Learning Good Interventions in Causal Graphs via Covering (Supplementary Material)

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A MISSING PROOFS FROM SECTION 3.1

We first provide a standard concentration bound which will be used in the analysis. Then, we restate and prove Lemmas 2, 3, and 4.

Lemma 1 (Hoeffding's Inequality). *Let $Z_1, \ldots, Z_n$ be independent bounded random variables with $Z_i \in [a_i, b_i]$, for all $i \in [n]$. Then, for all $\varepsilon \geq 0$:*

$$\mathbb{P}\left\{\left|\sum_{i=1}^{n}(Z_i - \mathbb{E}[Z_i])\right| \geq \varepsilon\right\} \leq 2\exp\left(-\frac{2\varepsilon^2}{\sum_{i=1}^{n}(b_i - a_i)^2}\right).$$

Lemma 2. *For estimates obtained via a covering intervention set $\mathcal{I}$, as in Algorithm 1, write $\mathcal{E}$ to denote the event that $|\Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right)| \leq \sqrt{\frac{|\mathcal{I}|(d+\log(NT))}{T}}$ for all vertices $i \in \mathcal{V}$. Then, $\Pr\{\mathcal{E}\} \geq \left(1 - \frac{2}{T}\right)$.*

Proof. Since $\mathcal{I}$ is a covering intervention set, for each conditional distribution $\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right)$, we have at least $\frac{T}{|\mathcal{I}|}$ independent samples. Now, we invoke Lemma 1, with $\varepsilon = \sqrt{\frac{|\mathcal{I}|\log(2^d NT)}{T}}$, and apply the union bound over all $i \in [N]$ and all assignments to $\mathrm{Pa}(i)$. This gives us the desired probability bound. □

Lemma 3. *For estimates obtained via a covering intervention set $\mathcal{I}$, as in Algorithm 1, the following event holds with probability at least $\left(1 - \frac{2}{T}\right)$:*

$$\sum_{\mathbf{z} \in Z(A)} |\mathcal{L}_{\mathbf{z}}| \leq 4(N\eta)^2 \qquad \text{for all } A \in \mathcal{A}.$$

Here, parameter $\eta = \sqrt{\frac{|\mathcal{I}|(d+\log(NT))}{T}}$ and T is moderately large T.

Proof. We will use the fact that each error term in $\mathcal{L}_{\mathbf{z}}$ satisfies the bound stated in Lemma 2. Moreover, we utilize the graph structure to marginalize variables that do not appear in an expansion of $\mathcal{L}_{\mathbf{z}}$.

$$\begin{aligned}\sum_{\mathbf{z} \in Z(A)} |\mathcal{L}_{\mathbf{z}}| &\leq \sum_{\mathbf{z} \in Z(A)} \sum_{k=2}^{|\mathcal{V}(A)|} \sum_{\substack{U \subseteq \mathcal{V}(A) \\ |U|=k}} \left(\prod_{i \in U} \left|\Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right)\right|\right)\left(\prod_{j \in \mathcal{V}(A)\setminus U} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right)\right) \\ &= \sum_{k=2}^{|\mathcal{V}(A)|} \sum_{\mathbf{z} \in Z(A)} \sum_{\substack{U \subseteq \mathcal{V}(A) \\ |U|=k}} \left(\prod_{i \in U} \left|\Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right)\right|\right)\left(\prod_{j \in \mathcal{V}(A)\setminus U} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right)\right).\end{aligned}$$

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First, we upper bound each term considered in the outer-most sum. Towards this, let $U = \{V_{x_1}, V_{x_2}, \dots, V_{x_k}\}$ to be a subset of vertices that appears in the inner sum. Here, $x_1 < x_2 < \dots < x_k$ and, as mentioned previously, the indexing of the vertices respects a topological ordering over the causal graph. In the derivation below, we will split the sum into k parts, $\sum_{\mathbf{z}_{[1:x_1]}} \sum_{\mathbf{z}_{(x_1:x_2]}} \dots \sum_{\mathbf{z}_{(x_k:N]}}$, and individually bound the marginalized probability distribution.

