

## Supplementary material for: Active Structure Learning of Causal DAGs via Directed Clique Trees

### A Meek Rules

In this section, we recall the *Meek rules* (Meek, 1995) for propagating orientations in DAGs. Of the standard four Meek rules, two of them only apply when the DAG contains v-structures. Since all DAGs that we need to consider do not have v-structures, we include only the first two rules here.

**Proposition 2** (Meek Rules under no v-structures).

1. **No colliders:** If  $a \rightarrow_G b \leftarrow_G c$  and  $a$  is not adjacent to  $c$ , then  $b \rightarrow_G c$ .

2. **Acyclicity:** If  $a \rightarrow_G b \rightarrow_G c$  and  $a$  is adjacent to  $c$ , then  $a \rightarrow_G c$ .

### B The running intersection property

A useful and well-known property of clique trees, used throughout proofs in the remainder of the appendix, is the following:

**Prop.** (Running intersection property). *Let  $\gamma = \langle C_1, \dots, C_K \rangle$  be the path between  $C_1$  and  $C_K$  in the clique tree  $T_G$ . Then  $C_1 \cap C_K \subseteq C_k$  for all  $C_k \in \gamma$ .*

We refer the interested reader to Maathuis et al. (2018).

### C Proof of Proposition 1

This proposition describes the connection between arrow-meets and intersection comparability. In order to prove this proposition, we begin by establishing the following propositions:

**Proposition 3.** *Suppose  $C_1$  and  $C_2$  are adjacent in  $T_G$ . Then for all  $v_1 \in C_1 \setminus C_2$ ,  $v_2 \in C_2 \setminus C_1$ ,  $v_1$  and  $v_2$  are not adjacent in  $G$ .*

*Proof.* We prove the contrapositive. Suppose  $v_1 \in C_1 \setminus C_2$  and  $v_2 \in C_2 \setminus C_1$  are adjacent. Then  $C'_3 = (C_1 \cap C_2) \cup \{v_1, v_2\}$  is a clique and belongs to some maximal clique  $C_3$ . For the induced subtree property to hold,  $C_3$  must lie between  $C_1$  and  $C_2$ , i.e.,  $C_1$  and  $C_2$  are not adjacent.  $\square$

**Proposition 4.** *Let  $D$  be a moral DAG, there are no undirected edges in any of its directed clique trees  $T_D$ , and therefore neither in its directed clique graph  $\Gamma_D$ .*

*Proof.* (By contradiction). Suppose  $v_2 \rightarrow_D v'_{12}$  for some  $v'_{12} \in C_1 \cap C_2$ ,  $v_2 \in C_2 \setminus C_1$ . By the assumption that  $D$  does not have v-structures and by Prop. 3,  $v_{12} \neq v'_{12}$ . Similarly, since  $v_{12} \rightarrow_D v_2$  (otherwise there would be a v-structure with  $v_1 \rightarrow_D v_{12}$ ) and  $v'_{12} \rightarrow_D v_1$  (otherwise there would be a collider with  $v_2 \rightarrow_D v'_{12}$ ). However, this induces a cycle  $v_1 \rightarrow_D v_{12} \rightarrow_D v_2 \rightarrow_D v'_{12} \rightarrow_D v_1$ .  $\square$

Now we can finally prove the final proposition:

**Proposition 1.** *Suppose  $C_1 \ast \rightarrow_{T_D} C_2$  and  $C_2 \leftarrow \ast_{T_D} C_3$  in  $T_D$ . Then these edges are intersection comparable. Equivalently in the contrapositive, if  $C_1 \ast \rightarrow_{T_D} C_2$  and  $C_2 \ast \leftarrow_{T_D} C_4$  are intersection incomparable, we can immediately deduce that  $C_2 \rightarrow_{T_D} C_4$ .*

*Proof.* We prove the contrapositive. If  $C_1 \cap C_2 \not\subseteq C_2 \cap C_3$  and  $C_1 \cap C_2 \not\subseteq C_2 \cap C_4$ , then there exist nodes  $v_{12} \in (C_1 \cap C_2) \setminus C_3$  and  $v_{23} \in (C_2 \cap C_3) \setminus C_1$ . Since  $v_{12}$  and  $v_{23}$  are both in the same clique  $C_2$  they are adjacent in the underlying DAG  $D$ , i.e.  $v_{12} -_D v_{23}$ . Moreover since  $C_1 \ast \rightarrow_{T_D} C_2$  by the definition of a directed clique graph, this edge is oriented as  $v_{12} \rightarrow_D v_{23}$ . Then by Prop. 4,  $C_2 \rightarrow_{T_D} C_3$ .  $\square$

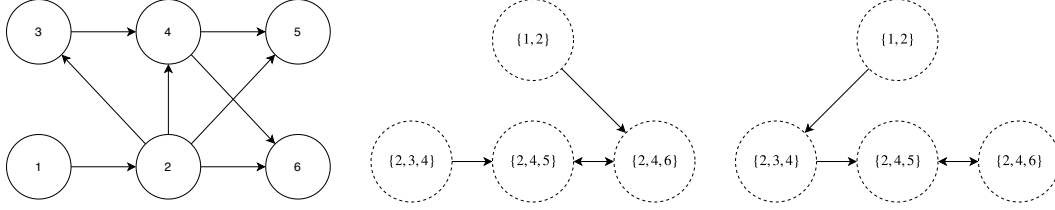


Figure 7: A DAG, its DCT with a conflicting source, and its DCG without a conflicting source.

