Chapter 6

Causal Structure Learning III: Experimental Design

In this lecture, we will discuss how one might *choose* interventions to learn the causal structure over variables. This moves of from the *passive* learning setting discussed in Chapter 5 to an *active* setting. For example, in genomics, a scientist can choose which genes to knockout in their experiments in their effort to learn a gene regulatory network.

6.1 Identifiability from Interventions

To begin, we will develop an understanding of which undirected edges in the essential graph can be oriented by an intervention. In doing so, we are assuming that we always have access to observational data: we will denote observational data by the "empty" intervention $I_\varnothing$, defined so that $\mathcal{X}(I_\varnothing) = \varnothing$, i.e., the empty intervention has no targets.

First, we extend our notion of an interventional causal graph from Chapter 1, which considered only a single intervention, to multiple interventions.

Definition 6.1. *Let $\mathcal{I} = \{I_\varnothing, I_1, \dots, I_K\}$ be a set of interventions on a structural causal model M with causal DAG $\mathcal{G}$ over nodes $\mathcal{X}$. Then the* **interventional causal graph**, *denoted $\mathcal{G}^{\mathcal{I}}$, is the DAG with:*

- *Nodes $\mathcal{X} \cup \mathcal{Z} \cup \{\zeta^*\}$, where $\mathcal{Z} = \{\zeta^{I_1}, \dots, \zeta^{I_K}\}$, and*

Z is intervention indicators - only one of them can be active at each time - which is Zeta^* - that denotes the node number of get intervend.

- *Edges as follows:*
  - *$X_i \to X_j$ for $X_i, X_j \in \mathcal{X}$ if $X_i \to X_j$ in $\mathcal{G}$,*
  - *$\zeta_k \to X_i$ for $X_i \in \mathcal{X}(I_k)$, $k \in [K]$, and*
  - *$\zeta^* \to \zeta_k$ for $k \in [K]$*

The interventional causal graph can be used to encode the interventions as follows. Suppose that the causal mechanisms of M are $\{f_{X_i}\}_{X_i \in \mathcal{X}}$ and the interventional causal mechanisms for I_k are $\{g_{X_i}^{I_k}\}_{X_i \in \mathcal{X}(I_k)}$. Let $\mathcal{I}(X_i) := \{I_k : X_i \in \mathcal{X}(I)\}$ be the set of interventions with X_i as an intervention target. Then

1. ζ^* takes values $0, 1, \dots, K$, with $\zeta^* = 0$ indicating that the variables $\mathcal{X}$ are generated from the SCM M, and $\zeta^* = k$ indicating that the variables are generated from the interventional SCM M^{I_k}.
2. The ζ_k variables are a deterministic function of ζ^*. If $\zeta^* = 0$, then $\zeta_k = 0$ for all k. Otherwise, if $\zeta^* = k$, then $\zeta_j = \mathbb{1}_{j=k}$.

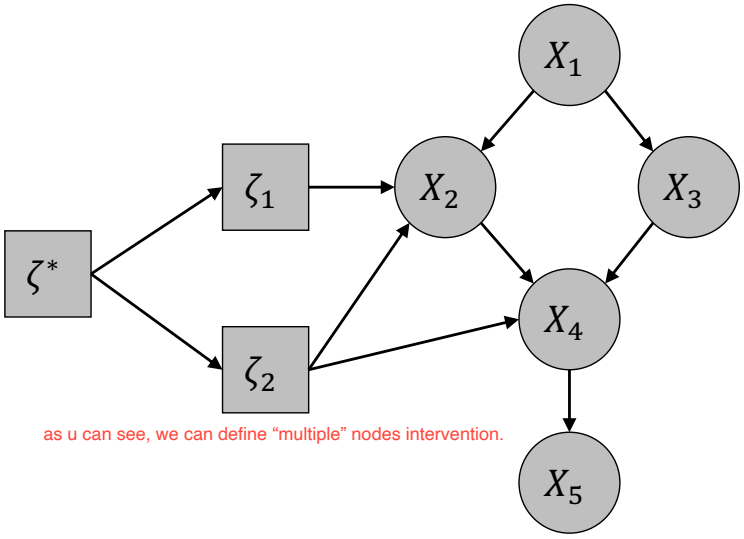

Figure 6.1: The interventional causal graph for $\mathcal{I} = \{I_\varnothing, I_1, I_2\}$, where $\mathcal{X}(I_1) = \{X_2\}$ and $\mathcal{X}(I_2) = \{X_2, X_4\}$.