$$
\begin{aligned}
&\sum_{\mathbf{z}\in Z(A)} \sum_{\substack{U\subseteq \mathcal{V}(A)\\ |U|=k}} \left(\prod_{i\in U} \left|\Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right)\right|\right) \left(\prod_{j\in\mathcal{V}(A)\setminus U} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right)\right) \\
&\le \sum_{\substack{U\subseteq \mathcal{V}(A)\\ |U|=k}} \sum_{\mathbf{z}\in Z(A)} \eta^k \left(\prod_{j\in\mathcal{V}(A)\setminus U} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right)\right) && \text{(via Lemma 2, } \left|\Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right)\right| \le \eta\text{)} \\
&= \sum_{\substack{U\subseteq \mathcal{V}(A)\\ |U|=k}} \eta^k \sum_{\mathbf{z}_{[1:\mathbf{x}_1]}\in Z_{[1:\mathbf{x}_1]}(A)} \left(\prod_{j_1\in\mathcal{V}_{[1:x_1)}(A)} \mathcal{P}\left(\mathbf{z}_{j_1} \mid \mathbf{z}_{\mathrm{Pa}(j_1)}\right)\right) \sum_{\mathbf{z}_{(x_1:\mathbf{x}_2]}\in Z_{(x_1:x_2]}(A)} \left(\prod_{j_2\in\mathcal{V}_{(x_1:x_2)}(A)} \mathcal{P}\left(\mathbf{z}_{j_2} \mid \mathbf{z}_{\mathrm{Pa}(j_2)}\right)\right) \dots \\
&\sum_{\mathbf{z}\in Z_{(x_i:x_{i+1}]}(A)} \left(\prod_{j_i\in\mathcal{V}_{(x_i:x_{i+1})}(A)} \mathcal{P}\left(\mathbf{z}_{j_i} \mid \mathbf{z}_{\mathrm{Pa}(j_i)}\right)\right) \dots \sum_{\mathbf{z}_{(x_k:N]}\in Z_{(x_k:N]}(A)} \left(\prod_{j_k\in\mathcal{V}_{(x_k:N]}(A)} \mathcal{P}\left(\mathbf{z}_{j_k} \mid \mathbf{z}_{\mathrm{Pa}(j_k)}\right)\right) && (1)
\end{aligned}
$$

The last term in the above expression can be bounded as follows

$$
\begin{aligned}
\sum_{\mathbf{z}_{(x_k:N]}\in Z_{(x_k:N]}(A)} \left(\prod_{j\in\mathcal{V}_{(x_k:N]}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right)\right) &= \sum_{\mathbf{z}_{(x_k:N]}\in Z_{(x_k:N]}(A)} \mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{(x_k:N]}(A) = \mathbf{z}_{(x_k:N]} | \mathrm{Pa}(\mathcal{V}_{(x_k:N]}(A))\right] \\
&= \mathbb{P}_{\mathrm{do}(A)}\left[V_N = 1 | \mathrm{Pa}\left(\mathcal{V}_{(x_k:N]}(A)\right)\right] \le 1.
\end{aligned}
$$

For all other terms, we have the following inequality

$$
\begin{aligned}
&\sum_{\mathbf{z}\in Z_{(x_i:x_{i+1}]}(A)} \left(\prod_{j\in\mathcal{V}_{(x_i:x_{i+1})}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right)\right) \\
&\qquad = \sum_{\mathbf{z}_{x_{i+1}}\in\{0,1\}} \sum_{\mathbf{z}_{(x_i:x_{i+1})}\in Z_{(x_i:x_{i+1})}(A)} \left(\prod_{j\in\mathcal{V}_{(x_i:x_{i+1})}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right)\right) \\
&\qquad = \sum_{\mathbf{z}_{x_{i+1}}\in\{0,1\}} \sum_{\mathbf{z}_{(x_i:x_{i+1})}\in Z_{(x_i:x_{i+1})}(A)} \mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{(x_i:x_{i+1})}(A) = \mathbf{z}_{(x_i:x_{i+1})} | \mathrm{Pa}\left(\mathcal{V}_{(x_i:x_{i+1})}(A)\right)\right] \\
&\qquad \le \sum_{\mathbf{z}_{x_{i+1}}\in\{0,1\}} 1 \\
&\qquad = 2.
\end{aligned}
$$

