

Appendices

A. Example of Comparison with the Influence Maximization Problem

Suppose $k = 1$. Figure 3 depicts a graph for which the optimal solution to the influence maximization problem is different from the optimal solution to the budgeted experiment design problems. Clearly, influencing vertex v_1 leads to influencing all the vertices in the graph, and hence, this vertex is the solution to the influence maximization problem. But, intervening on v_1 leads to discovering the orientation of only 3 edges, while intervening on, say v_2 , leads to discovering the orientation of 5 edges.

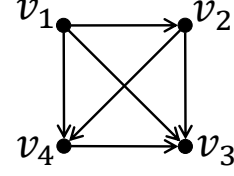


Figure 3. Example of comparison with the influence maximization problem.

B. Proof of Lemma 1

First we show that for a given directed graph $G_i \in \mathcal{G}$ the function $D(\mathcal{I}, G_i)$ is a monotonically increasing function of \mathcal{I} . In the proposed method, intervening on elements of \mathcal{I} , we first discover the orientation of the edges in $A_{G_i}^{(\mathcal{I})}$, and then applying the Meek rules, we possibly learn the orientation of some extra edges. Having $\mathcal{I}_1 \subseteq \mathcal{I}_2$ implies that $A_{G_i}^{(\mathcal{I}_1)} \subseteq A_{G_i}^{(\mathcal{I}_2)}$. Therefore using \mathcal{I}_2 , we have more information about the direction of edges. Hence, in the step of applying Meek rules, by soundness and order-independence of Meek algorithm, we recover the direction of more extra edges, i.e., $R(A_{G_i}^{(\mathcal{I}_1)}, G_i) \subseteq R(A_{G_i}^{(\mathcal{I}_2)}, G_i)$, which in turn implies that $D(\mathcal{I}_1, G_i) \leq D(\mathcal{I}_2, G_i)$. Finally, from the relation $\mathcal{D}(\mathcal{I}) = \frac{1}{|\mathcal{G}|} \sum_{G_i \in \mathcal{G}} D(\mathcal{I}, G_i)$, the desired result is immediate.

C. Proof of Lemma 2

The direction $R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*) \subseteq R(A_{G^*}^{(\mathcal{I}_1 \cup \mathcal{I}_2)}, G^*)$ is proved in the proof of Lemma 1. Also, as observed in the proof of Lemma 1, we have $R(A_{G^*}^{(\mathcal{I}_1 \cup \mathcal{I}_2)}, G^*) \subseteq R(R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*), G^*)$. Therefore, in order to prove that $R(A_{G^*}^{(\mathcal{I}_1 \cup \mathcal{I}_2)}, G^*) \subseteq R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*)$, it suffices to show that $R(R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*), G^*) \subseteq R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*)$, for which it suffices to show that if $e \notin R(A_{G^*}^{(\mathcal{I}_1)}, G^*)$ and $e \notin R(A_{G^*}^{(\mathcal{I}_2)}, G^*)$, then $e \notin R(R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*), G^*)$.

Proof by contradiction. Let $e \notin R(A_{G^*}^{(\mathcal{I}_1)}, G^*)$ and $e \notin R(A_{G^*}^{(\mathcal{I}_2)}, G^*)$, but its orientation is learned in the first iteration of applying Meek rules to $R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*) \cup A(\text{Ess}(G^*))$. Then, we have learned the orientation of e due to one of Meek rules (Verma & Pearl,

1992):

- *Rule 1.* $e = \{a, b\}$ is oriented as (a, b) if $\exists c$ s.t. $e_1 = (c, a) \in R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*) \cup A(\text{Ess}(G^*))$, and $\{c, b\} \notin \text{skeleton of } G^*$.
- *Rule 2.* $e = \{a, b\}$ is oriented as (a, b) if $\exists c$ s.t. $e_1 = (a, c) \in R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*) \cup A(\text{Ess}(G^*))$, and $e_2 = (c, b) \in R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*) \cup A(\text{Ess}(G^*))$.
- *Rule 3.* $e = \{a, b\}$ is oriented as (a, b) if $\exists c, d$ s.t. $e_1 = (c, b) \in R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*) \cup A(\text{Ess}(G^*))$, $e_2 = (d, b) \in R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*) \cup A(\text{Ess}(G^*))$, $\{a, c\} \in \text{skeleton of } G^*$, $\{a, d\} \in \text{skeleton of } G^*$, and $\{c, d\} \notin \text{skeleton of } G^*$.
- *Rule 4.* $e = \{a, b\}$ is oriented as (a, b) and $e = \{b, c\}$ is oriented as (c, b) if $\exists d$ s.t. $e_1 = (d, c) \in R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*) \cup A(\text{Ess}(G^*))$, $\{a, c\} \in \text{skeleton of } G^*$, $\{a, d\} \in \text{skeleton of } G^*$, and $\{b, d\} \notin \text{skeleton of } G^*$.

