SUPPLEMENTAL MATERIAL IDENTIFYING THE TYPES OF CAUSES USING OBSERVATIONAL DATA

A PREPRINT

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A Detailed Proofs

More concepts and lemmas are needed before we present the proofs of Lemmas, Theorems and Corollaries from our main text.

Let $\mathcal{C}=(V,E)$ be an undirected graph with vertex set V and edge set E. Given $S\subseteq E$, the subgraph $\mathcal{C}(S)$ of \mathcal{C} induced by S is an undirected graph with vertex set S and edge set $E(S)=\{(u,v)\in E|u,v\in S\}$. An induced subgraph $\mathcal{C}(S)$ is called complete if there is an edge between every pair of distinct nodes in S. A clique is a set of vertices such that the induced subgraph is complete. Moreover, a clique is maximal if it isn't contained in any other cliques.

Let $\pi=(v_0,v_1,...,v_k)$ denote a simple path with length equals to k. If $k\geq 2$, we say three consecutive vertices v_i,v_{i+1} and v_{i+2} form a triangle on π if v_i is adjacent to v_{i+2} . π is called triangle-free if it doesn't contain any triangle. We agree that any path with length equals to 2 is chordless and triangle-free. Generally, It can be shown that.

Lemma 2. In any chordal graph, a path is chordless if and only if it's triangle-free.

Proof. Let $\pi = (v_0, v_1, ..., v_k)$ denote a simple path with length $k \geq 2$. If π is chordless, then it's obviously triangle-free. Now suppose π is not chordless, then we can pick up a chord $v_i - v_j$ such that the subpath $\pi(v_i, v_j)$ has no chord except for $v_i - v_j$. If j = i + 2, then v_i, v_{i+1} and v_j form a triangle. If j > i + 2, then $v_i - v_{i+1} - ... - v_{j-1} - v_j$ with $v_i - v_j$ form a cycle with length greater than 3. However, since the graph is chordal, we must have a chord $v_k - v_l$ with $i \leq k, l \leq j$ and $l \geq k + 2$ and l - k < j - i, which is contrary to our assumption.

Lemma 2 is useful for finding chordless path, since checking whether a path is triangle-free is much easier. Another important result is,

Lemma 3. Let ρ be a cycle with length greater than 3 in a given chordal graph, and X be a vertex on ρ . If the two vertices adjacent to X on ρ are not adjacent to each other, then ρ has a chord of which X is an endpoint.

Proof. Let v_1 and v_2 be two vertices adjacent to X in ρ . Suppose that ρ doesn't have a chord of which X is an endpoint. Since ρ has length greater than 3, it must have a chord. Clearly, any chord of ρ separates ρ into two sub-cycles, and by our assumptions, it is easy to check that at least one sub-cycle contains X, v_1 and v_2 . If this sub-cycle still has a chord, then we can construct another cycle containing X, v_1 and v_2 but has shorter length. Finally, we will have a cycle containing X, v_1 and v_2 but has no chord. Since v_1 and v_2 are not adjacent, the length of this cycle should be greater than 3, Which is contradicted to the definition of chordal graph.

A chordal graph can be turned into a directed graph by orienting its edges. If the resulting directed graph of an orientation is a DAG without v-structure, then we call this orientation a v-structure-free acyclic orientation. Any v-structure-free acyclic orientation of a connected chordal graph has a unique source, i.e. a vertex which has no parent. Conversely, any vertex in a connected chordal graph can be the unique source in some v-structure-free acyclic orientation. The following lemma is useful.

Lemma 4. Let C be a connected chordal graph. For any chordless path π between two distinct vertices X and Y in C, there is a v-structure-free acyclic orientation of C such that π is a completely directed path from X to Y.

Proof. Let $\pi = (X = X_0, X_1, ..., X_N = Y)$ be a chordless path from X to Y. Consider a v-structure-free acyclic orientation of $\mathcal C$ whose unique source is X. Since X is the source, the edge $X - X_1$ should be oriented as $X \to X_1$. Assume that the subpath $\pi(X, X_{l-1})$ has been oriented as a completely directed path from X to X_{l-1} , then $X_{l-1} - X_l$ should be oriented as $X_{l-1} \to X_l$. Otherwise, $X_{l-2} \to X_{l-1} \leftarrow X_l$ forms a v-structure since by the chordless assumption X_{l-2} is not adjacent to X_l . By induction, π is a completely directed path from X to Y.