## D Proof of Lemma 2

**Lemma 2.** *For any moral DAG  $D$ , one can always construct a CDCT with no arrow-meets.*

*Proof.* To construct a CDCT with no arrow-meets, our approach is to first construct the DCT in a special way, so that after contraction, there are no arrow-meets. In particular, we need a DCT such that each bidirected component has at most one incoming edge. A DCT in which this does not hold is said to have *conflicting sources*, formally:

**Definition 11.** *A directed clique tree  $T_D$  has two conflicting sources  $C_0$  and  $C_{K+1}$ , if  $C_0 \rightarrow_{T_D} C_1$  and  $C_K \leftarrow_{T_D} C_{K+1}$ , and  $C_1$  and  $C_K$  are part of the same bidirected component  $B \in \mathcal{B}(T_D)$ , i.e.  $C_1, C_K \in B$ , possibly with  $C_1 = C_K$ .*

An example of a clique tree with conflicting sources is given in Fig. 7. The first DCT has conflicting sources  $\{1, 2\}$  and  $\{2, 3, 4\}$ , while the second DCT does not have conflicting sources.

We will now show that Algorithm 3 constructs a DCT with no conflicting sources. This is sufficient to prove 2, since after contraction, the resulting CDCT will have no arrow-meets.

First, Algorithm 3 constructs a weighted clique graph  $W_G$ , which is a complete graph over vertices  $\mathcal{C}(G)$ , with the edge  $C_1 -_{W_G} C_2$  having weight  $|C_1 \cap C_2|$ . We will show that at each iteration  $i$ , there are no conflicting sources in  $T_D$ . This is clearly true for  $i = 0$  since  $T_D$  has no edges to begin.

At a given iteration  $i$ , suppose that the candidate edge  $e = C_1 \rightarrow C_2$  is a maximum-weight edge that does not create a cycle, i.e.  $e \in E$ , but that it will induce conflicting sources. That is, the current  $T_D$  already contains  $C_2 \leftarrow C_3 \leftarrow \dots \leftarrow C_{K-1} \leftarrow C_K$ , where we choose  $C_K$  that has no parents. Note that we can do this by following any directed/bidirected edges upstream (away from  $C_2$ ), which must terminate since  $T_D$  is a tree and thus does not have cycles.

By Prop. 1,  $C_1 \cap C_2 \subseteq C_2 \cap C_3$ . In this case,  $C_1 \cap C_2 \subseteq C_2 \cap C_3$ , since  $C_2 \leftarrow C_3$  was already picked as an edge and thus cannot have less weight (in other words, it cannot have a smaller intersection) than  $C_1 \rightarrow C_2$ . Furthermore, since  $C_1 - C_2 - C_3$  is a valid subgraph of the clique tree, we must have  $C_1 \cap C_3 \subseteq C_2$  by the running intersection property of clique trees (see Appendix B). Combined with  $C_1 \cap C_2 \subseteq C_2 \cap C_3$ , we have  $C_1 \cap C_3 = C_1 \cap C_2$ . This means that  $C_1 - C_3$  is also a valid edge in the weighted clique graph and it has the same weight ( $C_1 \cap C_3$ ) as the  $C_1 - C_2$  edge ( $C_1 \cap C_2$ ). Moreover since  $C_1 \rightarrow C_2$  then this edge will also preserve the same orientations  $C_1 \rightarrow C_3$ . Thus,  $C_1 \rightarrow C_3$  is another candidate maximum-weight edge that does not create a cycle. We may continue this argument, replacing  $C_2$  by  $C_k$ , to show that  $C_1 \rightarrow C_K$  is a maximum weight edge that does not create a cycle. Since  $C_K$  has no parents, there are still no conflicting sources after adding  $C_1 \rightarrow C_K$ . Since we always pick a maximum-weight edge that does not create a cycle, this algorithm creates a maximum-weight spanning tree of  $W_G$  (Koller & Friedman, 2009), which is guaranteed to be a clique tree of  $G$  Koller & Friedman (2009).  $\square$

## E Proof of Lemma 3

The following lemma establishes that after finding the orientations of edges in the DCT, the only remaining unoriented edges are in the residuals.

**Lemma 3.** *The oriented edges of  $\mathcal{E}_{T_D}$  can be inferred directly from the oriented edges of  $T_D$ .*

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**Algorithm 3** CONSTRUCT\_DCT
 

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1: Input: DAG  $D$ 
2: let  $W_G$  be the weighted clique graph of  $G = \text{skel}(D)$ 
3: let  $T_D$  be the empty graph over  $V(W_G)$ 
4: for  $i = 1, \dots, |V(W_G)| - 1$  do
5:   let  $E$  be the set of maximum-weight edges of  $W_G$  that do not create a cycle when added to  $T_D$ 
6:   select  $e \in E$  s.t. there are no conflicting sources
7:   add  $e$  to  $T_D$ 
8: end for
9: Contract the bidirected components of  $T_D$  and create the CDCT  $\tilde{T}_D$ 
10: Return  $\tilde{T}_D$ 