Substituting in (1), we get

$$
\sum_{\mathbf{z}\in Z(A)} \sum_{\substack{U\subseteq \mathcal{V}(A)\\ |U|=k}} \left(\prod_{i\in U} \left|\Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right)\right|\right) \left(\prod_{j\in\mathcal{V}(A)\setminus U} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right)\right) \le \sum_{\substack{U\subseteq \mathcal{V}(A)\\ |U|=k}} (2\eta)^k = \binom{N}{k} (2\eta)^k
$$

Therefore, the sum $\sum_{\mathbf{z} \in Z(A)} |\mathcal{L}_{\mathbf{z}}|$ satisfies

$$
\begin{aligned}
\sum_{\mathbf{z} \in Z(A)} |\mathcal{L}_{\mathbf{z}}| &\leq \sum_{k=2}^{N} \binom{N}{k} (2\eta)^k \\
&= \sum_{k=0}^{N} \binom{N}{k} (2\eta)^k - 2N\eta - 1 \\
&= (1+2\eta)^N - 2N\eta - 1 \\
&\leq e^{2N\eta} - 2N\eta - 1 \\
&\leq 1 + 2N\eta + (2N\eta)^2 - 2N\eta - 1 && \text{(with } \eta \leq \tfrac{1}{2N}\text{)} \\
&\leq 4N^2\eta^2.
\end{aligned}
$$

The lemma stands proved. □

Lemma 4. *For estimates obtained via a covering intervention set $\mathcal{I}$, as in Algorithm 1, the following event holds with probability at least $\left(1 - \frac{2}{T}\right)$:*

$$
\left| \sum_{\mathbf{z} \in Z(A)} \mathcal{H}_{\mathbf{z}} \right| \leq \sqrt{\frac{N|\mathcal{I}| \log |\mathcal{A}| T}{T}} \qquad \textit{for all } A \in \mathcal{A}.
$$