Given a CPDAG \mathcal{G}^* , Andersson *et al.* (1997) proved that \mathcal{G}^* is a chain graph, which means the undirected subgraph \mathcal{G}^*_u of \mathcal{G}^* , i.e. an undirected graph obtained by deleting all the directed edges of \mathcal{G}^* , is the union of disjoint chordal graphs, and there is no partially directed cycle in the graph. Maathuis *et al.* (2009) pointed out that any v-structure-free acyclic orientation of the edges in \mathcal{G}^*_u corresponds to a DAG in the equivalence class represented by \mathcal{G}^* , and such an orientation can be considered separately for each of the disjoint chordal graphs. Moreover, local orientations of some edges are called *valid* if there is a v-structure-free acyclic orientation of \mathcal{C} such that the the directions of these edges in the v-structure-free acyclic orientation coincide with the local orientations. Maathuis *et al.* (2009) proved that,

Lemma 5. The orientations of the undirected edges adjacent to X are valid if and only if these new directed edges do not introduce v-structures.

A.1 Proof of Theorem 1

With the help of Lemma 4, we can prove Theorem 1.

Proof. Suppose there is a partially directed path from X to Y in \mathcal{G}^* . Without loss of generality, we can assume it has the following form: $X = X_0^1 - X_0^2 - \ldots - X_0^{k_0} \to X_1^1 - X_1^2 - \ldots - X_1^{k_1} \to \ldots \to X_n^1 - X_n^2 - \ldots - X_n^{k_n} = Y$. Since $X_1^1, X_1^2, \ldots, X_1^{k_1}$ are in the same chain component, $X_0^{k_0} \to X_1^1$ implies $X_0^{k_0} \to X_1^{k_1}$. Similarly, we have $X_i^{k_i} \to X_{i+1}^{k_{i+1}}$ for $i = 0, 1, 2, \ldots, n-1$. Hence $X_0^{k_0} \to X_1^{k_1} \to \ldots \to X_n^{k_n} = Y$ is a completely directed path from $X_0^{k_0}$ to Y. This means $X_0^{k_0}$ is an ancestor of Y in every DAG represented by \mathcal{G}^* . On the other hand, Lemma 4 indicates there is a v-structure-free acyclic orientation of the chain component containing X such that X is an ancestor of $X_0^{k_0}$. Combining these two observations we can conclude that X is a potential cause of Y. Conversely, if X is a potential cause of Y, then by the definition of CPDAG and potential cause, we can easily obtain the desired results.

A.2 Proof of Corollary 1

Proof. According to the definition of partially directed path, an undirected path is also partially directed, hence if X and Y are in the same chain component, they are potential causes of each other. Conversely, if X and Y are potential causes of each other, then by Theorem 1, there is a partially directed path from X to Y as well as a partially directed path from Y to X. Clearly, none of these two paths contains a directed edge, otherwise, a partially directed cycle would occur. Therefore, X and Y are connected by an undirected path, which means they are in the same chain component.

A.3 Proof of Corollary 2

This corollary is a trivial conclusion hence we omit the proof here.

A.4 Proof of Theorem 2

Proof. It is easy to verify that statement (1) is equivalent to statement (3), thus we only prove (2) \Leftrightarrow (3). The necessity is obvious, so we only need to prove the sufficiency. There is no loss of generality in assuming the path has the following form: $X = X_0 \to X_1^1 - X_1^2 - \dots - X_1^{k_1} \to \dots \to X_n^1 - X_n^2 - \dots - X_n^{k_n} = Y$. Similar to the proof of Theorem 1, we have $X \to X_1^{k_1}$ and $X_i^{k_i} \to X_{i+1}^{k_{i+1}}$ for i = 1, 2, ..., n-1. Hence, $\rho = (X, X_1^{k_1}, X_2^{k_2}, ..., X_n^{k_n} = Y)$ is a completely directed path from X to Y in \mathcal{G}^* , which means ρ is also a directed path in every DAG represented by \mathcal{G}^* .