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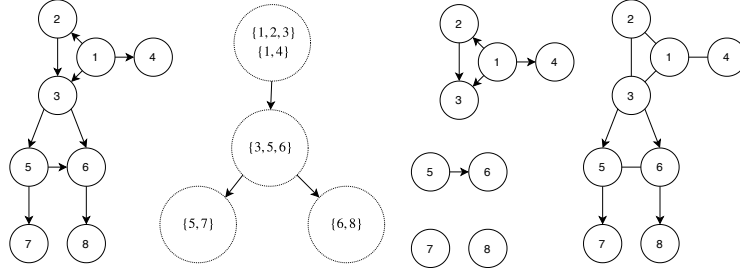


Figure 8: A DAG, its contracted directed clique tree, its residuals, and its residual essential graph.

489 *Proof.* In order to prove this theorem, we first introduce an alternative characterization of the  
 490 residual essential graph defined only in terms of the orientations in the contracted DCT and prove its  
 491 equivalence to Definition 12. Let  $\mathcal{E}_{\tilde{T}_D}$  have the same skeleton as  $D$ , with  $i \rightarrow_{\mathcal{E}_{\tilde{T}_D}} j$  if and only if  
 492  $j \in \text{Res}_{\tilde{T}_D}(B)$  and  $i \in P$ , for some  $B \in \mathcal{B}(\tilde{T}_D)$  and its unique parent  $P$ .

493 Suppose  $v_1 \rightarrow_D v_2$  for  $v_1 \in R_1$  and  $v_2 \in R_2$ , with  $R_1, R_2 \in \mathcal{R}(\tilde{T}_D)$  and  $R_1 \neq R_2$ . Let  
 494  $R_1 = \text{Res}_{\tilde{T}_D}(B_1)$  and  $R_2 = \text{Res}_{\tilde{T}_D}(B_2)$  for  $B_1, B_2 \in \mathcal{B}(\tilde{T}_D)$ . There must be at least one clique  
 495  $C_1 \in B_1$  that contains  $v_1$ , and likewise one clique  $C_2 \in B_2$  that contains  $v_2$ . Since  $v_1$  and  $v_2$  are  
 496 adjacent, by the induced subtree property there must be some maximal clique on the path between  
 497  $C_1$  and  $C_2$  which contains  $v_1$  and  $v_2$ . Let  $C_{12}$  be the clique on this path containing  $v_1$  and  $v_2$  that  
 498 is closest to  $C_1$ . Then, the next closest clique to  $C_1$  must not contain  $v_2$ , so we will call this clique  
 499  $C_{1 \setminus 2}$ . Since  $v_1 \rightarrow_D v_2$ , we know that  $C_{1 \setminus 2} \rightarrow_{T_D} C_{12}$ , hence  $C_{1 \setminus 2}$  and  $C_{12}$  are in different bidirected  
 500 components, and thus  $v_1 \rightarrow_D v_2$ .  $\square$

## 501 F Proof of Theorem 1

502 **Theorem 1.** An intervention set is a VIS for any general DAG  $D$  iff it contains VISes for each residual  
 503  $R \in \mathcal{R}(\tilde{T}_G)$  for all chain components  $G \in \mathcal{CC}(\mathcal{E}(D))$  of its essential graph  $\mathcal{E}(D)$ .

504 In order to prove the following theorem we start by introducing a few useful concepts and results.

### 505 F.1 Residual essential graphs

506 The residuals decompose the DAG into parts which must be separately oriented. Intuitively, after  
 507 adding orientations *between* all pairs of residuals, the inside of one residual is cut off from the insides  
 508 of other residuals. The following definition and lemma formalize this intuition.

509 **Definition 12.** The residual essential graph  $\mathcal{E}_{T_D}$  of  $D$  has the same skeleton as  $D$ , with  $v_1 \rightarrow_{\mathcal{E}_{T_D}} v_2$   
 510 iff  $v_1 \rightarrow_D v_2$  and  $v_1$  and  $v_2$  are in different residuals of  $\tilde{T}_D$ .

511 **Lemma 4.** The  $\mathcal{E}_{\text{res}}(D)$  is complete under Meek's rules (Meek, 1995).

512 *Proof.* Since Meek rules are sound and complete rules for orienting PDAGs (Meek, 1995), and in our  
 513 setting only two of the Meek rules apply (see Prop. 2 in Appendix A), it suffices to show that neither  
 514 applies for residual essential graphs.

515 First, suppose  $i \rightarrow_{\mathcal{E}_{\text{res}}(D)} j$  and  $j \rightarrow_{\mathcal{E}_{\text{res}}(D)} k$ . We must show that if  $i$  and  $k$  are adjacent, then  
 516  $i \rightarrow_{\mathcal{E}_{\text{res}}(D)} k$ , i.e. the acyclicity Meek rule does not need to be invoked.

517 We use the alternative characterization of  $\mathcal{E}_{\text{res}}(D)$  from the proof of Lemma ??, which establishes  
 518 that  $i \rightarrow_{\mathcal{E}} j$  iff.  $j \in \text{Res}_{\mathcal{T}_D}(B)$  and  $i \in P$  for some  $B \in \mathcal{B}(\tilde{T}_D)$  and its unique parent  $P$ .