3. The **system variables** $X_i \in \mathcal{X}$ have causal mechanisms

$$f^{\mathcal{I}}_{X_i}(\text{pa}_{\mathcal{G}^{\mathcal{I}}}(X_i)) = \mathbb{1}\{\zeta_k = 0, k \in \mathcal{I}(X_i)\} \cdot f_{X_i}(\text{pa}_{\mathcal{G}}(X_i), \varepsilon_i) + \sum_{k \in \mathcal{I}(X_i)} \mathbb{1}\{\zeta_k = 1\} \cdot g^{I_k}_{X_i}(\text{pa}_{\mathcal{G}}(X_i), \varepsilon_i)$$

Example 6.1. *An interventional causal graph with two interventions is shown in Figure 6.1. Note that we will often drop the node ζ^* and its outgoing edges, as they are implied.*

Claim 6.1. *Given a set of interventions $\mathcal{I}$, we can define a distribution over $\mathcal{X}^{\mathcal{I}} := \mathcal{X} \cup \mathcal{Z} \cup \{\zeta^*\}$ such that $\mathbb{P}_{\mathcal{X}^{\mathcal{I}}}(\mathcal{X} \mid \zeta_k = 1) = \mathbb{P}^{I_k}_{\mathcal{X}}(\mathcal{X})$*

Given a set of interventions, we may define a new form of equivalence between DAGs. In particular, we will consider $\mathcal{I}_{\perp\!\!\!\perp}(\mathcal{G}^{\mathcal{I}})$, the set of d-separations in the interventional causal graph $\mathcal{G}^{\mathcal{I}}$.

Definition 6.2. *Let $\mathcal{I}$ be a set of interventions such that $I_\varnothing \in \mathcal{I}$. We say that two DAGs $\mathcal{G}$ and $\mathcal{G}'$ are **$\mathcal{I}$-Markov equivalent** if $\mathcal{I}_{\perp\!\!\!\perp}(\mathcal{G}^{\mathcal{I}}) = \mathcal{I}_{\perp\!\!\!\perp}(\mathcal{G}'^{\mathcal{I}})$. We denote the set of all DAGs which are $\mathcal{I}$-Markov equivalent to $\mathcal{G}$ as $\mathcal{M}_{\mathcal{I}}(\mathcal{G})$.*

As in the observational case, we may define a single mixed graph to represent the $\mathcal{I}$-Markov equivalence class:

Definition 6.3. *The $\mathcal{I}$-essential graph of an $\mathcal{I}$-Markov equivalence class $\mathcal{M}_{\mathcal{I}}(\mathcal{G})$ is a mixed graph with:*

- *A directed edge $X_i \to X_j$ if $X_i \to X_j$ for all $\mathcal{G}' \in \mathcal{M}_{\mathcal{I}}(\mathcal{G})$, and*
- *An undirected edge $X_i - X_j$ if $X_i \to X_j$ for some $\mathcal{G}_1 \in \mathcal{M}_{\mathcal{I}}(\mathcal{G})$ and $X_i \leftarrow X_j$ for some $\mathcal{G}_2 \in \mathcal{M}(\mathcal{G})$.*

where is subscript I ?

Recall from Theorem 4.2 that two DAGs $\mathcal{G}$ and $\mathcal{G}'$ are Markov equivalent if and only if they have the same skeleton and unshielded colliders. By extension, two DAGs $\mathcal{G}$ and $\mathcal{G}'$ are $\mathcal{I}$-Markov equivalent if and only if $\mathcal{G}^{\mathcal{I}}$ and $\mathcal{G}'^{\mathcal{I}}$ have the same skeleton and unshielded colliders. This gives rise to a simple characterization of $\mathcal{I}$-Markov equivalence:

Proposition 6.1. *Let $\mathcal{I}$ be a set of interventions such that $I_\varnothing \in \mathcal{I}$. Two DAGs $\mathcal{G}$ and $\mathcal{G}'$ are $\mathcal{I}$-Markov equivalent if and only if:*

C1. *$\mathcal{G}$ and $\mathcal{G}'$ have the same skeleton and unshielded colliders, and*