A.5 Proof of Theorem 3

The proof of Theorem 3 is quiet complicated. First, we show that if X is a semi-invariant cause of Y, then at least two distinct variables in the chain component containing X are completely invariant cause of Y.

Lemma 6. Let \mathcal{G}^* be a CPDAG. X and Y are two distinct nodes that belong to different chain components. If X is the only completely invariant cause of Y in the chain component to which X belongs, then this chain component doesn't contain any other invariant cause of Y.

Proof. Let Z be a vertex in the chain component containing X, then every partially directed path between Z and Y passes through X. Since there is a v-structure-free orientation of the chain component whose unique source is X, there is a DAG in the Markov equivalence class represented by \mathcal{G}^* such that none of the vertex except X in the chain component is an ancestor of Y.

With the help of Lemma 6, we can prove,

Lemma 7. Let X, Z_1 , Z_2 ... Z_n be distinct vertices in a given chordal graph C. The following statements are equivalent.

- (1) $X \in an(\{Z_1, Z_2, ..., Z_n\})$ for every v-structure-free orientation of C;
- (2) there exists two distinct nodes Z_i , Z_j such that they are connected by a chordless path through X;
- (3) the subgraph over the critical set C of X with respect of $\{Z_1, Z_2, ..., Z_n\}$ in C is neither empty nor complete.

Proof. It is obvious that we only need to consider the case where $X, Z_1, Z_2 \dots Z_n$ are in the same connected component of C.

 $(2)\Rightarrow (1)$. If there exists two nodes Z_i, Z_j such that there is a chordless path π between Z_i and Z_j on which X is a intermediate node, then the two vertices adjacent to X on the path, say V_1 and V_2 , are not adjacent to each other. Hence, in any v-structure-free acyclic orientation of C, $V_1 \to X$ and $X \leftarrow V_2$ can't exist

simultaneously. Denote $\pi=(Z_i,...,V_1,X,V_2,...,Z_j)$, if $X\to V_1$, then X is an ancestor of Z_i since the subpath of a chordless path is still chordless. Similarly, if $X\to V_2$, then X is an ancestor of Z_j . Thus, $X\in an(Z_i,Z_j)\subseteq an(Z_1,Z_2,...,Z_n)$, which completes the proof of $(2)\Rightarrow (1)$.

- $(1)\Rightarrow (3)$. Clearly, C is not empty, and by Corollary 2, $n\geq 2$. If C induces a complete subgraph of C, then by Lemma 5, there is a v-structure-free acyclic orientation of C such that every vertex in C is a parent of X while every vertex in $adj(X)\setminus C$ is a child of X. We will prove that such an orientation leads to a DAG where $X\notin an(Z_1,Z_2,...,Z_n)$. In fact, if there is a completely directed path $\pi=(X=v_0,v_1,v_2,...,v_k=Z_i)$ from X to Z_i , then $v_1\notin C$, which means $k\geq 2$ and π is not chordless. Let $v_p-v_q, q\geq p+2$ be a chord on π . By acyclicity assumption, v_p must point at v_q . Therefore, $\pi(X,v_p)$, $v_p\to v_q$ and $\pi(v_q,Z_i)$ form a completely directed path from X to Z_i . If this path is not chordless, we can find another chord and construct a shorter path which is completely directed from X to Z_i . Finally, we will have a completely directed chordless path π' from X to Z_i . However, the vertex adjacent to X on π' is in critical set, thus the orientation of π' contradicts the assumption that every vertex in C is a parent of X.
- (3) \Rightarrow (2). If C doesn't induce a complete subgraph of C, then $\exists C_i, C_j \in C$, C_i and C_j are not adjacent. By the definition of critical set, we have two chordless paths, say π_i and π_j , which are from X to Z_p and Z_q respectively, such that C_i is adjacent to X on π_i and C_j is adjacent to X on π_j . We claim that π_i and π_j have no common vertex except for X. If not, let A be the common vertex such that among all the common vertices, A is closest to X on π_i , then the subpath $\pi_i(X,A)$ has no common vertex with subpath $\pi_j(X,A)$ other than X and X and X is simple to check that $\pi_i(X,A)$ and $\pi_j(X,A)$ form a cycle with length greater than X, and X and X are three consecutive vertices on this cycle. Since X are not adjacent, by Lemma X and X and some node X on this cycle. Notice that X is either a node on X and some node on X and some node on X and X are in or on X. This is contradicted to our assumptions. Since X and X have no common vertex except for X, X and X are distinct. Therefore, X and X constitute a path X from X to X which passes through X. As X and X are chordless, they are triangle-free. It follows from X and X are not adjacent that X is also triangle-free. The desired result comes from Lemma 2.