Proof. The definition of $\mathcal{H}_{\mathbf{z}}$ gives us

$$
\begin{aligned}
&\left| \sum_{\mathbf{z} \in Z(A)} \mathcal{H}_{\mathbf{z}} \right| \\
&= \left| \sum_{\mathbf{z} \in Z(A)} \sum_{i \in \mathcal{V}(A)} \Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right) \prod_{j \in \mathcal{V}(A), j \neq i} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right) \right| \\
&= \left| \sum_{i \in \mathcal{V}(A)} \sum_{\mathbf{z} \in Z(A)} \Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right) \prod_{j \in \mathcal{V}(A), j \neq i} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right) \right| \\
&= \left| \sum_{i \in \mathcal{V}(A)} \sum_{\substack{\mathbf{z}_{[1:i]} \in \\ Z_{[1:i]}(A)}} \Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right) \prod_{j \in \mathcal{V}_{[1:i)}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right) \sum_{\substack{\mathbf{z}_{(i:N]} \in \\ Z_{(i:N]}(A)}} \prod_{k \in \mathcal{V}_{(i:N]}(A)} \mathcal{P}\left(\mathbf{z}_k \mid \mathbf{z}_{\mathrm{Pa}(k)}\right) \right| \\
&= \left| \sum_{i \in \mathcal{V}(A)} \sum_{\substack{\mathbf{z}_{[1:i]} \in \\ Z_{[1:i]}(A)}} \Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right) \prod_{j \in \mathcal{V}_{[1:i)}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right) \sum_{\substack{\mathbf{z}_{(i:N]} \in \\ Z_{(i:N]}(A)}} \mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{(i:N]}(A) = \mathbf{z}_{(i:N]} \mid \mathrm{Pa}\left(\mathcal{V}_{(i:N]}(A)\right)\right] \right| \\
&= \left| \sum_{i \in \mathcal{V}(A)} \sum_{\substack{\mathbf{z}_{[1:i]} \in \\ Z_{[1:i]}(A)}} \Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right) \prod_{j \in \mathcal{V}_{[1:i)}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right) \mathbb{P}_{\mathrm{do}(A)}\left[V_N = 1 \mid \mathrm{Pa}\left(\mathcal{V}_{(i:N]}(A)\right)\right] \right| \\
&= \left| \sum_{i \in \mathcal{V}(A)} \sum_{\mathbf{z}_i \in \{0,1\}} \sum_{\substack{\mathbf{z}_{[1:i)} \in \\ Z_{[1:i)}(A)}} \Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right) \prod_{j \in \mathcal{V}_{[1:i)}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right) \mathbb{P}_{\mathrm{do}(A)}\left[V_N = 1 \mid \mathrm{Pa}\left(\mathcal{V}_{(i:N]}(A)\right)\right] \right| \\
&= \left| \sum_{i \in \mathcal{V}(A)} \sum_{\mathbf{z}_i \in \{0,1\}} \sum_{\substack{\mathbf{z}_{\mathrm{Pa}(i)} \in \\ Z_{\mathrm{Pa}(i)}(A)}} \Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right) \sum_{\substack{\mathbf{z}_{\mathrm{Ac}(i)} \in \\ Z_{\mathrm{Ac}(i)}(A)}} \prod_{j \in \mathcal{V}_{[1:i)}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right) \mathbb{P}_{\mathrm{do}(A)}\left[V_N = 1 \mid \mathrm{Pa}\left(\mathcal{V}_{(i:N]}(A)\right)\right] \right|
\end{aligned}
$$

Recall that $\mathrm{Ac}(i) = [1, i) \setminus \mathrm{Pa}(i)$ and write

$$c_i(z_i, \mathbf{z}_{\mathrm{Pa}(i)}) := \sum_{\substack{\mathbf{z}_{\mathrm{Ac}(i)} \in \\ Z_{\mathrm{Ac}(i)}(A)}} \prod_{j \in \mathcal{V}_{[1:i)}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right) \mathbb{P}_{\mathrm{do}(A)}\left[V_N = 1 \mid \mathrm{Pa}\left(\mathcal{V}_{(i:N]}(A)\right)\right] \tag{2}$$

Also, as a shorthand for $z_i = 1$ and $z_i = 0$ we will write 1_i and 0_i, respectively. With these notations, we have

$$\begin{aligned}\left|\sum_{\mathbf{z} \in Z(A)} \mathcal{H}_{\mathbf{z}}\right| &= \left|\sum_{i \in \mathcal{V}(A)} \sum_{\mathbf{z}_i \in \{0,1\}} \sum_{\mathbf{z}_{\mathrm{Pa}(i)} \in Z_{\mathrm{Pa}(i)}(A)} \Delta\mathcal{P}\left(\mathbf{z}_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right) c_i(\mathbf{z}_i, \mathbf{z}_{\mathrm{Pa}(i)})\right| \\ &= \left|\sum_{i \in \mathcal{V}(A)} \sum_{\mathbf{z}_{\mathrm{Pa}(i)} \in Z_{\mathrm{Pa}(i)}(A)} \Delta\mathcal{P}\left(1_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right) \left(c_i(1_i, \mathbf{z}_{\mathrm{Pa}(i)}) - c_i(0_i, \mathbf{z}_{\mathrm{Pa}(i)})\right)\right| \\ &\qquad \left(\text{since } \Delta\mathcal{P}\left(1_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right) = -\Delta\mathcal{P}\left(0_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right)\right)\end{aligned}$$