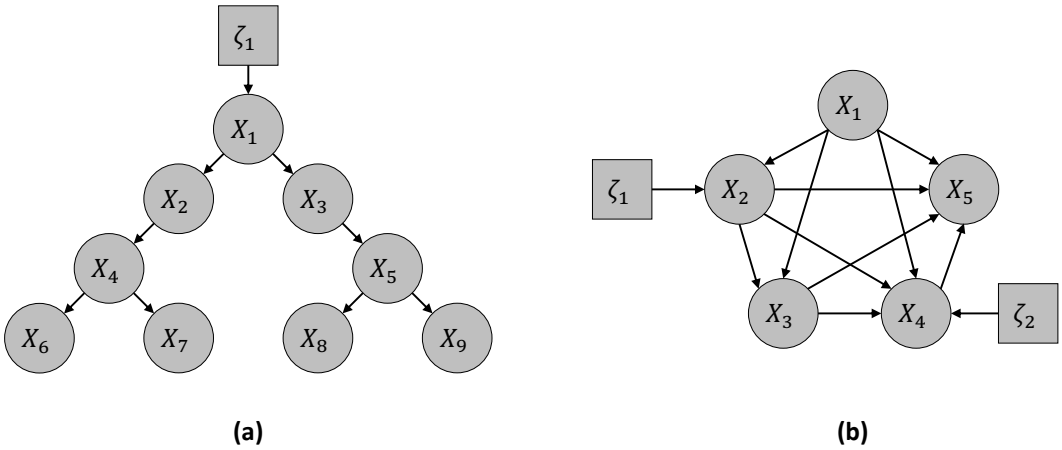

Figure 6.2: Verifying intervention sets for a tree graph and a complete graph.

C2. *for all $I_k \in \mathcal{I}$, $X_i \notin \mathcal{X}(I_k)$, $X_j \in \mathcal{X}(I_k)$, we have $X_i \to X_j$ in $\mathcal{G}$ if and only if $X_i \to X_j$ in $\mathcal{G}'$.*

Proof. Let $\mathcal{G}$ and $\mathcal{G}'$ be $\mathcal{I}$-Markov equivalent. It is clear that **C1** must hold. Further, for arbitrary I_k, suppose $X_i \notin \mathcal{X}(I_k)$ and $X_j \in \mathcal{X}(I_k)$. Then $\mathcal{G}^{\mathcal{I}}$ has an unshielded collider $X_i \to X_j \leftarrow \zeta_k$. Thus, $\mathcal{G}'^{\mathcal{I}}$ must have $X_i \to X_j \leftarrow \zeta_k$, in particular, $\mathcal{G}'$ must have $X_i \to X_j$. Symmetrically, if $X_i \to X_j$ in $\mathcal{G}'$, we must have $X_i \to X_j$ in $\mathcal{G}$. Thus, **C2** must hold.

Conversely, suppose that **C1** and **C2** hold. Let $X_i \to X_j$ be involved in an unshielded collider in $\mathcal{G}^{\mathcal{I}}$ but not in $\mathcal{G}$. Then there must exist $\zeta_k \in \mathcal{Z}$ such that $\zeta_k \to X_j$ but $\zeta_k \not\to X_i$. By **C2**, we have the same unshielded collider in $\mathcal{G}'^{\mathcal{I}}$. Symmetrically, if $X_i \to X_j$ is involved in an unshielded collider in $\mathcal{G}'^{\mathcal{I}}$ but not in $\mathcal{G}'$, then by **C2**, the same unshielded collider is in $\mathcal{G}^{\mathcal{I}}$. Thus, $\mathcal{G}^{\mathcal{I}}$ and $\mathcal{G}'^{\mathcal{I}}$ have the same skeleton and unshielded colliders, i.e., they are Markov equivalent. □

Example 6.2. *Let $\mathcal{G} = \{X_1 \to X_2\}$ and $\mathcal{G}' = \{X_1 \leftarrow X_2\}$. $\mathcal{G}$ and $\mathcal{G}'$ are Markov equivalent. Let $\mathcal{I} = \{I_1\}$. Then:*

- *If $\mathcal{X}(I_1) = \{X_1\}$, then $\mathcal{G}$ and $\mathcal{G}'$ are not $\mathcal{I}$-Markov equivalent, since $\zeta_1 \to X_1 \leftarrow X_2$ in $\mathcal{G}'$ but not in $\mathcal{G}$.*
- *Similarly, if $\mathcal{X}(I_1) = \{X_2\}$, then $\mathcal{G}$ and $\mathcal{G}'$ are not $\mathcal{I}$-Markov equivalent.*
- *However, if $\mathcal{X}(I_1) = \{X_1, X_2\}$, then $\mathcal{G}$ and $\mathcal{G}'$ are $\mathcal{I}$-Markov equivalent. For example, if we perform a do-intervention on both variables, then we can't tell which node is downstream of the other.*