519 Since  $j \rightarrow_{\mathcal{E}_{\text{res}}(D)} k$ , there must exist some component  $B_{jk} \in \mathcal{B}(\tilde{T}_D)$  containing  $j$  and  $k$  whose parent  
 520 component  $B_{j \setminus k}$  contains  $j$  but not  $k$ , i.e.  $B_{j \setminus k} \rightarrow_{\tilde{T}_D} B_{jk}$ . Likewise, there must be a component  $B_{ij}$   
 521 containing  $i$  and  $j$  whose parent component  $B_{i \setminus j}$  contains  $i$  but not  $j$ , i.e.  $B_{i \setminus j} \rightarrow_{\tilde{T}_D} B_{ij}$ . Moreover,  
 522 since there is a clique on  $\{i, j, k\}$ , there must be at least one component  $B_{ijk}$  containing  $i, j$  and  $k$ .

523 We will prove that  $B_{jk}$  and  $B_{j \setminus k}$  both contain  $i$ , which implies  $i \rightarrow_{\tilde{T}_D} k$ .

524 Let  $\gamma$  be the path in  $\tilde{T}_D$  between  $B_{i \setminus j}$  and  $B_{jk}$ . This path must contain the edge  $B_{j \setminus k} \rightarrow B_{jk}$ , since  
 525  $B_{i \setminus j}$  is upstream of  $B_{jk}$ , and  $\tilde{T}_D$  is a tree. By the induced subtree property on  $k$ , no component on  
 526 the path other than  $B_{jk}$  can contain  $k$ . Now consider the path between  $B_{ijk}$  and  $B_{i \setminus j}$ . By the induced  
 527 subtree property on  $k$ , this path must pass through  $B_{jk}$ . Finally, by the induced subtree property on  $i$ ,  
 528  $B_{jk}$  and  $B_{j \setminus k}$  must both contain  $i$ .

529 Now, we prove that also the first Meek rule is not invoked. Suppose  $i \rightarrow_{\mathcal{E}_{\text{res}}(D)} j$ , and  $j$  is adjacent to  
 530  $k$ . We must show that if  $i$  is not adjacent to  $k$ , then  $j \rightarrow_{\mathcal{E}_{\text{res}}(D)} k$ .

531 Since  $\{i, j, k\}$  do not form a clique, there must be distinct components containing  $i \rightarrow j$  and  $j \rightarrow k$ .  
 532 Let  $B_{ij}$  and  $B_{jk}$  denote the closest such components in  $\tilde{T}_D$ , which are uniquely defined since  $\tilde{T}_D$  is a  
 533 tree. Since  $i$  is upstream of  $k$ ,  $B_{ij}$  must be upstream of  $B_{jk}$ . Let  $P := \text{pa}_{\tilde{T}_D}(B_{jk})$ , we know  $j \in P$   
 534 since it is on the path between  $B_{ij}$  and  $B_{jk}$  (it is possible that  $P = B_{ij}$ ). Since we picked  $B_{jk}$  to be  
 535 the closest component to  $B_{ij}$  containing  $\{j, k\}$ , we must have  $k \notin P$ , so indeed  $j \rightarrow_G k$ .  $\square$

536 For an example of the residual essential graph, see Fig. 8. Lemma 4 implies that the residuals must be  
 537 oriented separately, since the orientations in one do not impact the orientations in others.

## 538 F.2 Proof for a moral DAG

539 We then prove the result for a moral DAG  $D$ :

540 **Lemma 5 (VIS Decomposition).** *An intervention set is a VIS for a moral DAG  $D$  iff it contains VISes*  
 541 *for each residual of  $\tilde{T}_D$ . This implies that finding a VIS for  $D$  can be decomposed in several smaller*  
 542 *tasks, in which we find a VIS for each of the residuals in  $\mathcal{R}(\tilde{T}_D)$ .*

543 *Proof.* We first prove that any VIS  $\mathcal{I}$  of  $D$  must contain VISes for each residual of  $D$ . Consider the  
 544 residual essential graph  $\mathcal{E}_{\text{res}}(D)$  of  $D$ . We show that if we intervene on a node  $c_1$  in the residual  
 545  $R_1 = \text{Res}_{\tilde{T}_D}(B_1)$  of some  $B_1 \in \mathcal{B}(\tilde{T}_D)$ , then the only new orientations are between nodes in  $R_1$ , or  
 546 in other words, each residual needs to be oriented independently.

547 By Definition 12, all edges between nodes in different residuals are already oriented in  $\mathcal{E}_{\text{res}}(D)$ . A  
 548 new orientation between nodes in  $R_1$  will not have any impact for the nodes in the other residuals,  
 549 which we can show by proving that Meek rules described in Prop. 2 would not apply outside of the  
 550 residual. In particular, Meek Rule 1 does not apply at all, since  $b$  and  $c$  must be in the same residual  
 551 since the edge is undirected, but then  $a$  is adjacent to  $c$  since it's a clique. Likewise,  $a -_{\mathcal{E}_{\text{res}}(D)} c$ , then  
 552  $a$  and  $b$  are in the same residual, so Meek Rule 2 only orients edges with both endpoints in the same  
 553 residual.

