Appendix of “An inclusion optimal algorithm for chain graph structure learning”

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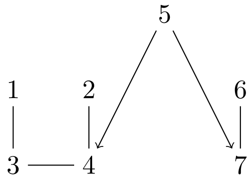
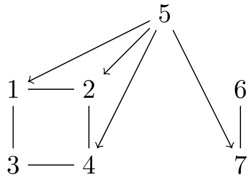
APPENDIX A: EXAMPLE RUN

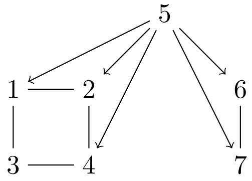
We show below an example run of the operation Fbsplit(K, L, G) presented in Figure 1 of the main text. Let G be the CG below, $K = \{1, 2, 3, 4, 6, 7\}$, and $L = \{3, 4, 7\}$.



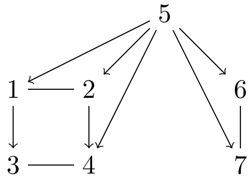
According to line 1, $L_1 = \{3, 4\}$ and $L_2 = \{7\}$. After having executed lines 2-4 for $i = 1$, G looks like the CG below.



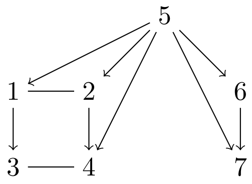
After having executed lines 2-4 for $i = 2$, G looks like the CG below.



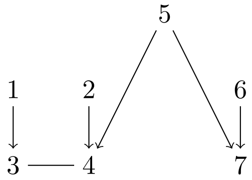
After having executed lines 5-8 for $i = 1$, G looks like the CG below. Note that according to line 6, $K_j = \{1, 2, 3, 4\}$.



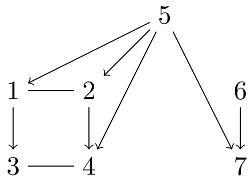
After having executed lines 5-8 for $i = 2$, G looks like the CG below. Note that according to line 6, $K_j = \{6, 7\}$.



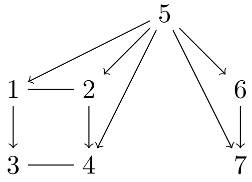
We show below an example run of the operation Fbmerge(L, R, G) presented in Figure 1 of the main text. Let G be the CG below, and $L = \{1, 2, 6\}$, and $R = \{3, 4, 7\}$.



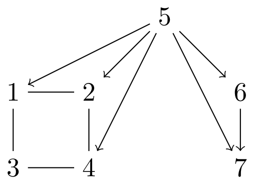
According to line 1, $R_1 = \{3, 4\}$ and $R_2 = \{7\}$. After having executed lines 2-4 for $i = 1$, G looks like the CG below.



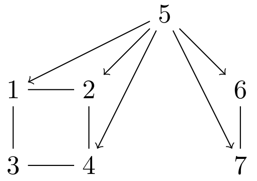
After having executed lines 2-4 for $i = 2$, G looks like the CG below.



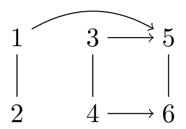
After having executed lines 5-8 for $i = 1$, G looks like the CG below. Note that according to line 6, $L_j = \{1, 2\}$.



After having executed lines 5-8 for $i = 2$, G looks like the CG below. Note that according to line 6, $L_j = \{6\}$.

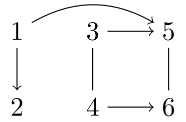


We show below an example run of the operation Construct $\beta(G,\ \alpha,\ \beta)$ presented in Figure 2 of the main text. Let G be the CG below and $\alpha = (\{1\}, \{5, 6\}, \{3, 4\}, \{2\})$.

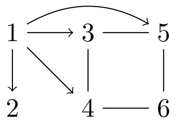


Initially, $H = G$. In the first iteration of the algorithm, $C = \{5, 6\}$, $\beta = (\{5, 6\})$, and the nodes $\{5, 6\}$ get removed from H. The algorithm jumps to line 3. In the second iteration, $C = \{3, 4\}$, $\beta = (\{3, 4\}, \{5, 6\})$, and the nodes $\{3, 4\}$ get removed from H. The algorithm jumps to line 3. In the third iteration, $C = \{1, 2\}$, $\beta = (\{1, 2\}, \{3, 4\}, \{5, 6\})$, and the nodes $\{1, 2\}$ get removed from H. The algorithm halts because $H = \emptyset$.

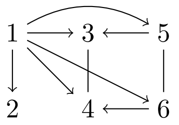
We finally show below an example run of the algorithm Method B3(G, α, β) presented in Figure 2 of the main text. Let G be the CG above and $\alpha = (\{1\}, \{5, 6\}, \{3, 4\}, \{2\})$. As shown above, $\beta = (\{1, 2\}, \{3, 4\}, \{5, 6\})$ after having executed line 1. In the first iteration of the algorithm, $C = \{2\}$, $K = \{1, 2\}$, G gets modified into the CG below by line 6 with $L = \{2\}$



and $\beta = (\{1\}, \{2\}, \{3, 4\}, \{5, 6\})$ by line 7, G does not get modified by line 10 but $\beta = (\{1\}, \{2, 3, 4\}, \{5, 6\})$ by line 11. The algorithm jumps to line 3. In the second iteration, $C = \{2\}$, $K = \{2, 3, 4\}$, G does not get modified by line 6 but $\beta = (\{1\}, \{3, 4\}, \{2\}, \{5, 6\})$ by line 7, G does not get modified by line 10 but $\beta = (\{1\}, \{3, 4\}, \{2, 5, 6\})$ by line 11. The algorithm jumps to line 3. In the third iteration, $C = \{2\}$, $K = \{2, 5, 6\}$, G does not get modified by line 6 but $\beta = (\{1\}, \{3, 4\}, \{5, 6\}, \{2\})$ by line 7. The algorithm jumps to line 2. In the fourth iteration, $C = \{3, 4\}$, $K = \{3, 4\}$, G gets modified into the CG below by line 10 with $L = \{3, 4\}$ and $R = \{5, 6\}$



and $\beta = (\{1\}, \{3, 4, 5, 6\}, \{2\})$ by line 11. The algorithm jumps to line 3. In the fifth iteration, $C = \{3, 4\}$, $K = \{3, 4, 5, 6\}$, G gets modified into the CG below by line 6 with $L = \{3, 4\}$



and $\beta = (\{1\}, \{5, 6\}, \{3, 4\}, \{2\})$ by line 7. The algorithm halts because $\beta = \alpha$.