Corollary 6.1. *Let $\mathcal{X}(I_k) = \{X_i\}$ and $I_k \in \mathcal{I}$. Then all edges incident to X_i are directed in $\mathcal{E}_{\mathcal{I}}(\mathcal{G})$.*

Proof. For $X_j \in \mathrm{pa}_{\mathcal{G}}(X_i)$, we have an unshielded collider $X_j \to X_i \leftarrow \zeta_k$ in $\mathcal{G}$. For $X_j \in \mathrm{ch}_{\mathcal{G}}(X_i)$, we have by Meek Rule 1 that $X_i \to X_j$. □

The case $\mathcal{X}(I_k) = \{X_i\}$ can be given the following interpretation. If $X_j \in \mathrm{pa}_{\mathcal{G}}(X_i)$, then $X_j \perp\!\!\!\perp_{\mathcal{G}^{\mathcal{I}}} \zeta_k \mid \mathcal{Z} \setminus \{\zeta_k\}$. Thus,

$$\mathbb{P}_{\mathcal{X}^{\mathcal{I}}}(X_j \mid \zeta_k = 1, \mathcal{Z} \setminus \{\zeta_k\} = 0) = \mathbb{P}_{\mathcal{X}^{\mathcal{I}}}(X_j \mid \zeta_k = 0, \mathcal{Z} \setminus \{\zeta_k\} = 0),$$

i.e., $\mathbb{P}^{I_k}_{\mathcal{X}}(X_j) = \mathbb{P}_{\mathcal{X}}(X_j)$, the marginal of X_j is unaffected by the intervention. However, for $X_j \in \mathrm{ch}_{\mathcal{G}}(X_i)$, we have $X_j \not\perp\!\!\!\perp_{\mathcal{G}^{\mathcal{I}}} \zeta_k \mid \mathcal{Z} \setminus \{\zeta_k\} = 0$, so under some form of faithfulness, we expect $\mathbb{P}^{I_k}_{\mathcal{X}}(X_j) \neq \mathbb{P}_{\mathcal{X}}(X_j)$.

6.2 Verifying Intervention Sets

In experimental design, we will often be interested in completely determining the causal graph. In particular, we will want our intervention set $\mathcal{I}$ to be a verifying intervention set, as we now define:

Definition 6.4. *Let $\mathcal{G}$ be a causal graph and $\mathcal{I}$ be a set of interventions. We call $\mathcal{I}$ a* **verifying intervention set** *for $\mathcal{G}$ if $|\mathcal{M}(\mathcal{G}^{\mathcal{I}})| = 1$.*

Example 6.3. *If $\mathcal{G}$ is a tree with root node X_i, then an intervention on X_i is a verifying intervention set. For a complete graph with topological order $X_1 < X_2 < \ldots < X_p$, the set of single-node intervention on all odd-numbered nodes is a verifying intervention set. See Figure 6.2.*

Remark 6.1. *Note that the definition of a verifying intervention set includes the graph $\mathcal{G}$, i.e., we cannot necessarily determine a verifying intervention set if we do not know $\mathcal{G}$. This motivates the term* ***verifying****: we can imagine that the set $\mathcal{I}$ is determined by a "teacher" who knows the graph $\mathcal{G}$. This set is told to a "student" who knows only the essential graph $\mathcal{E}(\mathcal{G})$. The student then performs the interventions in this set to verify that $\mathcal{G}$ is indeed the correct causal graph.*

Now, recall the **transformational characterization** of Markov equivalence from Chapter 5: for any two Markov equivalent graphs $\mathcal{G}$ and $\mathcal{G}'$, there is a set of covered edge reversals from $\mathcal{G}$ to $\mathcal{G}'$. This extends to $\mathcal{I}$-Markov equivalent graphs as follows:

Definition 6.5. *Let $\mathcal{G}$ be a DAG and $\mathcal{I}$ be a set of interventions. We call an edge $X_i \to X_j$ in $\mathcal{G}$ an $\mathcal{I}$-covered edge if it is a covered edge in $\mathcal{G}^{\mathcal{I}}$.*

Note that the set of $\mathcal{I}$-covered edges in $\mathcal{G}$ is exactly the set of covered edges in $\mathcal{G}^{\mathcal{I}}$: none of the $\zeta_k \to X_i$ edges are covered, since $\zeta^* \to \zeta_k$ but $\zeta^* \not\to X_i$.