In what follows, we show that the orientation of e cannot be learned due to any of the Meek rules unless it belongs to $R(A_{G^*}^{(\mathcal{I}_1)}, G^*)$ or $R(A_{G^*}^{(\mathcal{I}_2)}, G^*)$.

Rule 1.

Without loss of generality, assume $e_1 \in R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup A(\text{Ess}(G^*))$. Therefore, we should have the condition of rule 1 satisfied when only intervening on \mathcal{I}_1 as well, which implies that $e \in R(A_{G^*}^{(\mathcal{I}_1)}, G^*)$, which is a contradiction.

Rule 2.

If both e_1 and e_2 belong to $R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup A(\text{Ess}(G^*))$ (or $R(A_{G^*}^{(\mathcal{I}_2)}, G^*) \cup A(\text{Ess}(G^*))$), then we should have the condition of rule 2 satisfied when only intervening on \mathcal{I}_1 (or \mathcal{I}_2) as well, which implies that $e \in R(A_{G^*}^{(\mathcal{I}_1)}, G^*)$ (or $e \in R(A_{G^*}^{(\mathcal{I}_2)}, G^*)$), which is a contradiction. Therefore, it suffices to show that the case that e_1 belongs to exactly one of

$R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup A(Ess(G^*))$ or $R(A_{G^*}^{(\mathcal{I}_2)}, G^*) \cup A(Ess(G^*))$ and e_2 belongs only to the other one, does not happen. To this end, it suffices to show that there does not exist intervention target set \mathcal{I} such that $e_1 \in R(A_{G^*}^{(\mathcal{I})}, G^*) \cup A(Ess(G^*))$, and $e, e_2 \notin R(A_{G^*}^{(\mathcal{I})}, G^*) \cup A(Ess(G^*))$, i.e., there does not exist intervention target set \mathcal{I} that has structure S_0 , depicted in Figure 4, as a subgraph of $Ess(G^*)$ after applying the orientations learned from $R(A_{G^*}^{(\mathcal{I})}, G^*)$.

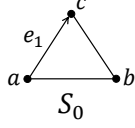


Figure 4. Structure S_0

If $e_1 \in A_{G^*}^{(\mathcal{I})}$, then $a \in \mathcal{I}$ or $c \in \mathcal{I}$, which implies $e \in A_{G^*}^{(\mathcal{I})}$ or $e_2 \in A_{G^*}^{(\mathcal{I})}$, respectively, and hence, $e \in R(A_{G^*}^{(\mathcal{I})}, G^*)$ or $e_2 \in R(A_{G^*}^{(\mathcal{I})}, G^*)$, respectively. Therefore, in either case, $e \in R(A_{G^*}^{(\mathcal{I})}, G^*)$, and S_0 will not be a subgraph. Therefore, $e_1 \notin A_{G^*}^{(\mathcal{I})}$, and hence, e_1 was learned by applying one of the Meek rules. We consider each of the rules in the following:

- If we have learned the orientation of e_1 from rule 1, then we should have had one of the structures in Figure 5 as a subgraph of $Ess(G^*)$ after applying the orientations learned from $R(A_{G^*}^{(\mathcal{I})}, G^*)$. In case of structure S_1 , using rule 1 on subgraph induced on vertices $\{v_1, a, b\}$, we will also learn (a, b) . In case of structure S_2 , using rule 4, we will also learn (b, c) . Therefore, we cannot learn only the direction of e_1 and hence, S_0 will not be a subgraph.