APPENDIX B: PROOFS

Lemma 1. *Let M denote an independence model, and α a chain $C_1, \ldots, C_n$. If M is a graphoid, then there exits a unique CG G_α that is a MI map of M relative to α. Specifically, for each node X of each block C_k of α, $Bd_{G_\alpha}(X)$ is the smallest subset B of $\cup_{j=1}^{k} C_j \setminus \{X\}$ s.t. $X \perp_M \cup_{j=1}^{k} C_j \setminus \{X\} \setminus B | B$.*[1]

Proof. Let X and Y denote any two non-adjacent nodes of G_α. Let k^* denote the smallest k s.t. $X, Y \in \cup_{j=1}^{k} C_j$. Assume without loss of generality that $X \in C_{k^*}$. Then, $X \perp_M \cup_{j=1}^{k^*} C_j \setminus \{X\} \setminus Bd_{G_\alpha}(X) | Bd_{G_\alpha}(X)$ by construction of G_α and, thus, $X \perp_M Y | \cup_{j=1}^{k^*} C_j \setminus \{X, Y\}$ by weak union. Then, G_α satisfies the pairwise block-recursive Markov property w.r.t. M and, thus, G_α is an I map of M. In fact, G_α is a MI map of M by construction of $Bd_{G_\alpha}(X)$.

Assume to the contrary that there exists another CG H_α that is a MI map of M relative to α. Let X denote any node s.t. $Bd_{G_\alpha}(X) \neq Bd_{H_\alpha}(X)$. Let $X \in C_k$. Then, $X \perp_M \cup_{j=1}^{k} C_j \setminus \{X\} \setminus Bd_{G_\alpha}(X) | Bd_{G_\alpha}(X)$ and $X \perp_M \cup_{j=1}^{k} C_j \setminus \{X\} \setminus Bd_{H_\alpha}(X) | Bd_{H_\alpha}(X)$ because G_α and H_α are MI maps of M. Then, $X \perp_M \cup_{j=1}^{k}$

[1] By convention, $X \perp_M \emptyset | \cup_{j=1}^{k} C_j \setminus \{X\}$.

$C_j \setminus \{X\} \setminus Bd_{G_\alpha}(X) \cap Bd_{H_\alpha}(X) | Bd_{G_\alpha}(X) \cap Bd_{H_\alpha}(X)$ by intersection. However, this contradicts the construction of $Bd_{G_\alpha}(X)$, because $Bd_{G_\alpha}(X) \cap Bd_{H_\alpha}(X)$ is smaller than $Bd_{G_\alpha}(X)$.

□

Lemma 2. *Let G and H denote two CGs s.t. $I(H) \subseteq I(G)$. For any component C of G, there exists a unique component of H that is maximal in H from the set of components of H that contain a descendant of C in G.*

Proof. By definition of CG, there exists at least one such component of H. Assume to the contrary that there exist two such components of H, say K and K'. Note that $Pa_H(K) \cap K' = \emptyset$ and $Pa_H(K') \cap K = \emptyset$ by definition of K and K'. Note also that no node of K or $Pa_H(K)$ is a descendant of K' in H by definition of K. This implies that $K' \perp_H K \cup Pa_H(K) \setminus Pa_H(K') | Pa_H(K')$ and, thus, $K \perp_H K' | Pa_H(K) \cup Pa_H(K')$ by weak union and symmetry.

That K and K' contain some descendants k and k' of C in G implies that there are descending routes from C to k and k' in G s.t. the nodes in the routes are descendant of C in G. Thus, there is a route between k and k' in G s.t. the nodes in the route are descendant of C in G. Note that no node in this route is in $Pa_H(K)$ or $Pa_H(K')$ by definition of K and K'. Then, $K \not\perp_G K' | Pa_H(K) \cup Pa_H(K')$. However, this contradicts the fact that $I(H) \subseteq I(G)$ because, as shown, $K \perp_H K' | Pa_H(K) \cup Pa_H(K')$.

□

Lemma 3. *Let G and H denote two CGs s.t. $I(H) \subseteq I(G)$. Let α denote a chain that is consistent with H. If no descendant of a node X in G is to the left of X in α, then the descendants of X in G are descendant of X in H too.*

Proof. Let D denote the descendants of X in G. Let C denote the component of G that contains X. Note that the descendants of C in G are exactly the set D. Then, there exists a unique component of H that is maximal in H from the set of components of H that contain a node from D, by Lemma 2.

Let K denote the component of H that contains X. Note that K is a component of H that is maximal in H from the set of components of H that contain a node from D, since no node of D is to the left of X in α. It follows from the paragraph above that K is the only such component of H.

□

Lemma 4. *Let G_α denote the MI map of the independence model induced by a CG G relative to a chain α. Then, Method B3(G, α) returns G_α.*

Proof. We start by proving that Method B3 halts at some point. When Method B3 is done with the rightmost block of α, the rightmost block of β contains all and only the nodes of the rightmost block of α. When Method B3 is done with the second rightmost block of α, the rightmost block of β contains all and only the nodes of the rightmost block of α, whereas the second rightmost block of β contains all and only the nodes of the second rightmost block of α. Continuing with this reasoning, one can see that when Method B3 is done with all the blocks of α, β coincides with α and thus Method B3 halts.