Since $\mathcal{I}$ is a covering intervention set, for each pair $(i, \mathbf{z}_{\mathrm{Pa}(i)})$, there exists an intervention $I \in \mathcal{I}$ such that intervening $\mathrm{do}(I)$ provides a sample from the conditional probability distribution $\mathbb{P}[V_i = 1 \mid \mathrm{Pa}(V_i) = \mathbf{z}_i]$. Hence, Line 2 of the algorithm provides at least $\frac{T}{|\mathcal{I}|}$ independent samples from the conditional distribution $\mathbb{P}[V_i = 1 \mid \mathrm{Pa}(V_i) = \mathbf{z}_i]$. We write the s^{th} sample for this conditional distribution by $Y_s(i, \mathbf{z}_{\mathrm{Pa}(i)})$. Now, we have

$$\left|\sum_{\mathbf{z} \in Z(A)} \mathcal{H}_{\mathbf{z}}\right| = \left|\sum_{i \in \mathcal{V}(A)} \sum_{\substack{\mathbf{z}_{\mathrm{Pa}(i)} \in \\ Z_{\mathrm{Pa}(i)}(A)}} \frac{|\mathcal{I}|}{T} \left(\sum_{s=1}^{T/|\mathcal{I}|} Y_s(i, \mathbf{z}_{\mathrm{Pa}(i)}) - \mathcal{P}\left(1_i \mid \mathbf{z}_{\mathrm{Pa}(i)}\right)\right) \left(c_i(1_i, \mathbf{z}_{\mathrm{Pa}(i)}) - c_i(0_i, \mathbf{z}_{\mathrm{Pa}(i)})\right)\right|$$

We will apply Hoeffding's inequality (Lemma 1) to bound the above expression. Note that in this expression, besides $Y_s(i, \mathbf{z}_{\mathrm{Pa}(i)})$-s, all the other terms are deterministic. In particular, we show in Claim 5 (stated and proved below) that $\sum_{\mathbf{z}_{\mathrm{Pa}(i)} \in Z_{\mathrm{Pa}(i)}(A)} (c(1_i, \mathbf{z}_{\mathrm{Pa}(i)}) - c(0_i, \mathbf{z}_{\mathrm{Pa}(i)}))^2 \leq 1$, for all i. Hence, for any $A \in \mathcal{A}$, Lemma 1 gives us

$$\begin{aligned}\mathbb{P}\left(\left|\sum_{\mathbf{z} \in Z(A)} \mathcal{H}_{\mathbf{z}}\right| \geq \varepsilon\right) &\leq 2 \exp\left(\frac{-T\varepsilon^2}{|\mathcal{I}| \sum_{i \in \mathcal{V}(A)} \sum_{\mathbf{z}_{\mathrm{Pa}(i)} \in Z_{\mathrm{Pa}(i)}(A)} (c_i(1_i, \mathbf{z}_{\mathrm{Pa}(i)}) - c_i(0_i, \mathbf{z}_{\mathrm{Pa}(i)}))^2}\right) \\ &\leq 2 \exp\left(\frac{-T\varepsilon^2}{|\mathcal{I}|\,|\mathcal{V}(A)|}\right) \qquad \text{(via Claim 5)} \\ &\leq 2 \exp\left(\frac{-T\varepsilon^2}{|\mathcal{I}|\, N}\right).\end{aligned}$$

Setting $\varepsilon = \sqrt{\frac{N\,|\mathcal{I}| \log(|\mathcal{A}| T)}{T}}$ and taking union bound over all $A \in \mathcal{A}$, gives us the required probability bound. This completes the proof of the lemma. ☐

We next establish the claim used in the proof of Lemma 4.