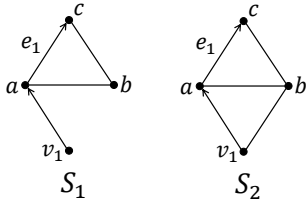


Figure 5. Rule 1

- If we have learned the orientation of e_1 from rule 3, then we have had one of the structures in Figure 6 as a subgraph of $Ess(G^*)$ after applying the orientations learned from $R(A_{G^*}^{(\mathcal{I})}, G^*)$. In case of structures S_3 and S_4 , using rule 1 on subgraph induced on vertices $\{v_2, c, b\}$, we will also learn (c, b) . In case of structure S_5 , using rule 3 on subgraph induced on vertices $\{b, v_2, c, v_1\}$, we will also learn (b, c) . Therefore, we cannot learn only the direction of e_1 and hence, S_0 will not be a subgraph.

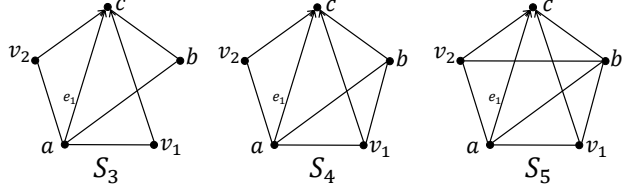


Figure 6. Rule 3

- If we have learned the orientation of e_1 from rule 4, then we have had one of the structures in Figure 7 as a subgraph of $Ess(G^*)$ after applying the orientations learned from $R(A_{G^*}^{(\mathcal{I})}, G^*)$. In case of structures S_6 , using rule 1 on subgraph induced on vertices $\{v_1, c, b\}$, we will also learn (c, b) . In case of structure S_7 , using rule 1 on subgraph induced on vertices $\{v_2, v_1, b\}$, we will also learn (v_1, b) , and then using rule 4 on subgraph induced on vertices $\{b, a, v_2, v_1\}$, we will also learn (a, b) . In case of structures S_8 , using rule 4 on subgraph induced on vertices $\{b, v_2, v_1, c\}$, we will also learn (b, c) . Therefore, we cannot learn only the direction of e_1 and hence, S_0 will not be a subgraph.

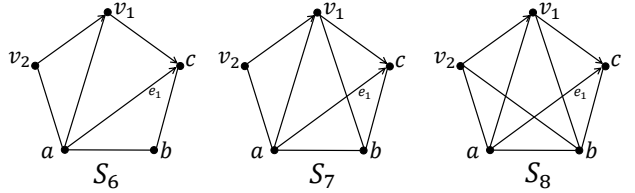


Figure 7. Rule 4

- If we have learned the orientation of e_1 from rule 2, then we should have had one of the structures in Figure 8 as a subgraph of $Ess(G^*)$ after applying the orientations learned from $R(A_{G^*}^{(\mathcal{I})}, G^*)$. In case of structure S_9 , using rule 1 on subgraph induced on vertices $\{v_1, c, b\}$, we will also learn (c, b) and hence, S_0 will not be a subgraph. In case of structure S_{10} , if $v_1 \in \mathcal{I}$, then the direction of the edge $\{v_1, b\}$ will be also known. If the direction of this edge is (v_1, b) , then using rule 2 on subgraph induced on vertices $\{a, v_1, b\}$, we will also learn (a, b) ; otherwise, using rule 2 on subgraph induced on vertices $\{b, v_1, c\}$, we will also learn (c, b) . Therefore, $v_1 \notin \mathcal{I}$. Also, as mentioned earlier, $a \notin \mathcal{I}$. Therefore, we have learned the orientation of (a, v_1) from applying Meek rules.

In the triangle induced on vertices $\{v_1, b, a\}$, we have learned only the orientation of one edge, which is (a, v_1) . But as seen in structures S_1 to S_9 , all of them lead to learning the orientation of at least 2 edges of a triangle. In the following, we will show that a structure

of form S_{10} , does not lead to learning the orientation of only (a, v_1) and making S_{10} a subgraph either.

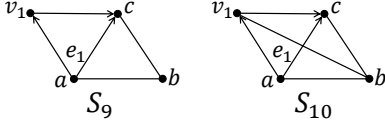


Figure 8. Rule 2

Suppose we had learned (a, v_1) via a structure of form S_{10} , as depicted in Figure 9(a). Using rule 4 on subgraph induced on vertices $\{v_2, v_1, c, b\}$, we will also learn (b, c) . Therefore, we should have the edge $\{v_2, c\}$ too. Also, using rule 2 on triangle induced on vertices $\{v_2, v_1, c\}$, the orientation of this edges should be (v_2, c) . Therefore, in order to have S_{10} as a subgraph, we need to have the structure depicted in Figure 9(b) as a subgraph. As seen in Figure 9(b), we again have a structure similar to S_{10} : a complete skeleton K_5 , which contains (v_j, c) , (a, v_j) , $\{v_j, b\}$, for $j \in \{1, 2\}$ and (v_2, v_1) , with a triangle on vertices $\{v_2, b, a\}$, in which we have learned only the orientation of (a, v_2) .