Finally, we can prove our main result.

Proof of Theorem 3. (3) \Rightarrow (2) and (2) \Rightarrow (1) can be easily derived from Lemma 7, so we omit the proof here. For (1) \Rightarrow (3), let Z be the set of all completely invariant causes of Y. By Corollary 2 and Lemma 6, X and Y belong to different chain components and $Z \neq \emptyset$. Suppose (3) doesn't hold, then by Lemma 7 X is not an invariant cause of Z, which means there is a DAG $\mathcal G$ in the markov equivalence class such that $X \notin an(Z)$. Since X is a semi-invariant cause of Y, it follows that there is a completely directed path from X to Y in $\mathcal G$. Let π be such a path, then none of the vertices on π is in Z. Recall that X and Y belong to different chain components, hence by the definition of CPDAG there are two consecutive vertices on π such that the edge between them is directed in $\mathcal G^*$. Let v_1 and v_2 be such two vertices with $v_1 \to v_2$ and $\pi(X, v_1)$ corresponds to an undirected path in $\mathcal G^*$, then by Theorem 2, v_1 is a completely invariant cause of Y. However, $v_1 \notin Z$, which is contrary to the definition of Z.

A.6 Proof of Theorem 4

Proof. First we prove statement (1). Suppose X is not a potential cause of Y, that is, X has no causal effect on Y, then for every DAG $\mathcal G$ in the Markov equivalence class represented by $\mathcal G^*$, Y is a non-descendent of X. Therefore, $X \perp \!\!\!\perp Y|pa(X)$ by Markov Property. On the other hand, if X is a potential cause of Y, then by definition there is a DAG $\mathcal G$ in the Markov equivalence class represented by $\mathcal G^*$ in which X is an ancestor of Y. Assume π is the directed path from X to Y in $\mathcal G$. Since every vertex on π is a non-collider and none of them is in pa(X), $X \not\perp \!\!\!\perp Y|pa(X)$.

Statement (2) is simply a restatement of statement (1), thus we omit the proof.

Next we prove statement (3). If X is a completely invariant cause of Y, then clearly $X \not\perp \!\!\! \perp Y|pa(X)$. By Theorem 2, let π be the directed path from X to Y in \mathcal{G}^* , then for any DAG \mathcal{G} in the Markov equivalence

class represented by \mathcal{G}^* , π is directed, which means π has no collider. However, none of the vertices on π is a member of pa(X) or sib(X), since otherwise, a directed cycle or a partially directed cycle would occur in \mathcal{G}^* . Therefore, π is active given $pa(X) \cup sib(X)$, which means $X \not\perp Y | pa(X) \cup sib(X)$. Conversely, suppose X is not a completely invariant cause of Y. Since $X \not\perp Y | pa(X)$ implies X is a potential cause of Y, X must be a semi-invariant or non-invariant cause of Y. In the following, we will prove in both cases $X \perp Y | pa(X) \cup sib(X)$ holds. By Lemma 5, there is a DAG \mathcal{G} in the Markov equivalence class represented by \mathcal{G}^* such that $ch_{\mathcal{G}}(X) = sib(X) \cup ch(X)$ and $pa_{\mathcal{G}}(X) = pa(X)$. Here, $ch_{\mathcal{G}}(X)$ and $pa_{\mathcal{G}}(X)$ means the children set and parents set of X in \mathcal{G} , respectively. Consider a path π from X to Y in \mathcal{G} . Without loss of generality, we can assume $\pi = (X, V_1, ..., V_n, Y)$. If $V_1 \in pa_{\mathcal{G}}(X)$, then π is blocked by $pa(X) \cup sib(X)$ since V_1 cannot be a collider on π . If $V_1 \in ch(X)$, then π is not directed, since otherwise, the corresponding path in \mathcal{G}^* would be a a partially directed path from X to Y where the node adjacent to X is a child of X. Therefore, there must be a collider on π . Let V_i is the collider nearest to X. If $V_i \in an(pa(X) \cup sib(X))$, there exists a partially directed cycle in \mathcal{G}^* , which is impossible. Thus $V_i \notin an(pa(X) \cup sib(X))$, and π is blocked by $pa(X) \cup sib(X)$. Finally, in the case where $V_1 \in sib(X)$, if V_1 is a non-collider, π is clearly blocked by $pa(X) \cup sib(X)$. If V_1 is a collider, then V_2 is adjacent to X, which means $V_2 \notin ch(X)$, since otherwise, both $X \to V_2 \to V_1 - X$ and $X \to V_2 - V_1 - X$ are partially directed cycles. However, V_2 is a non-collider on π and $V_2 \notin ch(X)$ implies $V_2 \in pa(X) \cup sib(X)$. Hence, π is blocked by $pa(X) \cup sib(X)$. This completes the proof of statement (3).