Thus, we have the following corollary of Theorem 5.3.

Corollary 6.2. *Let $\mathcal{G}'$ and $\mathcal{G}$ be $\mathcal{I}$-Markov equivalent. Then there is a sequence of $\mathcal{I}$-covered edge reversals from $\mathcal{G}$ to $\mathcal{G}'$.*

This gives us a simple way of characterizing verifying intervention sets.

Definition 6.6. *We say that $\mathcal{I}$ is a* **separating set** *for $\mathcal{G}$ if, for any covered edge $X_i \to X_j$ in $\mathcal{G}$, there exists some $I_k \in \mathcal{I}$ such that $X_i \in \mathcal{X}(I_k)$ and $X_j \notin \mathcal{X}(I_k)$.*

Theorem 6.1 (Choo et al. (2022))**.** *$\mathcal{I}$ is a verifying intervention set for $\mathcal{G}$ if and only if it is a separating set for $\mathcal{G}$.*

Proof. If $\mathcal{I}$ is a separating set, then there are no $\mathcal{I}$-covered edges in $\mathcal{G}$, so there are no graphs which are $\mathcal{I}$-Markov equivalent to $\mathcal{G}$. That is, $\mathcal{I}$ is a verifying intervention set. Conversely, if $\mathcal{I}$ is not a separating set, then there exists a covered edge $X_i \to X_j$ that is $\mathcal{I}$-covered, so there is a graph which is $\mathcal{I}$-Markov equivalent to $\mathcal{G}$. That is, $\mathcal{I}$ is not a verifying intervention set. □

Example 6.4. *For a tree graph $\mathcal{G}$ with root X_i, the only covered edges are of the form $X_i \to X_j$ for $X_j \in \mathrm{ch}_{\mathcal{G}}(X_i)$. Hence, for a tree graph, an intervention set with only an intervention targeting X_i is a separating set.*

For a complete graph $\mathcal{G}$ with topological order $X_1 < X_2 < \ldots < X_p$, the covered edges are $X_1 \to X_2, X_2 \to X_3, \ldots, X_{p-1} \to X_p$. Thus, if $\mathcal{I}$ is a separating set for $\mathcal{G}$, then for every pair of nodes (X_i, X_{i+1}), one must be intervened. Thus, just even-numbered nodes suffice.

6.3 Non-adaptive intervention policies

Definition 6.7. *A (noiseless)* **non-adaptive intervention policy** π *is a map from an essential graph $\mathcal{E}(\mathcal{G})$ to a set of interventions $\mathcal{I}$.*

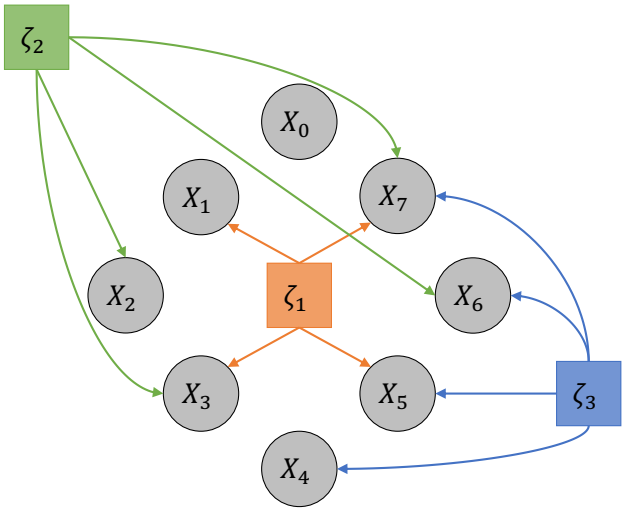

Figure 6.3: A sufficient set of interventions $\mathcal{I}$ for orienting all edges in a complete graph, following the construction in Theorem 6.2.

It is often natural to place restrictions on the allowed interventions, for example, restricting their size.