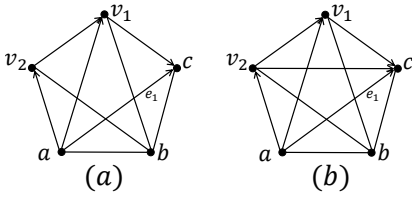


Figure 9. Step of the induction.

We claim that this procedure always repeats, i.e., at step i , we end up with skeleton K_i , which contains (v_j, c) , (a, v_j) , $\{v_j, b\}$, for $j \in \{1, \dots, i\}$ and (v_k, v_j) , for $1 \leq j < k \leq i$, with a triangle induced on vertices $\{v_i, b, a\}$, in which we have learned only the orientation of (a, v_i) . We prove this claim by induction. We have already proved the base of the induction above. For the step of the induction, suppose the hypothesis is true for $i - 1$. Add vertex v_i to form a structure of form S_{10} for (a, v_{i-1}) . v_i should be adjacent to v_j , for $j \in \{1, \dots, i - 2\}$; otherwise, using rule 4 on subgraph induced on vertices $\{v_i, v_{i-1}, v_j, b\}$, we will also learn (b, v_j) . Moreover, using rule 2 on triangle induced on vertices $\{v_i, v_{i-1}, v_j\}$, the direction of $\{v_i, v_j\}$ should be (v_i, v_j) . Also, using rule 4 on subgraph induced on vertices $\{v_i, v_{i-1}, c, b\}$, we will also learn (b, c) . Therefore, we should have the edge $\{v_i, c\}$ too.

We showed that S_0 is a subgraph only if S_{10} is a subgraph, and S_{10} is a subgraph only if the structure in Figure 9(b) is a subgraph, and this chain of required subgraphs continue. Therefore, since the order of the

graph is finite, there exist a step where since we cannot add a new vertex, it is not possible to have one of the required subgraphs, and hence we conclude that S_0 is not a subgraph.

Rule 3.

Since edges e_1 and e_2 form a v-structure, they should appear in $A(Ess(G^*))$ as well. Therefore, we should have the condition of rule 3 satisfied when only intervening on \mathcal{I}_1 as well, which implies that $e \in R(A_{G^*}^{(\mathcal{I}_1)}, G^*)$, which is a contradiction.

Rule 4.

Without loss of generality, assume $e_1 \in R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup A(Ess(G^*))$. Therefore, we should have the condition of rule 4 satisfied when only intervening on \mathcal{I}_1 as well, which implies that $e \in R(A_{G^*}^{(\mathcal{I}_1)}, G^*)$, which is a contradiction.

The argument above proves that there is no edge e such that $e \notin R(A_{G^*}^{(\mathcal{I}_1)}, G^*)$ and $e \notin R(A_{G^*}^{(\mathcal{I}_2)}, G^*)$, but $e \in R(R(A_{G^*}^{(\mathcal{I}_1)}, G^*) \cup R(A_{G^*}^{(\mathcal{I}_2)}, G^*), G^*)$.

D. Proof of Theorem 3

Let $\mathcal{I}^* = \{v_1^*, \dots, v_k^*\} \in \arg \max_{\mathcal{I}: \mathcal{I} \subseteq V, |\mathcal{I}|=k} \mathcal{D}(\mathcal{I})$. We have

$$\begin{aligned} \mathcal{D}(\mathcal{I}^*) &\stackrel{(a)}{\leq} \mathcal{D}(\mathcal{I}^* \cup \mathcal{I}_i) = \mathcal{D}(\mathcal{I}_i) \\ &+ \sum_{j=1}^k [\mathcal{D}(\mathcal{I}_i \cup \{v_1^*, \dots, v_j^*\}) - \mathcal{D}(\mathcal{I}_i \cup \{v_1^*, \dots, v_{j-1}^*\})] \\ &\stackrel{(b)}{\leq} \mathcal{D}(\mathcal{I}_i) + \sum_{j=1}^k [\mathcal{D}(\mathcal{I}_i \cup \{v_j^*\}) - \mathcal{D}(\mathcal{I}_i)], \end{aligned} \quad (3)$$