That Method B3 halts at some point implies that it performs a finite sequence of m modifications to G due to the fbsplit and fbmerging in lines 6 and 10. Let G_t denote the CG resulting from the first t modifications to G, and let $G_0 = G$. Specifically, Method B3 constructs G_{t+1} from G_t by either

- adding an edge $X - Y$ due to line 3 of Fbsplit or Fbmerge,
- adding an edge $X \rightarrow Y$ due to line 4 of Fbsplit or Fbmerge,
- performing all the component splits due to lines 5-8 of Fbsplit, or
- performing all the component mergings due to lines 5-8 of Fbmerge.

Note that none of the modifications above introduces new separation statements. This is trivial to see for the first and second modification. To see it for the third and fourth modification, recall that the splits and the mergings are part of a fbsplit and a fbmerging respectively and, thus, they are feasible. Therefore, $I(G_{t+1}) \subseteq I(G_t)$ for all $0 \leq t < m$ and, thus, $I(G_m) \subseteq I(G_0)$.

We continue by proving that G_t is consistent with β for all $0 \leq t \leq m$. Since this is true for G_0 due to line 1, it suffices to prove that if it is true for G_t then it is true for G_{t+1} for all $0 \leq t < m$. We consider the following four cases.

Case 1 Method B3 constructs G_{t+1} from G_t by adding an edge $X - Y$ due to line 3 of Fbsplit or Fbmerge. It suffices to note that X and Y are in the same block of G_t and β.

Case 2 Method B3 constructs G_{t+1} from G_t by adding an edge $X \rightarrow Y$ due to line 4 of Fbsplit.

It suffices to note that X is to the left of Y in β, because G_t is consistent with β.

Case 3 Method B3 constructs G_{t+1} from G_t by adding an edge $X \to Y$ due to line 4 of Fbmerge. Note that X is to the left of R in β, because β is consistent with G_t. Then, X is to the left of L in β, because L is the left neighbor of R in β and $X \notin L$. Then, X is to the left of Y in β, because $Y \in L$.

Case 4 Method B3 constructs G_{t+1} from G_t by either performing all the component splits due to lines 5-8 of Fbsplit or performing all the component mergings due to lines 5-8 of Fbmerge. Note that the splits and the mergings are feasible, since they are part of a fbsplit and a fbmerging respectively. Therefore, G_{t+1} is a CG. Moreover, note that β is modified immediately after the fbsplit and the fbmerging so that it is consistent with G_{t+1}.

Note that G_m is not only consistent with β but also with α because, as shown, β coincides with α when Method B3 halts. In order to prove the lemma, i.e. that $G_m = G_\alpha$, all that remains to prove is that $I(G_\alpha) \subseteq I(G_m)$. To see it, note that $G_m = G_\alpha$ follows from $I(G_\alpha) \subseteq I(G_m)$, $I(G_m) \subseteq I(G_0)$, the fact that G_m is consistent with α, and the fact that G_α is the unique MI map of $I(G_0)$ relative to α. Recall that G_α is guaranteed to be unique by Lemma 1, because $I(G_0)$ is a graphoid.

The rest of the proof is devoted to prove that $I(G_\alpha) \subseteq I(G_m)$. Specifically, we prove that if $I(G_\alpha) \subseteq I(G_t)$ then $I(G_\alpha) \subseteq I(G_{t+1})$ for all $0 \leq t < m$. Note that this implies that $I(G_\alpha) \subseteq I(G_m)$ because $I(G_\alpha) \subseteq I(G_0)$ by definition of MI map. First, we prove it when Method B3 constructs G_{t+1} from G_t by either performing all the component splits due to lines 5-8 of Fbsplit or performing all the component mergings due to lines 5-8 of Fbmerge. Note that the splits and the mergings are feasible, since they are part of a fbsplit and a fbmerging respectively. Therefore, $I(G_{t+1}) = I(G_t)$. Thus, $I(G_\alpha) \subseteq I(G_{t+1})$ because $I(G_\alpha) \subseteq I(G_t)$.

Now, we prove that if $I(G_\alpha) \subseteq I(G_t)$ then $I(G_\alpha) \subseteq I(G_{t+1})$ when Method B3 constructs G_{t+1} from G_t by adding a directed or undirected edge due to lines 3 and 4 of Fbsplit and Fbmerge. Specifically, we prove that if there is an S-active route ρ^{AB}_{t+1} between two nodes A and B in G_{t+1}, then there is an S-active route between A and B in G_α. We prove this result by induction on the number of occurrences of the added edge in ρ^{AB}_{t+1}. We assume without loss of generality that the added edge occurs in ρ^{AB}_{t+1} as few or fewer times than in any other S-active route between A and B in G_{t+1}. We call this the minimality property of ρ^{AB}_{t+1}. If the number of occurrences of the added edge in ρ^{AB}_{t+1} is zero, then ρ^{AB}_{t+1} is an S-active route between A and B in G_t too and, thus, there is an S-active route between A and B in G_α since $I(G_\alpha) \subseteq I(G_t)$. Assume as induction hypothesis that the result holds for up to n occurrences of the added edge in ρ^{AB}_{t+1}. We now prove it for $n+1$ occurrences. We consider the following four cases.

Case 1 Method B3 constructs G_{t+1} from G_t by adding an edge $X - Y$ due to line 3 of Fbsplit. Note that $X - Y$ occurs in ρ^{AB}_{t+1}.[2] Assume that $X - Y$ occurs in a collider section of ρ^{AB}_{t+1}. Note that X and Y must be in the same component of G_t for line 3 of Fbsplit to add an edge $X - Y$. This component also contains a node Z that is in S because, otherwise, ρ^{AB}_{t+1} would not be S-active in G_{t+1}.[3] Note that there is a route $X - \ldots - Z - \ldots - Y$ in G_t. Then, we can replace any occurrence of $X - Y$ in a collider section of ρ^{AB}_{t+1} with $X - \ldots - Z - \ldots - Y$, and thus construct an S-active route between A and B in G_{t+1} that violates the minimality property of ρ^{AB}_{t+1}. Since this is a contradiction, $X - Y$ only occurs in non-collider sections of ρ^{AB}_{t+1}. Let $\rho^{AB}_{t+1} = \rho^{AX}_{t+1} \cup X - Y \cup \rho^{YB}_{t+1}$. Note that $X, Y \notin S$ because, otherwise, ρ^{AB}_{t+1} would not be S-active in G_{t+1}. For the same reason, ρ^{AX}_{t+1} and ρ^{YB}_{t+1} are S-active in G_{t+1}. Then, there are S-active routes ρ^{AX}_{α} and ρ^{YB}_{α} between A and X and between Y and B in G_α by the induction hypothesis.