Definition 6.8. *Let Π_K denote the set of intervention policies such that $|\mathcal{X}(I_t)| \leq K$ for all t. As a special case, Π_∞ denotes the set of all intervention policies (i.e., with no bounds on the number of targets in each intervention).*

The **minimum cost identification** problem is

$$\min_{\pi \in \Pi_K} \ \text{cost}(\mathcal{I}) \quad \text{s.t. } |\mathcal{M}_{\mathcal{I}}(\mathcal{G})| = 1$$

Remark 6.2. *We will consider a simple cost function, $\text{cost}(\mathcal{I}) = |\mathcal{I}|$, so that we simply want to minimize the number of interventions. One may consider more complex cost functions, for example, where each node X_i has an associated cost $\text{cost}(X_i)$, and $\text{cost}(\mathcal{I}) = \sum_{I_k \in \mathcal{I}} \sum_{X_i \in \mathcal{X}(I_k)} \text{cost}(X_i)$.*

Theorem 6.2. *Let $\mathcal{E}(\mathcal{G})$ be a complete graph on $p \geq 3$ nodes and consider non-adaptive intervention policies in Π_∞. Then $\lfloor \log_2 p \rfloor + 1$ interventions are sufficient and, in the worst case, necessary to identify $\mathcal{G}$.*

Proof. **Sufficiency.** For an integer m, let $b(m)$ denote its binary representation, i.e., $b(6) = 110$. Label the nodes $0, \ldots, p-1$ and let $\mathcal{I}$ be the set of interventions with $I_k = \{m : b(m)_k = 1\}$ for $k = 1, \ldots, \lfloor \log_2 p \rfloor + 1$. Since any two numbers differ in their binary representation in at least one position, $\mathcal{I}$ is a separating set.

Worst-case Necessity. Consider $p = 3$. For any intervention set with one single-node intervention on X_i, in the worst case, X_i is the source node and the edge between the other two nodes is unoriented. For any intervention set with one two-node intervention on X_i and X_j, in the worst case, X_i and X_j are downstream of the other node, and the edge between X_i and X_j is unoriented.

Assume the result holds for $q < p$. Consider an intervention on $K \leq p$. In the worst case, all $p - K$ non-intervened nodes are upstream of the K intervened nodes. Thus, the problem splits into two complete graphs of size $p-K$ and size K. By the induction hypothesis, one of the graphs requires at least $\lfloor \log_2 \frac{p}{2} \rfloor + 1 = \lfloor \log_2 p \rfloor$ interventions. this should be ceiling? □

Example 6.5. *An example of the construction for $\mathcal{I}$ is depicted in Figure 6.3.*

A similar result holds for general essential graphs. In particular, we will characterize the structure of essential graphs.

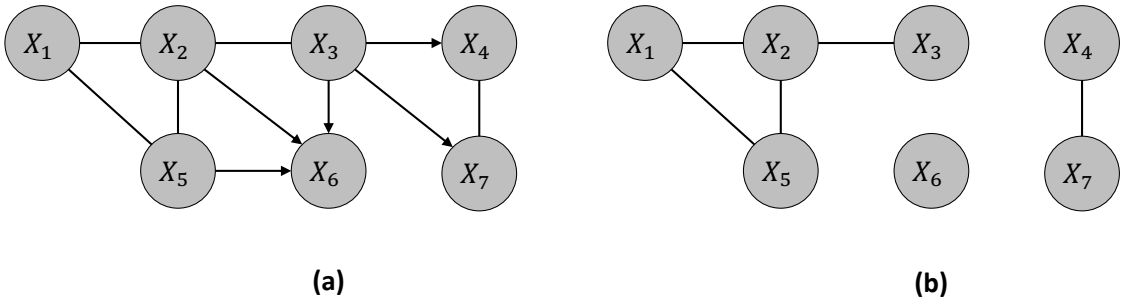

Figure 6.4: **(a)** A chain graph and **(b)** its chain components.

Definition 6.9. *Let $\mathcal{G}$ be a partially directed acyclic graph (PDAG). A* **partially directed cycle** *is a sequence $\gamma_1, \ldots, \gamma_M$ of nodes such that $\gamma_m - \gamma_{m+1}$ or $\gamma_m \to \gamma_{m+1}$ for all $m = 1, \ldots, M-1$, and such that at least one edge in the path is directed.*

$\mathcal{G}$ is a **chain graph** *if it has no partially directed cycles. In this case, the* **chain components** *of a chain graph are the connected components of the subgraph containing only undirected edges.*

Example 6.6. *Figure 6.4 shows a chain graph and its chain components.*

Proposition 6.2. *An essential graph is a chain graph.* chain graph is chordal graph

Further, the chain components of an $\mathcal{I}$-essential graph have a special structure.