554 Now, we show that if  $\mathcal{I}$  contains VISes for each residual of  $D$ , then it is a VIS for  $D$ . We will  
 555 accomplish this by inductively showing that all edges in each bidirected component are oriented. Let  
 556  $\gamma = \langle B_1, \dots, B_n \rangle$  be a path from the root of  $\tilde{T}_D$  to a leaf of  $\tilde{T}_D$ . As our base case, all edges in  $B_1$   
 557 are oriented, since  $B_1 = \text{Res}_{\tilde{T}_D}(B_1)$ . Now, as our induction hypothesis, suppose that all edges in  
 558  $B_{i-1}$  are oriented.

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**Algorithm 4** FIND\_MVIS\_DCT

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1: Input: Moral DAG  $D$ 
2: let  $\tilde{T}_D$  be the contracted directed clique tree of  $D$ 
3: let  $S = \emptyset$ 
4: for component  $B$  of  $T_D$  do
5:   let  $R = \text{Res}_{\tilde{T}_D}(B)$ 
6:   let  $S' = \text{FIND\_MVIS\_ENUMERATION}(G[R])$ 
7:   let  $S = S \cup S'$ 
8: end for
9: Return  $S$ 
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559 The edges between nodes in  $B_i$  are partitioned into three categories: edges with both endpoints also  
560 in  $B_{i-1}$ , edges with both endpoints in  $\text{Res}_{\tilde{T}_D}(B_i)$ , and edges with one endpoint in  $B_{i-1}$  and one  
561 endpoint in  $\text{Res}_{\tilde{T}_D}(B_i)$ . The first category of edges are directed by the induction hypothesis, and  
562 the second category of edges are directed by the assumption that  $\mathcal{I}$  contains VISes for each residual.  
563 It remains to show that all edges in the third category are oriented. Each of these edges has one  
564 endpoint in some  $C_{i-1} \in B_{i-1}$  and one endpoint in some  $C_i$  in  $B_i$ , so we can fix some  $C_{i-1}$  and  $C_i$   
565 and argue that all edges from  $C_{i-1} \cap C_i$  to  $C_i \setminus C_{i-1}$  are oriented.

566 Since  $C_{i-1} \rightarrow_{R_D} C_i$ , there exists some  $c_{i-1} \in C_{i-1} \setminus C_i$  and  $c' \in C_i \cap C_{i-1}$  such that  $c_{i-1} \rightarrow_D c'$ .  
567 By Prop. 3,  $c_{i-1}$  is not adjacent to any  $c_i \in C_i \setminus C_{i-1}$ , so Meek Rule 1 ensures that  $c' \rightarrow_D c_i$  is  
568 oriented. For any other node  $c'' \in C_{i-1} \cap C_i$ , either  $c' \rightarrow_D c''$ , in which case Meek Rule 2 ensures  
569 that  $c_{i-1} \rightarrow_D c''$  and the same argument applies, or  $c'' \rightarrow_D c'$ , in which case Meek Rule 2 ensures  
570 that  $c'' \rightarrow_D c_i$ .  $\square$

### 571 E.3 Proof for a general DAG

572 We can now easily prove the theorem for any DAG  $D$ :

573 **Theorem 1.** *An intervention set is a VIS for any general DAG  $D$  iff it contains VISes for each residual*  
574  *$R \in \mathcal{R}(\tilde{T}_D)$  for all chain components  $G \in \mathcal{CC}(\mathcal{E}(D))$  of its essential graph  $\mathcal{E}(D)$ .*

575 *Proof.* By the previous result (Lemma 5) and Lemma 1 from (Hauser & Bühlmann, 2012).  $\square$

## 576 G Algorithm for finding an MVIS

577 An algorithm using the decomposition into residuals to compute a minimal verifying intervention set  
578 (MVIS) is described in Algorithms 4 and 5. Compared to running Algorithm 5 on any moral DAG,  
579 using Algorithm 4 ensures that we only have to enumerate over subsets of the nodes in each residual,  
580 which in general require far fewer interventions. Moreover, the residual of any component containing  
581 a single clique is itself a clique, which have easily characterized MVISes, and Algorithm 5 efficiently  
582 computes.

## 583 H Proof of Theorem 2

584 First, we prove the following proposition:

585 **Proposition 5.** *Let  $D$  be a moral DAG,  $\mathcal{E} = \mathcal{E}(D)$  and let  $\tilde{T}_D$  contain a single bidirected component.*  
586 *Then  $m(D) \geq \left\lfloor \frac{\omega(\mathcal{E})}{2} \right\rfloor$ .*

587 *Proof.* Let  $C_1 \in \arg \max_{C \in \mathcal{C}(\mathcal{E})} |C|$ . By the running intersection property (see Appendix B), for  
588 any clique  $C_2$ ,  $C_1 \cap C_2 \subseteq C_2 \cap C_{\text{adj}}$  for  $C_{\text{adj}}$  adjacent to  $C_2$  in  $T_D$ . Since  $C_{\text{adj}} \leftrightarrow_{T_D} C_2$ , we have  
589  $v_{12} \rightarrow_D v_{2 \setminus 1}$  for all  $v_{12} \in C_1 \cap C_2$  and  $v_{2 \setminus 1} \in C_2 \setminus C_1$ , i.e. there is no node in  $D$  outside of  $C_1$   
590 that points into  $C_1$ . Thus, since the Meek rules only propagate downward, intervening on any nodes  
591 outside of  $C_1$  does not orient any edges within  $C_1$ . Finally, since  $C_1$  is a clique, each consecutive