Again, Statement (4) is simply a restatement of statement (2). We omit the proof here. \Box

A.7 Proof of Lemma 1

Before we prove Lemma 1, we present Algorithm 4, which slightly generalizes Algorithm 1. The main differences between Algorithm 1 and 4 are the elements in S. In Algorithm 4, We introduce a number to each element in S and this number is related to the number of loops.

Algorithm 4 is a variant of Breadth-First-Search. It starts from X, by adding $\{(X,\emptyset,0,\emptyset)\}$ to a waiting queue S. Each quadruple in S consists of T, P, n and A. The first element, T, is the vertex we will visit, which stands for an endpoint of a chordless path starting from X denoted by $\pi(X,T)$, the second element P is the vertex adjacent to T on $\pi(X,T)$, the third element n is the unique ID of the subpath $\pi(X,P)$ and the forth element is the vertex adjacent to X on $\pi(X,T)$. During the k-th loop, we take the first element (T,P,n,A) out of S and add (T,P,n,k) to the front of F, which stores the found paths. Each quadruple in F contains 4 elements, namely T, P, n and k. The first three elements have the meanings as they are in S, while the forth element k means the current number of loops, which is also the ID of the chordless path $\pi(X,T)$. Next, if $T \in Z$, we add A into C since by definition A is a member of the critical set. Otherwise, we extend the current path $\pi(X,T)$ to a longer chordless path by appending a vertex adjacent to T but not adjacent to T. More precisely, let T0 be a such vertex, the chordless path T1 and the edge T2 generate a new chordless path T2. We label T3. We label T4 by number T5 and add T5 to the end of T5, since T6 is still the vertex adjacent to T5 on this new path. Of course, such a vertex T6 may not exist and if so, no quadruple will be added to T5.

Basically, The output F is a linearization of a tree. Given the output queue F of Algorithm 4, each element in F except for $(X,\emptyset,0,1)$ represents a chordless path that starts with X. More specifically, let $(T,P,n,k) \in F$ and $T \neq X$, (T,P,n,k) represents a chordless path starting with X and ending with T. To recover this path, we first add T into a queue, and find the quadruple after (T,P,n,k) in F whose forth element is n. Clearly, the first element of this quadruple is P. Again, add P into the queue. Repeat the above procedures until we reach $(X,\emptyset,0,1)$ and add X into the queue. Finally, reverse the queue to get a chordless path starting with X and ending with T.