Definition 6.10. *Given an undirected graph $\mathcal{G}$ and an undirected cycle in $\mathcal{G}$, a* **chord** *is an edge that is not in the cycle, but connects two nodes in the cycle.*

An undirected graph is **chordal** *if all cycles of length ≥ 4 have a chord.*

Proposition 6.3. *The chain components of an $\mathcal{I}$-essential graph $\mathcal{E}_\mathcal{I}(\mathcal{G})$ are chordal. Further, the orientations in one chain component of $\mathcal{E}_\mathcal{I}(\mathcal{G})$ are logically independent of the orientation of other chain components of $\mathcal{E}_\mathcal{I}(\mathcal{G})$.*

Proof. Suppose there is a chordless cycle $\gamma_1 - \gamma_2 - \ldots - \gamma_M - \gamma_1$. Since $\mathcal{E}_\mathcal{I}(\mathcal{G})$ is an essential graph, we have $\gamma_1 \to \gamma_2$ for some $\mathcal{G}'$ in the represented $\mathcal{I}$-MEC. Since the cycle is chordless, the Meek rules imply that we have $\gamma_1 \to \gamma_2 \to \ldots \to \gamma_M \to \gamma_1$, a directed cycle in $\mathcal{G}'$. Thus, there cannot be a chordless cycle.

That the chain components are logically independent follows from the Meek rules. □

Chordal graphs have very nice theoretical and computational properties that make them easy to use for experimental design. We will see that the difficulty of experimental design is closely related to the size of the largest clique in a chordal graph:

Definition 6.11. *The* **clique number** *of an undirected graph $\mathcal{G}$, denoted $\omega(\mathcal{G})$, is the size of the largest clique in $\mathcal{G}$.*

Definition 6.12. *A* **k-coloring** *of a graph over nodes $\mathcal{X}$ is a map $c : \mathcal{X} \to [k]$ such that $c(X_i) \neq c(X_j)$ for any two adjacent nodes X_i and X_j.*

The **chromatic number** *of a graph is the smallest number of colors which forms a coloring.*

Proposition 6.4. *In a chordal graph $\mathcal{G}$, the chromatic number equals $\omega(\mathcal{G})$. Furthermore, an optimal coloring can be computed in linear time (in the number of nodes + the number of edges).*

Theorem 6.3. *Let $\mathcal{E}(\mathcal{G})$ be a chordal graph on $p \geq 3$ nodes and consider non-adaptive intervention policies in Π_∞. Then $\lfloor \omega(\mathcal{E}(\mathcal{G})) \rfloor + 1$ interventions are sufficient to identify $\mathcal{G}$.*

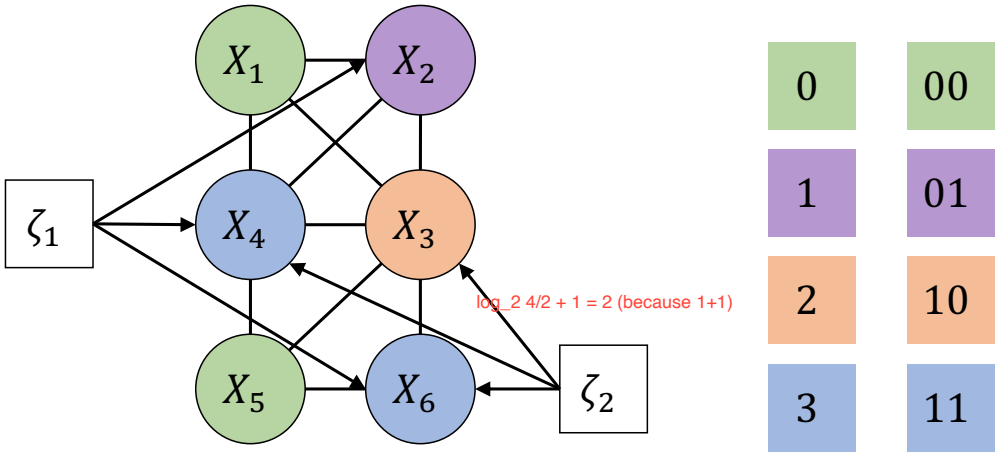

Figure 6.5: A coloring of a chordal graph and intervention assignments as constructed in Theorem 6.3.

Proof. Let c be a coloring of $\mathcal{G}$ and let b denote the binary representation of an integer m. Let $\mathcal{I}$ be the set of interventions with $I_k = \{m : b(c(m))_k = 1\}$ for $k = 1, \ldots, \lfloor \log_2 \omega(\mathcal{E}(\mathcal{G})) \rfloor + 1$. □

The same number of interventions is also, in the worst case, necessary to identify $\mathcal{G}$. The proof is similar to that of Theorem 6.2, so we will not repeat it here.