Claim 5.

$$\sum_{\mathbf{z}_{\mathrm{Pa}(i)} \in Z_{\mathrm{Pa}(i)}(A)} (c(1_i, \mathbf{z}_{\mathrm{Pa}(i)}) - c(0_i, \mathbf{z}_{\mathrm{Pa}(i)}))^2 \leq 1.$$

Proof. The definition of $c(\mathbf{z}_i, \mathbf{z}_{\mathrm{Pa}(i)})$ (see equation (2)) gives us

$$\begin{aligned}&|c(1_i, \mathbf{z}_{\mathrm{Pa}(i)}) - c(0_i, \mathbf{z}_{\mathrm{Pa}(i)})| \\ &= \Bigg|\sum_{\mathbf{z} \in Z_{\mathrm{Ac}(i)}(A)} \prod_{j \in \mathcal{V}_{[1:i)}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right) \mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{[i+1:N]}(A) = \mathbf{z}_{[i+1:N]} \mid \mathrm{Pa}\left(\mathcal{V}_{[1:i]}(A)\right) = (\mathbf{z}_{[1:i)} \cup 1_i)\right] -\end{aligned}$$

$$\sum_{\mathbf{z}\in Z_{\mathrm{Ac}(i)}(A)} \prod_{j\in\mathcal{V}_{[1:i)}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right) \mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{[i+1:N]}(A) = \mathbf{z}_{[i+1:N]} \mid \mathrm{Pa}\left(\mathcal{V}_{[1:i]}(A)\right) = (\mathbf{z}_{[1:i)} \cup 0_i)\right]\Bigg|$$

$$= \Bigg|\sum_{\mathbf{z}\in Z_{\mathrm{Ac}(i)}(A)} \prod_{j\in\mathcal{V}_{[1:i)}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right) \Big(\mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{[i+1:N]}(A) = \mathbf{z}_{[i+1:N]} \mid \mathrm{Pa}(\mathcal{V}_{[1:i]}(A)) = (\mathbf{z}_{[1:i)} \cup 1_i)\right] -$$

$$\mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{[i+1:N]}(A) = \mathbf{z}_{[i+1:N]} \mid \mathrm{Pa}(\mathcal{V}_{[1:i]}(A)) = (\mathbf{z}_{[1:i)} \cup 0_i)\right]\Big)\Bigg|$$

$$\leq \sum_{\mathbf{z}\in Z_{\mathrm{Ac}(i)}(A)} \prod_{j\in\mathcal{V}_{[1:i)}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right) \Big|\mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{[i+1:N]}(A) = \mathbf{z}_{[i+1:N]} \mid \mathrm{Pa}(\mathcal{V}_{[1:i]}(A)) = (\mathbf{z}_{[1:i)} \cup 1_i)\right] -$$

$$\mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{[i+1:N]}(A) = \mathbf{z}_{[i+1:N]} \mid \mathrm{Pa}(\mathcal{V}_{[1:i]}(A)) = (\mathbf{z}_{[1:i)} \cup 0_i)\right]\Big|$$

$$\leq \sum_{\mathbf{z}\in Z_{\mathrm{Ac}(i)}(A)} \prod_{j\in\mathcal{V}_{[1:i)}(A)} \mathcal{P}\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}(j)}\right)$$

$$= \mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{\mathrm{Pa}(i)}(A) = \mathbf{z}_{\mathrm{Pa}(i)}\right].$$

Hence, under intervention $A \in \mathcal{A}$, we have

$$\begin{aligned}\sum_{\mathbf{z}_{\mathrm{Pa}(i)}\in Z_{\mathrm{Pa}(i)}(A)} (c(1_i, \mathbf{z}_{\mathrm{Pa}(i)}) - c(0_i, \mathbf{z}_{\mathrm{Pa}(i)}))^2 &\leq \sum_{\mathbf{z}_{\mathrm{Pa}(i)}\in Z_{\mathrm{Pa}(i)}(A)} |c(1_i, \mathbf{z}_{\mathrm{Pa}(i)}) - c(0_i, \mathbf{z}_{\mathrm{Pa}(i)})| \\ &\leq \sum_{\mathbf{z}_{\mathrm{Pa}(i)}\in Z_{\mathrm{Pa}(i)}(A)} \mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{\mathrm{Pa}(i)}(A) = \mathbf{z}_{\mathrm{Pa}(i)}\right] \\ &\leq 1.\end{aligned}$$

This completes the proof of the claim. □

B REGRET ANALYSIS FOR SEMI MARKOV BAYESIAN NETWORKS (SMBNS)