Let $X - X' - \ldots - Y' - Y$ be a route in G_t s.t. the nodes in $X' - \ldots - Y'$ are in L.[4] Such a route must exist for line 3 of Fbsplit to add an edge $X - Y$. Note that X and X' are adjacent in G_α since $I(G_\alpha) \subseteq I(G_t)$. In fact, $X \to X'$ is in G_α. To see it, recall that Method B3 is currently considering the block C of α, and that it has previously considered all the blocks of α to the right of C in α. Then, K only contains nodes from C or from blocks to the left of C in α. However, $X \notin C$ because $X \in K \setminus L$ and $L = K \cap C$. Then, X is to the left of C in α. Thus, $X \to X'$ is in G_α because $X' \in L \subseteq C$. Likewise, $Y \to Y'$ is in G_α. Note also that $X' - \ldots - Y'$ is in G_α. To see it, note that the adjacencies in $X' - \ldots - Y'$ are preserved in G_α since $I(G_\alpha) \subseteq I(G_t)$. Moreover, these adjacencies correspond to undirected edges in G_α, because the nodes in $X' - \ldots - Y'$ are in L and thus in the same block of G_α, since $L \subseteq C$. Furthermore, a node in $X' - \ldots - Y'$ is in S because, otherwise, $\rho^{AX}_{t+1} \cup X - X' - \ldots - Y' - Y \cup \rho^{YB}_{t+1}$

[2] Note that maybe $A = X$ and/or $Y = B$.

[3] Note that maybe $Z = X$ or $Z = Y$.

[4] Note that maybe $X' = Y'$.

would be an S-active route between A and B in G_{t+1} that would violate the minimality property of ρ^{AB}_{t+1}. Then, $\rho^{AX}_{\alpha} \cup X \to X' - \ldots - Y' \leftarrow Y \cup \rho^{YB}_{\alpha}$ is an S-active route between A and B in G_α.

Case 2 Method B3 constructs G_{t+1} from G_t by adding an edge $X \to Y$ due to line 4 of Fbsplit. Note that $X \to Y$ occurs in ρ^{AB}_{t+1}.[5] Assume that $X \to Y$ occurs as a collider edge in ρ^{AB}_{t+1}, i.e. $X \to Y$ occurs in a subroute of ρ^{AB}_{t+1} of the form $X \to Y - \ldots - Z \leftarrow W$.[6] Note that a node in $Y - \ldots - Z$ is in S because, otherwise, ρ^{AB}_{t+1} would not be S-active in G_{t+1}. Let $X \to X' - \ldots - Y' - Y$ be a route in G_t s.t. the nodes in $X' - \ldots - Y'$ are in L.[7] Such a route must exist for line 4 of Fbsplit to add an edge $X \to Y$. Then, we can replace $X \to Y - \ldots - Z \leftarrow W$ with $X \to X' - \ldots - Y' - Y - \ldots - Z \leftarrow W$ in ρ^{AB}_{t+1}, and thus construct an S-active route between A and B in G_{t+1} that violates the minimality property of ρ^{AB}_{t+1}. Since this is a contradiction, $X \to Y$ never occurs as a collider edge in ρ^{AB}_{t+1}. Let $\rho^{AB}_{t+1} = \rho^{AX}_{t+1} \cup X \to Y \cup \rho^{YB}_{t+1}$. Note that $X, Y \notin S$ because, otherwise, ρ^{AB}_{t+1} would not be S-active in G_{t+1}. For the same reason, ρ^{AX}_{t+1} and ρ^{YB}_{t+1} are S-active in G_{t+1}. Then, there are S-active routes ρ^{AX}_{α} and ρ^{YB}_{α} between A and X and between Y and B in G_α by the induction hypothesis.

Let $X \to X' - \ldots - Y' - Y$ denote a route in G_t s.t. the nodes in $X' - \ldots - Y'$ are in L.[8] Such a route must exist for line 4 of Fbsplit to add an edge $X \to Y$. Note that $X' - \ldots - Y'$ is in G_α. To see it, note that the adjacencies in $X' - \ldots - Y'$ are preserved in G_α since $I(G_\alpha) \subseteq I(G_t)$. Moreover, these adjacencies correspond to undirected edges in G_α, because the nodes in $X' - \ldots - Y'$ are in L and thus in the same block of G_α, since $L \subseteq C$. Furthermore, a node in $X' - \ldots - Y'$ is in S because, otherwise, $\rho^{AX}_{t+1} \cup X \to X' - \ldots - Y' - Y \cup \rho^{YB}_{t+1}$ would be an S-active route between A and B in G_{t+1} that would violate the minimality property of ρ^{AB}_{t+1}. Moreover, note that X and X' are adjacent in G_α since $I(G_\alpha) \subseteq I(G_t)$. In fact, $X \to X'$ is in G_α. To see it, recall that Method B3 is currently considering the block C of α, and that it has previously considered all the blocks of α to the right of C in α. Then, no block to the left of K in β has a node from C or from a block to the right of C in α. Note that X is to the left of K in β, because β is consistent with G_t. Thus, $X \to X'$ is in G_α since $X' \in L \subseteq C$. Likewise, note that Y' and Y are adjacent in G_α since $I(G_\alpha) \subseteq I(G_t)$. In fact, $Y' \leftarrow Y$ is in G_α. To see it, note that K only contains nodes from C or from blocks to the left of C in α. However, $Y \notin C$ because $Y \in K \setminus L$ and $L = K \cap C$. Then, Y is to the left of C in α. Thus, $Y' \leftarrow Y$ is in G_α because $Y' \in L \subseteq C$. Then, $\rho^{AX}_{\alpha} \cup X \to X' - \ldots - Y' \leftarrow Y \cup \rho^{YB}_{\alpha}$ is an S-active route between A and B in G_α.