Example 6.7. *An example of the construction from Theorem 6.3 is given in Figure 6.5.*

6.4 Adaptive intervention policies

In practice, we might consider running experiments *sequentially* instead of in parallel. Thus, for the t-th intervention, we can make use of the orientations discovered by the $t-1$ interventions, denoted $\mathcal{I}_{t-1}$, already performed to make our choice.

Definition 6.13. *A (noiseless)* **adaptive intervention policy** π *is a set of maps* π_t*, where each* π_t *is a map from a sequence of* $(\mathcal{I})$*-essential graphs* $\mathcal{E}_{\mathcal{I}_0}(\mathcal{G}), \mathcal{E}_{\mathcal{I}_1}(\mathcal{G}), \mathcal{E}_{\mathcal{I}_{t-1}}(\mathcal{G})$ *to an intervention* I_t*.*

In the adaptive setting, it is natural to take a *greedy* approach to picking each intervention.

Definition 6.14. *The* **greedy minimax entropy policy** *picks* I_t *as follows:*

$$I_t \in \arg\min_{I_t'} \max_{\mathcal{G}' \in \mathcal{M}_{\mathcal{I}_{t-1}}(\mathcal{G})} |\mathcal{M}_{\mathcal{I}_{t-1} \cup \{I_t'\}}(\mathcal{G})|$$

Theorem 6.4. *Let* $\mathcal{E}(\mathcal{G})$ *be a tree graph, and consider adaptive intervention policies in* Π_1*. Then* $\lceil \log_2 p \rceil + 1$ *interventions are sufficient to identify* $\mathcal{G}$*.*

Proof. An intervention on X_i splits a tree into components, with at most one component upstream of X_i (otherwise, we would form an unshielded collider at X_i). By the first Meek rule, all edges downstream of X_i are oriented. Thus, for the worst case $\mathcal{G}' \in \mathcal{M}_{\mathcal{I}_{t-1}}$, the largest component is upstream of X_i. The size of this component is minimized by picking a **central node**, which is guaranteed to split the tree into components with at most $p/2$ nodes. Thus, we reduce the problem size by $1/2$ at each time, ending in at most $\lceil \log_2 p \rceil$ steps. □

Remark 6.3. *Greenewald et al. (2019) showed that the expected number of interventions used by the greedy minimax entropy policy is at most twice the expected number of interventions used by the optimal intervention policy in* Π_1*. In particular, this shows that the optimal intervention policy in* Π_1 *can differ from the size of the smallest verifying intervention set (which is of size one in the case of a tree) by a factor of* $\log_2 p$*. This factor was also recently shown to be achievable for any graph, see Choo et al. (2022).*

6.5 Additional Readings

- **Maximum information gain:** In this lecture, we considered minimizing the cost of a set of interventions, subject to the constraint that these interventions fully orient the DAG $\mathcal{G}$. One may also be interested in the "dual" of this problem, where we are given a budget B, and we wish to maximize some measure of information about the $\mathcal{I}$-essential graph (e.g., the number of oriented edges) subject to $\text{cost}(\mathcal{I}) \leq B$. See for example Ghassami et al. (2018).
- **Targeted experimental design:** We considered picking interventions with the end goal of fully orienting the graph. However, this may be overkill, for example if we only care about determining the structure of some subgraph. In such cases, we may design more targeted intervention policies, see for example Agrawal et al. (2019).

Bibliography

Agrawal, R., Squires, C., Yang, K., Shanmugam, K., and Uhler, C. (2019). Abcd-strategy: Budgeted experimental design for targeted causal structure discovery. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 3400–3409. PMLR.

Choo, D., Shiragur, K., and Bhattacharyya, A. (2022). Verification and search algorithms for causal dags. *arXiv preprint arXiv:2206.15374*.

Ghassami, A., Salehkaleybar, S., Kiyavash, N., and Bareinboim, E. (2018). Budgeted experiment design for causal structure learning. In *International Conference on Machine Learning*, pages 1724–1733. PMLR.

Greenewald, K., Katz, D., Shanmugam, K., Magliacane, S., Kocaoglu, M., Boix Adsera, E., and Bresler, G. (2019). Sample efficient active learning of causal trees. *Advances in Neural Information Processing Systems*, 32.