where (a) follows from Lemma 1, and (b) follows from Theorem 1. Define $\hat{\mathcal{D}}_{i,v,1}$ and $\hat{\mathcal{D}}_{i,v,2}$ as the first and second calls of subroutine in i -th step for variable vv , respectively. By the assumption of the theorem we have

$$\mathcal{D}(\mathcal{I}_i \cup \{v_j^*\}) - \epsilon \mathcal{D}(\mathcal{I}_i \cup \{v_j^*\}) < \hat{\mathcal{D}}_{i,v_j^*,1}(\mathcal{I}_i \cup \{v_j^*\}),$$

with probability larger than $1 - \delta$. Therefore

$$\mathcal{D}(\mathcal{I}_i \cup \{v_j^*\}) < \hat{\mathcal{D}}_{i,v_j^*,1}(\mathcal{I}_i \cup \{v_j^*\}) + \epsilon \mathcal{D}(\mathcal{I}^*),$$

with probability larger than $1 - \delta$. Similarly

$$\begin{aligned} \hat{\mathcal{D}}_{i,v_j^*,2}(\mathcal{I}_i) &< \mathcal{D}(\mathcal{I}_i) + \epsilon \mathcal{D}(\mathcal{I}_i) & w.p. > 1 - \delta, \\ \Rightarrow -\mathcal{D}(\mathcal{I}_i) &< -\hat{\mathcal{D}}_{i,v_j^*,2}(\mathcal{I}_i) + \epsilon \mathcal{D}(\mathcal{I}^*) & w.p. > 1 - \delta, \end{aligned}$$

Therefore,

$$\begin{aligned} \mathcal{D}(\mathcal{I}_i \cup \{v_j^*\}) - \mathcal{D}(\mathcal{I}_i) &< \hat{\mathcal{D}}_{i,v_j^*,1}(\mathcal{I}_i \cup \{v_j^*\}) \\ &- \hat{\mathcal{D}}_{i,v_j^*,2}(\mathcal{I}_i) + 2\epsilon\mathcal{D}(\mathcal{I}^*) \quad w.p. > 1 - 2\delta. \end{aligned} \quad (4)$$

Also, by the definition of the greedy algorithm,

$$\begin{aligned} \hat{\mathcal{D}}_{i,v_j^*,1}(\mathcal{I}_i \cup \{v_j^*\}) - \hat{\mathcal{D}}_{i,v_j^*,2}(\mathcal{I}_i) \\ \leq \hat{\mathcal{D}}_{i,v_{i+1},1}(\mathcal{I}_i \cup \{v_{i+1}\}) - \hat{\mathcal{D}}_{i,v_{i+1},2}(\mathcal{I}_i) \\ = \hat{\mathcal{D}}_{i,v_{i+1},1}(\mathcal{I}_{i+1}) - \hat{\mathcal{D}}_{i,v_{i+1},2}(\mathcal{I}_i), \end{aligned} \quad (5)$$

and similar to (4), we have

$$\begin{aligned} \hat{\mathcal{D}}_{i,v_{i+1},1}(\mathcal{I}_{i+1}) - \hat{\mathcal{D}}_{i,v_{i+1},2}(\mathcal{I}_i) &< \mathcal{D}(\mathcal{I}_{i+1}) \\ - \mathcal{D}(\mathcal{I}_i) + 2\epsilon\mathcal{D}(\mathcal{I}^*) \quad w.p. > 1 - 2\delta. \end{aligned} \quad (6)$$

Therefore, from equations (4), (5), and (6) we have

$$\mathcal{D}(\mathcal{I}_i \cup \{v_j^*\}) - \mathcal{D}(\mathcal{I}_i) < \mathcal{D}(\mathcal{I}_{i+1}) - \mathcal{D}(\mathcal{I}_i) + 4\epsilon\mathcal{D}(\mathcal{I}^*), \quad (7)$$

