *Let G be a DAG and F be the moral graph of G . Then F must have at least one simplicial node.*

Proof Since each DAG has at least one leaf, by Proposition 2 F have at least one simplicial node. \square

Corollary 6 *Let G be a DAG and F be the moral graph of G . If a node x is not a simplicial node in F , then it must not be a leaf in G .*

Proposition 3 *Let G be a DAG and F be the moral graph of G . Let S^1 be the set of simplicial nodes in F and F_1 be the induced subgraph of F over $X \setminus S^1$. Then there must exist at least one simplicial node after removing from F' all the edges between $N(X_i), \forall X_i \in S^1$.*

Proof Let F'_1 be the result of removing from F_1 all the edges between $N(X_i), \forall X_i \in S^1$. The corresponding directed graph G' of F'_1 must be a subgraph of the DAG G , so also acyclic. Assuming F'_1 has no simplicial nodes, by Corollary 6 G' has no leaf, which is a contradiction. \square

Here are some issues worth discussing:

1. Application: the backtracking algorithm can now be applied when learning MBs in parallel. What if there are conflicts between two MBs, which one should give up? Need to estimate uncertainty?
2. Simplicial nodes in the first step always contain the leaves.
3. Those nodes that become simplicial in the next step without having to delete any edges contain the leaves in the next step.
4. So wrs can be used to test if a MB family is consistent with a DAG, it would be good if we can also find out how many consistent DAGs or essential graphs are there for this MB family.
5. also it would be good if we can explore wrs into details, such as what dag nodes become simplicial nodes in wrs recursion, and if no edges need to be deleted from a simplicial node's neighbours then what's this simplicial node?

6. maybe there is a path from s.t. every step is a moral graph of a dag, perhaps can be proved by delete an edge from a dag.

Questions: If a graph F is known to be wrs, does it help to decide if a subgraph/-supergraph different by one edge from F is wrs or not?

Answer: Probably not. If it is, then we know a base case, any graph can be reached from this base case, hence any graph can be efficiently tested.

4 Appendix

4.1 Polytree

Proposition 4 *Let $T = (V, E)$ be a polytree and F be the moral graph of T . Then F is a chordal graph.*

Proof Assuming F is not a chordal graph, there must exist a chordless $C_m \subset F$ for $m \geq 4$. F being moral implies that the C_m shares an edge with a simplicial clique K_n for $n \geq 3$. Hence, there are multiple paths between a node in the C_m and the simplicial node in the K_n via different neighbours of the simplicial node. Hence, the assumption leads to a contradiction to T being singly connected. \square

The converse of Proposition 4 is not true. For example, the chordal moral graph in Figure 7 comes from a non-singly connected DAG.

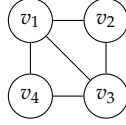


Fig. 7: A chordal graph that comes from moralizing a non-singly connected DAG.

Corollary 7 *Let B_X be a set of Markov blankets over a variable set X . The problem of testing if B_X is consistent with a polytree tree is in polynomial time.*

Proof Chordality can be verified in polynomial time [?]. \square

Idea: Since it is in polynomial time to check if a set of learned B_X is consistent with a DAG or not, we could start the structure discovery process by learning a polytree over all variables in X . Then gradually build up a DAG from a polytree. In addition, because a polytree is a subset of DAGs, so there would be less number of consistent polytrees to a chordal graph than consistent DAGs to a WRS graph.