Case 3 Method B3 constructs G_{t+1} from G_t by adding an edge $X - Y$ due to line 3 of Fbmerge. Note that $X - Y$ occurs in ρ^{AB}_{t+1}. We consider two cases.

Case 3.1 Assume that $X - Y$ occurs in a collider section of ρ^{AB}_{t+1}. Let $\rho^{AB}_{t+1} = \rho^{AZ}_{t+1} \cup Z \to X' - \ldots - X - Y - \ldots - Y' \leftarrow W \cup \rho^{WB}_{t+1}$.[9] Note that $Z, W \notin S$ because, otherwise, ρ^{AB}_{t+1} would not be S-active in G_{t+1}. For the same reason, ρ^{AZ}_{t+1} and ρ^{WB}_{t+1} are S-active in G_{t+1}. Then, there are S-active routes ρ^{AZ}_{α} and ρ^{WB}_{α} between A and Z and between W and B in G_α by the induction hypothesis.

Let R_i denote the component of G_t in R that Fbmerge is processing when the edge $X - Y$ gets added. Recall that Method B3 is currently considering the block C of α, and that it has previously considered all the blocks of α to the right of C in α. Then, R_i only contains nodes from C or from blocks to the left of C in α. In other words, $R_i \subseteq \cup_{j=1}^{k^*} C_j \setminus \{X, Y\}$ where $C_{k^*} = C$ (recall that $X, Y \in L \subseteq C$). Therefore, $X \not\perp_{G_t} Y | \cup_{j=1}^{k^*} C_j \setminus \{X, Y\}$ because X and Y must be in $Pa_{G_t}(R_i)$ for line 3 of Fbmerge to add an edge $X - Y$. Then, X and Y are adjacent in G_α because, otherwise, $X \perp_{G_\alpha} Y | \cup_{j=1}^{k^*} C_j \setminus \{X, Y\}$ which would contradict that $I(G_\alpha) \subseteq I(G_t)$. In fact, $X - Y$ is in G_α because X and Y are in the same block of α, since $X, Y \in L \subseteq C$.

Note that $X' - \ldots - X$ and $Y - \ldots - Y'$ are in G_α. To see it, note that the adjacencies in $X' - \ldots - X$ and $Y - \ldots - Y'$ are preserved in G_α since $I(G_\alpha) \subseteq I(G_t)$. Moreover, these adjacencies correspond to undirected edges in G_α, because the nodes in $X' - \ldots - X$ and $Y - \ldots - Y'$ are in L since $X, Y \in L$ and, thus, they are in the same block of G_α since $L \subseteq C$. Then, $X' - \ldots - X - Y - \ldots - Y'$ is in G_α. Furthermore, a node in $X' - \ldots - X - Y - \ldots - Y'$ is in S because, otherwise, ρ^{AB}_{t+1} would not be S-active in G_{t+1}. Note also that Z and X' are adjacent in G_α since

[5] Note that maybe $A = X$ and/or $Y = B$.

[6] Note that maybe $Y = Z$ and/or $W = X$.

[7] Note that maybe $X' = Y'$.

[8] Note that maybe $X' = Y'$.

[9] Note that maybe $A = Z$, $X' = X$, $Y' = Y$, $W = Z$ and/or $W = B$.

$I(G_\alpha) \subseteq I(G_t)$. In fact, $Z \to X'$ is in G_α. To see it, recall that Method B3 is currently considering the block C of α, and that it has previously considered all the blocks of α to the right of C in α. Then, no block to the left of L in β has a node from C or from a block to the right of C in α. Note that Z is to the left of L in β, because β is consistent with G_t. Thus, $Z \to X'$ is in G_α since $X' \in L \subseteq C$. Likewise, $Y' \leftarrow W$ is in G_α. Then, $\rho_\alpha^{AZ} \cup Z \to X' - \ldots - X - Y - \ldots - Y' \leftarrow W \cup \rho_\alpha^{WB}$ is an S-active route between A and B in G_α.

Case 3.2 Assume that $X - Y$ occurs in a non-collider section of ρ_{t+1}^{AB}. Note that this implies that G_t has a descending route from X to A or to a node in S, or from Y to B or to a node in S. Assume without loss of generality that G_t has a descending route from Y to B or to a node in S.

Let R_i denote the component of G_t in R that Fbmerge is processing when the edge $X - Y$ gets added. Let L_Y denote the component of G_t that contains the node Y. Let D denote the component of G_α that is maximal in G_α from the set of components of G_α that contain a descendant of L_Y in G_t. Recall that D is guaranteed to be unique by Lemma 2, because $I(G_\alpha) \subseteq I(G_t)$. We now show that some $d \in D$ is a descendant of R_i in G_t. We consider four cases.

Case 3.2.1 Assume that $D \cap L_Y \neq \emptyset$. It suffices to consider any $d \in R_i$. To see it, recall that Method B3 is currently considering the block C of α, and that it has previously considered all the blocks of α to the right of C in α. Then, R_i only contains nodes from C or from blocks to the left of C in α. Thus, d is not to the right of the nodes of $D \cap L_Y$ in α, since $L_Y \subseteq L \subseteq C$. Moreover, d is not to the left of the nodes of $D \cap L_Y$ in α because, otherwise, there would be a contradiction with the definition of D. Then, $d \in D$.

Case 3.2.2 Assume that $D \cap L_Y = \emptyset$ and $D \cap R_i \neq \emptyset$. It suffices to consider any $d \in D \cap R_i$.

Case 3.2.3 Assume that $D \cap L_Y = \emptyset$, $D \cap R_i = \emptyset$, and some $d \in D$ was a descendant of some $r \in R_i$ in G_0. Recall that Method B3 is currently considering the block C of α, and that it has previously considered all the blocks of α to the right of C in α. Then, R_i only contains nodes from C or from blocks to the left of C in α. Then, r was not in the blocks of α previously considered, since $r \in R_i$. Therefore, no descendant of r in G_0 is currently to the left of r in β and, thus, the descendants of r in G_0 are descendant of r in G_t by Lemma 3, because $I(G_t) \subseteq I(G_0)$ and β is consistent with G_t. Then, d is a descendant of r and thus of R_i in G_t.