with probability larger than $1 - 4\delta$. Plugging (7) back in (3), we get

$$\begin{aligned} \mathcal{D}(\mathcal{I}^*) &< \mathcal{D}(\mathcal{I}_i) + \sum_{j=1}^k [\mathcal{D}(\mathcal{I}_{i+1}) - \mathcal{D}(\mathcal{I}_i) + 4\epsilon\mathcal{D}(\mathcal{I}^*)] \\ &= \mathcal{D}(\mathcal{I}_i) + k[\mathcal{D}(\mathcal{I}_{i+1}) - \mathcal{D}(\mathcal{I}_i)] + 4k\epsilon\mathcal{D}(\mathcal{I}^*), \end{aligned}$$

with probability larger than $1 - 4k\delta$. Therefore,

$$\begin{aligned} \mathcal{D}(\mathcal{I}^*) - \mathcal{D}(\mathcal{I}_i) \\ < k[\mathcal{D}(\mathcal{I}^*) - \mathcal{D}(\mathcal{I}_i)] - k[\mathcal{D}(\mathcal{I}^*) - \mathcal{D}(\mathcal{I}_{i+1})] + 4k\epsilon\mathcal{D}(\mathcal{I}^*), \end{aligned}$$

with probability larger than $1 - 4k\delta$. Defining $a_i := \mathcal{D}(\mathcal{I}^*) - \mathcal{D}(\mathcal{I}_i)$, and noting that $a_0 = \mathcal{D}(\mathcal{I}^*)$, by induction we have

$$\begin{aligned} a_k &= \mathcal{D}(\mathcal{I}^*) - \mathcal{D}(\mathcal{I}_k) \\ &< \left(1 - \frac{1}{k}\right)^k \mathcal{D}(\mathcal{I}^*) + 4\epsilon\mathcal{D}(\mathcal{I}^*) \sum_{j=0}^{k-1} \left(1 - \frac{1}{k}\right)^j \\ &< \left[\frac{1}{e} + 4\epsilon k\right] \mathcal{D}(\mathcal{I}^*) \quad w.p. > 1 - 4k^2\delta. \end{aligned}$$

It concludes that

$$\mathcal{D}(\mathcal{I}_k) > \left(1 - \frac{1}{e} - 4\epsilon k\right) \mathcal{D}(\mathcal{I}^*) \quad w.p. > 1 - 4k^2\delta.$$

Therefore, for $\epsilon = \frac{\epsilon'}{4k}$ and $\delta = \frac{\delta'}{4k^2}$, Algorithms 1 is a $(1 - \frac{1}{e} - \epsilon')$ -approximation algorithm with probability larger than $1 - \delta'$.

E. Proof of Theorem 4

We run the algorithm for k iterations. In each iteration, we execute the function $\hat{\mathcal{D}}(\cdot)$ using Subroutine 1 for at most n vertices. Furthermore, in this subroutine, we generate N random DAGs by calling the function `RANDEDGE`, where in (Ghassami et al., 2018) it is shown that the complexity of each call is $O(n^\Delta)$. Hence, the computational complexity of the algorithm is $O(knN \times n^\Delta)$.

F. Proof of Lemma 3

We require the following lemma for the proof:

Lemma 4. *A chordal graph has a directed cycle only if it has a directed cycle of size 3.*

Proof. If the directed cycle is of size 3 itself, the claim is trivial. Suppose the cycle C_n is of size $n > 3$. Relabel the vertices of C_n to have $C_n = (v_1, \dots, v_n, v_1)$. Since the graph is chordal, C_n has a chord and hence we have a triangle on vertices $\{v_i, v_{i+1}, v_{i+2}\}$ for some i . If the direction of $\{v_i, v_{i+2}\}$ is (v_{i+2}, v_i) , we have the directed cycle $(v_i, v_{i+1}, v_{i+2}, v_i)$ which is of size 3. Otherwise, we have the directed cycle $C_{n-1} = (v_1, \dots, v_i, v_{i+2}, \dots, v_n, v_1)$ on $n-1$ vertices. Relabeling the vertices from 1 to $n-1$ and repeating the above reasoning concludes the lemma. \square

Proof of Lemma 3. All the components in the undirected subgraph of $Ess(G^*)$ are chordal (Hauser & Bühlmann, 2012). Therefore, by Lemma 4, to insure that a generated directed graph is a DAG, it suffices to make sure that it does not have any directed cycles of length 3, which is one of the checks that we do in the proposed procedure. For checking if the generated DAG is in the same Markov equivalence class as G^* , it suffices to check if they have the same set of v-structures (Verma & Pearl, 1991), which is the other check that we do in the proposed procedure. \square