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**Algorithm 5** FIND\_MVIS\_ENUMERATION
 

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1: Input: DAG  $D$ 
2: if  $D$  is a clique then
3:   Let  $\pi$  be a topological ordering of  $D$ 
4:   Let  $S$  include even-indexed element of  $\pi$ 
5:   Return  $S$ 
6: end if
7: for  $s = 1, \dots, |V(D)|$  do
8:   for  $S \subseteq V(D)$  with  $|S| = s$  do
9:     if  $S$  fully orients  $D$  then
10:      Return  $S$ 
11:    end if
12:   end for
13: end for

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592 pair of nodes in the topological order of  $C_1$  must have at least one of the nodes intervened, which  
 593 requires  $\left\lfloor \frac{|C_1|}{2} \right\rfloor$  interventions.  $\square$

594 Now we can prove the following result for a moral DAG  $D$ :

595 **Lemma 6.** *Let  $D$  be a moral DAG and let  $G = \text{skel}(D)$ . Then  $m(D) \geq \left\lfloor \frac{\omega(G)}{2} \right\rfloor$ , where  $\omega(G)$  is the*  
 596 *size of the largest clique in  $G$ .*

597 Consider a path  $\gamma$  from the source of  $\tilde{T}_D$  to the bidirected component containing the largest clique, i.e.,  
 598  $\gamma = \langle B_1, \dots, B_Z \rangle$ . For each component, pick  $C_i^* \in \arg \max_{C \in B_i} |C|$ . Also, let  $R_i = \text{Res}_{\tilde{T}_D}(B_i)$ .  
 599 We will prove by induction that  $\sum_{i=1}^z m(D[R_i]) \geq \max_{i=1}^z \left\lfloor \frac{|C_i^*|}{2} \right\rfloor$  for any  $z = 1, \dots, Z$ . As a base  
 600 case, it is true for  $z = 1$ , since  $R_1 = B_1$  and by Prop. 5.

601 Suppose the lower bound holds for  $z - 1$ . If  $C_z^*$  is not the unique maximizer of  $\left\lfloor \frac{|C_i^*|}{2} \right\rfloor$  over  
 602  $i = 1, \dots, z$ , the lower bound already holds. Thus, we consider only the case where  $B_z$  is the unique  
 603 maximizer.

604 Let  $S_z = C_z^* \cap B_{z-1}$ . By the running intersection property (see Appendix B),  $S_z$  is contained in the  
 605 clique  $C_{\text{adj}}$  in  $B_{z-1}$  which is adjacent to  $C_z^*$  in  $T_D$ . Since  $C_{\text{adj}}$  is distinct from  $C_z^*$ ,  $|C_{\text{adj}}| \geq |S_z| + 1$ ,  
 606 and by the induction hypothesis we have that

$$\begin{aligned}
 \sum_{i=1}^{z-1} m(D[R_i]) &\geq \max_{i=1, \dots, z-1} \left\lfloor \frac{|C_i^*|}{2} \right\rfloor \\
 &\geq \left\lfloor \frac{|C_{z-1}^*|}{2} \right\rfloor \\
 &\geq \left\lfloor \frac{|C_{\text{adj}}|}{2} \right\rfloor \\
 &\geq \left\lfloor \frac{|S_z| + 1}{2} \right\rfloor
 \end{aligned}$$

607 Finally, applying Prop. 5,

$$\begin{aligned}
 \left\lfloor \frac{|S_z| + 1}{2} \right\rfloor + m(D[R_z]) &\geq \left\lfloor \frac{|S_z| + 1}{2} \right\rfloor + \left\lfloor \frac{|C_z^* \cap R_z|}{2} \right\rfloor \\
 &\geq \left\lfloor \frac{|C_z^*|}{2} \right\rfloor
 \end{aligned}$$

608 where the last equality holds since  $|S_z| + |C_z^* \cap R_z| = |C_z^*|$  and by the property of the floor function  
 609 that  $\left\lfloor \frac{a+1}{2} \right\rfloor + \left\lfloor \frac{b}{2} \right\rfloor \geq \left\lfloor \frac{a+b}{2} \right\rfloor$ , which can be easily checked.