Case 3.2.4 Assume that $D \cap L_Y = \emptyset$, $D \cap R_i = \emptyset$, and no node of D was a descendant of a node of R_i in G_0. As shown in Case 3.2.3, the descendants of any node $r \in R_i$ in G_0 are descendant of r in G_t too. Therefore, no descendant of r in G_0 was to the left of the nodes of D in α because, otherwise, a descendant of r and thus of L_Y in G_t would be to the left of the nodes of D in α, which would contradict the definition of D. Recall that no descendant of r in G_0 was in D either. Note also that the nodes of D are to the left of the nodes of R_i in α, by definition of D and the fact that $D \cap R_i = \emptyset$. These observations have two consequences. First, the components of G containing a node from D were still in H when any component of G containing a node from R_i became a terminal component of H in Construct β. Thus, Construct β added the components of G containing a node from D to β after having added the components of G containing a node from R_i. Second, Construct β did not interchange in β any component of G containing a node from D with any component of G containing a node from R_i.

Recall that Method B3 is currently considering the block C of α, and that it has previously considered all the blocks of α to the right of C in α. Note that the nodes of D were not in the blocks of α previously considered because, otherwise, C and thus the nodes of L_Y (recall that $L_Y \subseteq L \subseteq C$) would be to the left of D in α, which would contradict the definition of D. Therefore, the nodes of D are currently still to the left of R_i in β. Note that the only component to the left of R_i in β that contains a descendant of L_Y in G_t is precisely L_Y, because L is the left neighbor of R in β, $L_Y \subseteq L$, and β is consistent with G_t. However, $D \cap L_Y = \emptyset$. Thus, D contains no descendant of L_Y in G_t, which contradicts the definition of D. Thus, this case never occurs.

We continue with the proof of Case 3.2. Let

$\rho_{t+1}^{AB} = \rho_{t+1}^{AX} \cup X - Y \cup \rho_{t+1}^{YB}$.[10] Note that $X, Y \notin S$ because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1}. For the same reason, ρ_{t+1}^{AX} and ρ_{t+1}^{YB} are S-active in G_{t+1}. Note that X and Y must be in $Pa_{G_t}(R_i)$ for line 3 of Fbmerge to add an edge $X - Y$. Then, no descendant of R_i in G_t is in S because, otherwise, there would be an S-active route ρ_t^{XY} between X and Y in G_t and, thus, $\rho_{t+1}^{AX} \cup \rho_t^{XY} \cup \rho_{t+1}^{YB}$ would be an S-active route between A and B in G_{t+1} that would violate the minimality property of ρ_{t+1}^{AB}. Then, there is an S-active descending route ρ_t^{rd} from some $r \in R_i$ to some $d \in D$ in G_t because, as shown, D contains a descendant of R_i in G_t. Then, $\rho_{t+1}^{AX} \cup X \to X' - \ldots - r \cup \rho_t^{rd}$ is an S-active route between A and d in G_{t+1}.[11] Likewise, $\rho_{t+1}^{BY} \cup Y \to Y' - \ldots - r \cup \rho_t^{rd}$ is an S-active route between B and d in G_{t+1}, where ρ_{t+1}^{BY} denotes the route resulting from reversing ρ_{t+1}^{YB}.[12] Therefore, there are S-active routes ρ_α^{Ad} and ρ_α^{Bd} between A and d and between B and d in G_α by the induction hypothesis.

Recall that we assumed without loss of generality that G_t has a descending route from Y to a node E s.t. $E = B$ or $E \in S$. Note that E is a descendant of L_Y in G_t and, thus, E is a descendant of d in G_α by definition of D and the fact that $d \in D$. Let ρ_α^{dE} denote the descending route from d to E in G_α. Assume without loss of generality that G_α has no descending route from d to B or to a node of S that is shorter than ρ_α^{dE}. We now consider two cases.

Case 3.2.5 Assume that $E = B$. Note that ρ_α^{dE} is S-active in G_α by definition and the fact that $d \notin S$. To see the latter, recall that no descendant of R_i in G_t (among which is d) is in S. Thus, $\rho_\alpha^{Ad} \cup \rho_\alpha^{dE}$ is an S-active route between A and B in G_α.

Case 3.2.6 Assume that $E \in S$. Let ρ_α^{dB} and ρ_α^{Ed} denote the routes resulting from reversing ρ_α^{Bd} and ρ_α^{dE}. Consider the route $\rho_\alpha^{Ad} \cup \rho_\alpha^{dB}$ between A and B in G_α. If this route is S-active, then we are done. If it is not S-active in G_α, then d occurs in a collider section of $\rho_\alpha^{Ad} \cup \rho_\alpha^{dB}$ that has no node in S. Then, we can replace each such occurrence of d with $\rho_\alpha^{dE} \cup \rho_\alpha^{Ed}$ and, thus construct an S-active route between A and B in G_α.

Case 4 Method B3 constructs G_{t+1} from G_t by adding an edge $X \to Y$ due to line 4 of Fbmerge. Note that $X \to Y$ occurs in ρ_{t+1}^{AB}. We consider two cases.