Proof. We only need to prove the correctness of Algorithm 4. Let C_t be the true critical set. The construction above shows that each element in F represents a chordless path starting with X, which means $C \subset C_t$. Therefore, to prove the correctness of Algorithm 4, it suffices to show that for each element A in C_t , there

Algorithm 4 Finding the critical set

Require: an undirected graph \mathcal{G}_u^* , a variable X, and a set Z, **Ensure:** the critical set C of X with respect to Z in \mathcal{G}_u^* , a sequence F that stores chordless paths. 1: Initialize $C = \emptyset$, and waiting queue $S = \{(X, \emptyset, 0, \emptyset)\}$, and $F = \emptyset$, 3: **while** S is not empty **do** 4: k=k+1, 5: take the first element (T, P, n, A) out of S and add (T, P, n, k) to the front of F, if $T \notin Z$ and $P \neq \emptyset$ then 7: for $\alpha \in adj(T)$ such that $\alpha \notin adj(P) \cup \{P\}$ do 8: if P = X then add (α, T, k, T) to the end of S, 9: 10: add (α, T, k, A) to the end of S, 11: 12: end if end for 13: 14: else if $T \notin Z$ then for $\alpha \in adj(T)$, do 15: add (α, T, k, α) it to the end of S, 16: 17: end for 18: else 19: add A into C if it's not in C, 20: end if 21: end while 22: return C, F

is a quadruple (T, P, n, k) in F such that $T \in Z$ and A is the vertex adjacent to X on the corresponding chordless path.

Let $A \in C_t$ and $\pi = (X, A, V_2, ..., V_m)$ be a chordless path such that $V_m \in Z$ and no intermediate vertex on the path is in Z. For convenience, we set $V_0 = X, V_1 = A, V - 1 = \emptyset, n_0 = 1, n_{-1} = 0$. During the first loop, $(X,\emptyset,0,1)$ is added into F and (A,X,1,A) is added into S since A is adjacent to X. Since S is a queue, there exists n_1 such that (A,X,1,A) will be took out from S during the n_1 -th loop. Clearly, if m=1, then $A \in Z$, and A will be added to C during the n_1 -th loop. Suppose m>1, since X and V_2 are not adjacent, during the n_1 -th loop, $(A,X,1,n_1)$ is added to F and (V_2,A,n_1,A) is added to S. Assume that during the n_{m-1} -th loop, $(V_{m-1},V_{m-2},n_{m-2},A)$ was took out from S, and (V_m,V_{m-1},n_{m-1},A) was added to S, then there exists n_m such that (V_m,V_{m-1},n_{m-1},A) will be took out from S during the n_m -th loop and $(V_m,V_{m-1},n_{m-1},n_m)$ will be added into F. Since $V_m \in Z$, A will be added to C. It can be checked that $(V_m,V_{m-1},n_{m-1},n_m)$ corresponds to the chordless path π , which proves the existence.

Next we will prove that there is only one quadruple in F corresponding to π . Suppose that $(V_m,V_{m-1},s_{m-1},s_m)$ and $(V_m,V_{m-1},t_{m-1},t_m)$ are two different quadruples in F which both correspond to π . By above discussion, the construction procedure of the path will visit a sequence of quadruples in F. Let $(V_i,V_{i-1},s_{i-1},s_i)$ and $(V_i,V_{i-1},t_{i-1},t_i)$ i=0,1,...,m are two sequences of quadruples which the procedure visited, starting from $(V_m,V_{m-1},s_{m-1},s_m)$ and $(V_m,V_{m-1},t_{m-1},t_m)$, respectively. Since the forth element of a quadruple is the number of loops when the quadruple enters the queue, $s_m \neq t_m$. If $s_{m-1} = t_{m-1}$, we have $(V_{m-1},V_{m-2},s_{m-2},s_{m-1}) = (V_{m-1},V_{m-2},t_{m-2},t_{m-1})$, which means (V_m,V_{m-1},s_{m-1},A) is added to S twice during the s_{m-1} -th loop. This is contrary to Algorithm 4, hence $s_{m-1} \neq t_{m-1}$. By induction, $s_i \neq t_i$ for i=0,1,...m. However, $s_0 = t_0 = 1$. This completes the proof of uniqueness. \square

A.8 Proof of Theorem 5

The proof follows from Theorem 1 to Theorem 4, as well as Lemma 1.

References

Steen A. Andersson, David Madigan, and Michael D. Perlman. A characterization of markov equivalence classes for acyclic digraphs. *The Annals of Statistics*, 25(2):505–541, 04 1997.

Marloes H. Maathuis, Markus Kalisch, and Peter Bühlmann. Estimating high-dimensional intervention effects from observational data. *The Annals of Statistics*, 37(6A):3133–3164, 12 2009.