---

**Algorithm 6** CLIQUEINTERVENTION

---

```

1: Input: Clique  $C$ 
2: while  $C -_{\Gamma_D} C'$  unoriented for some  $C'$  do
3:   if  $\exists v$  non-dominated in  $C$  then
4:     Pick  $v \in C$  at random among non-dominated nodes.
5:   else
6:     Pick  $v \in C$  at random.
7:   end if
8:   Intervene on  $v$ .
9: end while
10: Output:  $P_{\text{up}}(C)$ 

```

---



---

**Algorithm 7** EDGEINTERVENTION

---

```

1: Input: Adjacent cliques  $C, C'$ 
2: while  $C -_{\Gamma_D} C'$  unoriented do
3:   Pick  $v \in C \cap C'$  at random.
4:   Intervene on  $v$ .
5: end while
6: Output:  $P_{\text{up}}(C)$ 

```

---

610 Finally we can prove the theorem:

611 **Theorem 2.** *Let  $D$  be any DAG. Then  $m(D) \geq \sum_{G \in \text{cc}(\mathcal{E}(D))} \left\lfloor \frac{\omega(G)}{2} \right\rfloor$ , where  $\omega(G)$  is the size of the*  
612 *largest clique in each of the chain components  $G$  of the essential graph  $\mathcal{E}(D)$ .*

613 *Proof.* By Lemma 6 and Lemma 1 in Hauser & Bühlmann (2012). □

## 614 I Clique and Edge Interventions

615 We present the procedures that we use for clique- and edge-interventions in Algorithm 6 and Algo-  
616 rithm 7, respectively.

## 617 J Identify-Upstream Algorithm

618 Given the clique graph, a simple algorithm to identify the upstream branch consists of performing an  
619 edge-intervention on each pair of parents of  $C$  to discover which is the most upstream. However, if  
620 the number of parents of  $C$  is large, this may consist of many interventions. The following lemma  
621 establishes that the only parents which are candidates for being the most upstream are those whose  
622 intersection with  $C$  is the smallest:

623 **Proposition 6.** *Let  $P_{\text{up}}(C) \in \text{pa}_{\Gamma_D}(C)$  be the parent of  $C$  which is upstream of all other parents.*  
624 *Then  $P_{\text{up}}(C) \in \mathcal{P}_{\Gamma_D}(C)$ , where  $\mathcal{P}_{\Gamma_D}(C)$  is the set of parents of  $C$  in  $\Gamma_D$  with the smallest intersection*  
625 *size, i.e.,  $P \in \mathcal{P}_{\Gamma_D}(C)$  if and only if  $P \rightarrow_{\Gamma_D} C$  and  $|P \cap C| \leq |P' \cap C|$  for all  $P' \in \text{pa}_{\Gamma_D}(C)$ .*

626 *Proof.* We begin by citing a useful result on the relationship between clique trees and clique graphs  
627 when the clique contains an intersection-comparable edge:

628 **Lemma 7** (Galinier et al. (1995)). *If  $C_1 -_{T_G} C_2 -_{T_G} C_3$  and  $C_1 \cap C_2 \subseteq C_2 \cap C_3$ , then  $C_1 -_{\Gamma_G} C_3$ .*

629 **Corollary 1.** *If  $C_1 -_{T_G} C_2 -_{T_G} C_3$  and  $C_1 \cap C_2 \subseteq C_2 \cap C_3$ , then  $C_1 \cap C_3 = C_1 \cap C_2$ .*

630 *Proof.* By the running intersection property of clique trees (see Appendix B),  $C_1 \cap C_3 \subseteq C_2$ .  
631 Combined with  $C_1 \cap C_2 \subseteq C_2 \cap C_3$  and simple set logic, the result is obtained. □

---

**Algorithm 8** IDENTIFYUPSTREAM
 

---

```

1: Input: Clique  $C$ 
2: for  $P_1, P_2 \in \mathcal{P}_{\Gamma_D}(C)$  do
3:   perform an edge-intervention on  $P_1 -_{\Gamma_D} P_2$ 
4: end for
5: Output:  $P_{\text{up}}(C)$ 

```

---

Every parent of  $C$  is adjacent in  $\Gamma_D$  to every other parent of  $C$  by Prop. 1 and Lemma 7, and since every edge has at least one arrowhead, there can be at most one parent of  $C$  that does not have an incident arrowhead.

Now we show that this parent must be in  $\mathcal{P}_{\Gamma_D}(C)$ . Corollary 1 implies that for any triangle in  $\Gamma_G$ , two of the edge labels (corresponding to intersections of their endpoints) must be equal. If  $P \in \mathcal{P}_{\Gamma_D}(C)$  and  $P' \in \text{pa}_{T_D}(C) \setminus \mathcal{P}_{\Gamma_D}(C)$ , then the labels of  $P \rightarrow_{\Gamma_D} C$  and  $P' \rightarrow_{\Gamma_D} C$  are of different size and thus cannot match. Therefore, the label of  $P \cap P' = P \cap C$ . Finally, since we already know  $P \rightarrow_{\Gamma_D} C$ , it must also be the case that  $P \rightarrow_{\Gamma_D} P'$ .  $\square$

### K Proof of Theorem 3

We start by proving bounds for each of the two phases:

**Lemma 8.** *Algorithm 2 uses at most  $\lceil \log_2 |\mathcal{C}| \rceil$  clique-interventions. Moreover, assuming  $T_G$  is intersection-incomparable, Algorithm 2 uses no edge-interventions.*

*Proof.* Since  $T_G$  is intersection-incomparable, after a clique-intervention on  $C$ , orientations propagate in all but at most one branch of  $T_G$  out of  $C$ . By the definition of a central node, the one possible remaining branch has at most half of the nodes from the previous time step, so the number of edges in  $T_G$  reduces by at least half after each clique-intervention. Thus, there can be at most  $\lceil \log_2 |\mathcal{C}| \rceil$  clique-interventions.  $\square$

For ease of notation, we will overload the symbol  $\text{CC}$  for the chain components of a chain graph  $G$  to take a DAG as an argument, and return the subgraphs corresponding to the chain components of its essential graph. Formally,  $\text{CC}(D) = \{D[V(G)] \mid G \in \text{CC}(\mathcal{E}(D))\}$ .