Case 4.1 Assume that $X \to Y$ occurs as a collider edge in ρ_{t+1}^{AB}. Let $\rho_{t+1}^{AB} = \rho_{t+1}^{AX} \cup X \to Y \cup \rho_{t+1}^{YB}$.[13] Note that $X \notin S$ because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1}. For the same reason, ρ_{t+1}^{AX} is S-active in G_{t+1}. Then, there is an S-active route ρ_α^{AX} between A and X in G_α by the induction hypothesis. Let R_i denote the component of G_t in R that Fbmerge is processing when the edge $X \to Y$ gets added. Recall that Method B3 is currently considering the block C of α, and that it has previously considered all the blocks of α to the right of C in α. Then, R_i only contains nodes from C or from blocks to the left of C in α. In other words, $R_i \subseteq \cup_{j=1}^{k^*} C_j \setminus \{X, Y\}$ where k^* is the smallest k s.t. $X, Y \in \cup_{j=1}^{k} C_j$ (recall that $Y \in L \subseteq C$). Therefore, $X \not\perp_{G_t} Y | \cup_{j=1}^{k^*} C_j \setminus \{X, Y\}$ because X and Y must be in $Pa_{G_t}(R_i)$ for line 4 of Fbmerge to add an edge $X \to Y$. Then, X and Y are adjacent in G_α because, otherwise, $X \perp_{G_\alpha} Y | \cup_{j=1}^{k^*} C_j \setminus \{X, Y\}$ which would contradict that $I(G_\alpha) \subseteq I(G_t)$. In fact, $X \to Y$ is in G_α. To see it, recall that Method B3 is currently considering the block C of α, and that it has previously considered all the blocks of α to the right of C in α. Then, no block to the left of L in β has a node from C or from a block to the right of C in α. Note that X is to the left of R in β, because β is consistent with G_t. Then, X is to the left of L in β, because L is the left neighbor of R in β and $X \notin L$. Thus, $X \to Y$ is in G_α because $Y \in L \subseteq C$. We now consider two cases.

Case 4.1.1 Assume that $\rho_{t+1}^{YB} = Y - \ldots - Y \leftarrow X \cup \rho_{t+1}^{XB}$. Note that a node in $Y - \ldots - Y$ is in S because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1}. For the same reason, ρ_{t+1}^{XB} is S-active in G_{t+1}. Then, there is an S-active route ρ_α^{XB} between X and B in G_α by the induction hypothesis. Note that $Y - \ldots - Y$ is in G_α. To see it, note that the adjacencies in $Y - \ldots - Y$ are preserved in G_α since $I(G_\alpha) \subseteq I(G_t)$. Moreover, these adjacencies correspond to undirected edges in G_α, because the nodes in $Y - \ldots - Y$ are in L since $Y \in L$ and, thus, they are in the same block of G_α since $L \subseteq C$. Then,

[10] Note that maybe $A = X$ and/or $Y = B$.

[11] Note that maybe $X' = r$.

[12] Note that maybe $Y' = r$.

[13] Note that maybe $A = X$ and/or $Y = B$.

$\rho_\alpha^{AX} \cup X \rightarrow Y - \ldots - Y \leftarrow X \cup \rho_\alpha^{XB}$ is an S-active route between A and B in G_α.

Case 4.1.2 Assume that $\rho_{t+1}^{YB} = Y - \ldots - Z \leftarrow W \cup \rho_{t+1}^{WB}$.[14] Note that $W \notin S$ and a node in $Y - \ldots - Z$ is in S because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1}. For the same reason, ρ_{t+1}^{WB} is S-active in G_{t+1}. Then, there is an S-active route ρ_α^{WB} between W and B in G_α by the induction hypothesis. Note that $Y - \ldots - Z$ is in G_α. To see it, note that the adjacencies in $Y - \ldots - Z$ are preserved in G_α since $I(G_\alpha) \subseteq I(G_t)$. Moreover, these adjacencies correspond to undirected edges in G_α, because the nodes in $Y - \ldots - Z$ are in L since $Y \in L$ and, thus, they are in the same block of G_α since $L \subseteq C$. Moreover, note that Z and W are adjacent in G_α since $I(G_\alpha) \subseteq I(G_t)$. In fact, $Z \leftarrow W$ is in G_α. To see it, recall that no block to the left of L in β has a node from C or from a block to the right of C in α. Note that W is to the left of L in β, because β is consistent with G_t. Thus, $Z \leftarrow W$ is in G_α since $Z \in L \subseteq C$. Then, $\rho_\alpha^{AX} \cup X \rightarrow Y - \ldots - Z \leftarrow W \cup \rho_\alpha^{WB}$ is an S-active route between A and B in G_α.

Case 4.2 Assume that $X \rightarrow Y$ occurs as a non-collider edge in ρ_{t+1}^{AB}. The proof of this case is the same as that of Case 3.2, with the only exception that $X - Y$ should be replaced by $X \rightarrow Y$.

□

Theorem 1. *Given two CGs G and H s.t. $I(H) \subseteq I(G)$, Method G2H(G, H) transforms G into H by a sequence of directed and undirected edge additions and feasible splits and mergings s.t. after each operation in the sequence G is a CG and $I(H) \subseteq I(G)$.*

Proof. Note from line 1 that α denotes a chain that is consistent with H. Let G_α denote the MI map of $I(G)$ relative to α. Recall that G_α is guaranteed to be unique by Lemma 1, because $I(G)$ is a graphoid. Note that $I(H) \subseteq I(G)$ implies that G_α is a subgraph of H. To see it, note that $I(H) \subseteq I(G)$ implies that we can obtain a MI map of $I(G)$ relative to α by just removing edges from H. However, G_α is the only MI map of $I(G)$ relative to α.

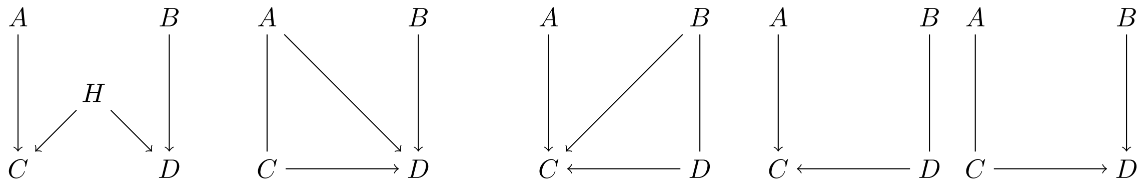
Then, it follows from the proof of Lemma 4 that line 2 transforms G into G_α by a sequence of directed and undirected edge additions and feasible splits and mergings, and that after each operation in the sequence G is a CG and $I(G_\alpha) \subseteq I(G)$. Thus, after each operation in the sequence $I(H) \subseteq I(G)$ because $I(H) \subseteq I(G_\alpha)$ since, as shown, G_α is a subgraph of H. Finally, line 3 transforms G from G_α to H by a sequence of edge additions. Of course, after each edge addition G is a CG and $I(H) \subseteq I(G)$ because G_α is a subgraph of H.

□

Theorem 2. *For any probability distribution p for which the composition property holds, the CKES algorithm finds a CG that is inclusion optimal w.r.t. p.*

Proof. Let R, S and T be three random variables. Let $H(R|S)$ denote the conditional entropy of R given S. Then, $H(R|S,T) \leq H(R|S)$ and, moreover, $H(R|S,T) = H(R|S)$ iff $R \perp_p T|S$ (Cover and Thomas, 1991, Chapter 2). Therefore, $H(Y|Bd_G(Y))$ stays the same when removing the edge $X \rightarrow Y$ from G in line 4. Likewise, $H(X|Bd_G(X))$ and $H(Y|Bd_G(Y))$ stay the same when removing $X - Y$ from G in line 5. On the other hand, $H(Y|Bd_G(Y))$ decreases when adding the edge $X \rightarrow Y$ to G in line 6. Likewise, $H(X|Bd_G(X))$ or $H(Y|Bd_G(Y))$ decreases when adding the edge $X - Y$ to G in line 7. Let us define the score of a CG G as $\sum_{X \in V} H(X|Bd_G(X))$. Now, note that the algorithm cannot enter an endless loop, i.e. it cannot perform a sequence of edge additions and removals so that the CGs before and after the sequence coincide. To see it, assume the contrary and note that such a sequence must contain both edge additions and removals. However, such a sequence would imply that the score of the CG after the sequence is smaller than the score of the CG before the sequence, which is a contradiction. If the algorithm cannot enter an endless loop, then the algorithm must reach a CG G such that no edge can be added or removed from it in lines 3-7, because the number of CGs is finite. Moreover, $I(G) \subseteq I(p)$. To see it, assume the contrary. Then, according to the local Markov property and the composition property, there must exist two nodes X and Y such that $X \notin Sd_G(Y) \cup Bd_G(Y)$, $X \not\perp_p Y|Bd_G(Y)$ but $X \perp_G Y|Bd_G(Y)$. Then, a new edge can be added to G in line 6 or 7, which is a contradiction. Obviously, $I(G) \subseteq I(p)$ still holds after G has been updated in line 8. Therefore, the next execution of lines 3-7 may remove edges from G but it never adds edges to G. Consequently, the algorithm must reach a CG G such that no edge can be removed from it, because the number of edges that can be removed is finite. At this point, the algorithm executes line 8 repeatedly. This implies that the algorithm terminates at some point, because any CG can be transformed in any other equivalent CG via a sequence of feasible

[14] Note that maybe $Y = Z$, $W = X$ and/or $W = B$. Note that $Y \neq Z$ or $W \neq X$, because the case where $Y = Z$ and $W = X$ is covered by Case 4.1.1.



The w-structure CG
(a)

Inclusion optimal CGs
(b)

CGs learnt by the LCD algorithm
(c)

Figure 1: CGs In The Experiment.

Table 1: Average Results For Gaussian Data.

CG structure	Recall		Precision	
	CKES	LCD	CKES	LCD
n=100	0.54	0.61	0.75	0.44
n=30000	0.57	0.57	1.00	0.57

merges and splits (Studený et al., 2009, Corollary 7).

Finally, we show that there is no model G' such that $I(G) \subset I(G') \subseteq I(p)$ when the algorithm has terminated in G. Assume the contrary. Theorem 1 says that there must exist a model H such that $I(G) = I(F) \subset I(H) \subseteq \ldots \subseteq I(G') \subseteq I(p)$ and H can be reached by a single edge removal from a CG F which is in the equivalence class of G.[15] However this edge must be between two nodes X and Y in F such that $X \in Bd_F(Y)$ and $X \perp_p Y | Bd_F(Y) \setminus X$ because $I(H) \subseteq I(p)$. This now contradicts the assumption since we know that the algorithm only can terminate if there exists no such edge for any CG in the equivalence class of G. Hence, we have a contradiction.

□

APPENDIX C: ADDITIONAL EXPERIMENT

In this experiment, we want to show how the algorithms handle an unfaithful probability distribution that satisfies the composition property. Chickering and Meek (2002) performed a similar experiment and we used the same setup. Specifically, we used the w-structure seen in Figure 1a as CG structure. From this structure, 10 Gaussian probability distributions were generated and sampled into sample sets in the same way as we did for the experiment in our paper. We then removed the H variable from the sample sets. This meant that the algorithms tried to model the (in)dependencies in Figure 1a with only A, B, C and D as nodes. It can be shown that this is impossible (i.e. that there exists no faithful CG for this probability distribution) and that the inclusion optimal CGs are those seen in Figure 1b (Chickering and Meek, 2002). As performance measures, we computed the recall of the separations over $\{A, B, C, D\}$ in the 5-node CG sampled, and the precision of the separations in the 4-node CGs learnt. This meant that it was impossible to find a CG with perfect precision and recall, but that the best inclusion optimal CG had precision 1 and recall 0.57. The results obtained are shown in Figure 1. The table show average results over the 10 sample sets in the experiment. The results for categorical data are similar and, thus, they are not included here.

Running the example above by hand with perfect information, it can be seen that the CKES algorithm will end up in one of the CGs seen in Figure 1b. The LCD algorithm on the other hand ends up in one of the CGs shown in Figure 1c, which do not include the original independence model. The experimental results obtained with large sample sets (30000 samples) are shown in Figure 1 and coincide with the theoretical results just described. For the smaller sample sets (100 samples), the same trend observed in the experiment in our paper can be seen here (i.e. the CKES algorithm learning a CG with higher precision and the LCD algorithm learning a CG with higher recall). Therefore, we reach here the same conclusion as we did previously: Since the goal of structural learning is to find a model representing an I map of the probability distribution at hand, the CKES algorithm achieves better results than the LCD algorithm.

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