**Lemma 9.** *The second phase of Algorithm 1 (line 6-8) uses at most  $\sum_{C \in \mathcal{C}(D')} |\text{Res}_{\tilde{T}_{D'}}(C)| - 1$  single-node interventions for the moral DAG  $D' \in \text{CC}(D)$ .*

*Proof.* Eberhardt et al. (2006) show that  $n - 1$  single-node interventions suffice to determine the orientations of all edges between  $n$  nodes. We sum this value over all residuals.  $\square$

**Theorem 3.** *Assuming  $\Gamma_G$  is intersection-incomparable, Algorithm 1 uses at most  $(3\lceil \log_2 \mathcal{C}_{\max} \rceil + 2)m(D)$  single-node interventions, where  $\mathcal{C}_{\max} = \max_{G \in \text{CC}(\mathcal{E}(D))} |\mathcal{C}(G)|$ .*

*Proof.* Consider a moral DAG  $D' \in \text{CC}(D)$ . We will show that Algorithm 1 uses at most  $(3\lceil \log_2 |\mathcal{C}(\mathcal{E}(D))| \rceil + 2)m(D')$  single-node interventions. The result then follows since  $m(D) = \sum_{D' \in \text{CC}(D)} m(D')$ , the total number of interventions used by Algorithm 1 is the sum over the number interventions used for each chain component, and  $\mathcal{C}_{\max} \geq |\mathcal{C}(\mathcal{E}(D))|$  for all  $D'$ .

Assume that for each clique-intervention in Algorithm 2, we intervene on every node in the clique. Then, the number of single-node interventions used by each clique intervention is upper-bounded by  $\omega(G)$ . By Theorem 2 and the simple algebraic fact that  $\forall a \in \mathbb{N}, a \leq 3\lfloor \frac{a}{2} \rfloor$  (which can be proven simply by noting that if  $a$  is even  $a \leq 3\frac{a}{2}$  and if  $a$  is odd  $a \leq 3\frac{a-1}{2}$ ),  $\omega(G) \leq 3m(D)$ , Algorithm 2 uses at most  $3m(D)$  single-node interventions. Next, by Lemma 5 and Lemma 9, and the fact that  $\forall a \in \mathbb{N}, a - 1 \leq 2\lfloor \frac{a}{2} \rfloor$ , the second phase of Algorithm 1 uses at most  $2m(D)$  single-interventions.  $\square$



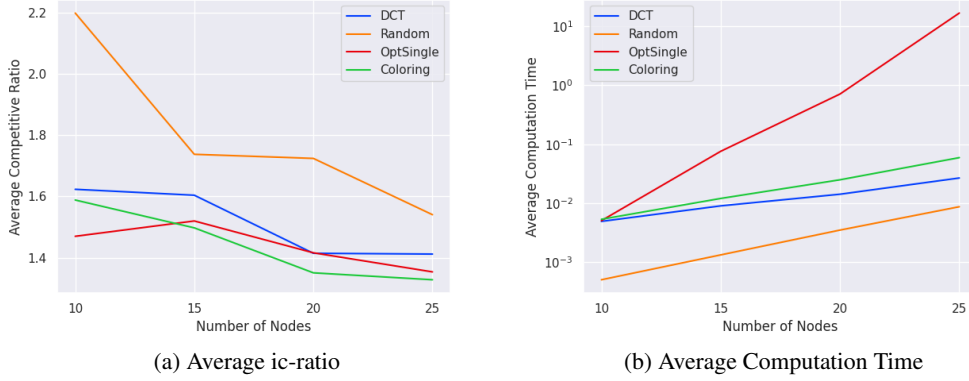
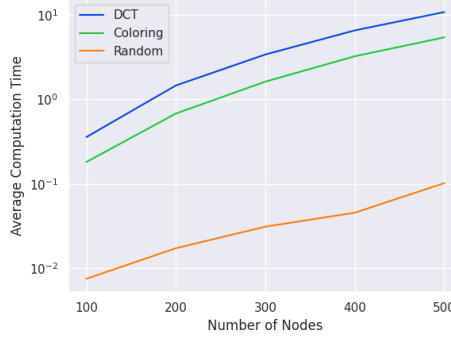


Figure 9: Comparison (over 100 random synthetic DAGs)



(a) Average Computation Time

## L Additional Experimental Results

### L.1 Scalability of OptSingle

We use the same graph generation procedure as outlined in Section 5. We compare OptSingle, Coloring, DCT, and ND-Random on graphs of up to 25 nodes in Fig. 9. We observe that at 25 nodes, OptSingle already takes more than 2 orders of magnitude longer than either the Coloring or DCT policies to select its interventions, while achieving comparable performance in terms of average competitive ratio.

### L.2 Computation time for large tree-like graphs

In this section, we report the results on average computation time associated with Fig. 6c from Section 5. We find similar scaling for our DCT policy and the Coloring policy, both taking about 5-10 seconds for graphs of up to 500 nodes.