We introduce the notion of *pseudo parents* of a vertex in an SMBN graph $\mathcal{G}$, which we will use throughout the proof. Recall that $\mathcal{V}$ denotes the set of vertices, and they conform to a topological ordering. We assume that each c-component C_i maintains the ordering. For an intervention A, consider any c-component $C \in \mathcal{C}(A)$ with vertices $(U_1, U_2, \ldots, U_m)$, the pseudo parents of a vertex U_j is defined as

$$\mathrm{Pa}'(j) \coloneqq \mathrm{Pa}(\{U_1, U_2, \ldots U_j\}) \cup \{U_1, U_2, \ldots U_{j-1}\} \tag{3}$$

For any SMBN graph with in-degree at most d and c-components of size at most ℓ, the size $|\mathrm{Pa}'(j)|$ is at most $d\ell + \ell$. Furthermore, note that the set $\mathrm{Pa}'(j)$ will always precede the vertex V_j in any topological ordering of the graph.

The next lemma shows that the distribution of any c-component conditioned on its parents, $\mathcal{P}_{\mathbf{z}_{\mathrm{Pa}(C)}}(\mathbf{z}_C)$, can be factorized into the distribution of individual vertices conditioned on its pseudo parents. This allows us to extend the techniques used for the regret analysis of fully observable graphs (Section 3.1) to the case of SMBNs. Intuitively, one can view the factorization of an SMBN (under an intervention A) as a factorization over a fully observable graph where each vertex V_j has the set $\mathrm{Pa}'(j)$ as its parents.

Lemma 6. *For any intervention A and any c-component $C \in \mathcal{C}(A)$, consisting of vertices $\{U_1, U_2 \ldots U_m\}$, we have*

$$\mathcal{P}_{\mathbf{z}_{\mathrm{Pa}(C)}}(\mathbf{z}_C) = \prod_{j\in C} \mathcal{P}_A\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}'(j)}\right)$$

Here $\mathrm{Pa}'(j)$ denotes the set of pseudo parents as defined in equation (3).

Proof. First, note that intervening on parent vertices of a c-component (under intervention A) is the same as conditioning on them. Specifically,

$$\mathcal{P}_{\mathbf{z}_{\mathrm{Pa}(C)}}(\mathbf{z}_C) = \mathcal{P}_A\left(\mathbf{z}_C \mid \mathbf{z}_{\mathrm{Pa}(C)}\right)$$

Further, the chain rule of conditional probability gives us

$$\mathcal{P}_A\left(\mathbf{z}_C \mid \mathbf{z}_{\mathrm{Pa}(C)}\right) = \prod_{j \in C} \mathbb{P}_{\mathrm{do}(A)}\left[U_j = \mathbf{z}_j \mid \mathrm{Pa}(C) = \mathbf{z}_{\mathrm{Pa}(C)}, (U_1 \dots U_{j-1}) = \mathbf{z}_{(U_1 \dots U_{j-1})}\right]$$

Next, we use the notion of d-separation (see [Pearl, 2009]) to argue that conditioning on just the set $\mathrm{Pa}'(j)$ is sufficient. In particular, note that the set $Y = \mathrm{Pa}(\{U_{j+1} \dots U_m\})$ is d-separated from vertex U_j by the set $X = \mathrm{Pa}(\{U_1 \dots U_j\}) \cup (\{U_1 \dots U_{j-1}\})$. This is due to the fact that all paths from a vertex in Y to U_j are either blocked by a collider vertex in $\{U_{j+1} \dots U_m\}$ (and the collider vertex is not included X), or the path is blocked by a vertex in X. This implies that conditioned on X, U_j is independent of all vertices in Y [Pearl, 2009] . Formally, we write

$$\begin{aligned}
&\mathbb{P}_{\mathrm{do}(A)}\left[U_j = \mathbf{z}_j \mid \mathrm{Pa}(C) = \mathbf{z}_{\mathrm{Pa}(C)}, (U_1 \dots U_{j-1}) = \mathbf{z}_{(U_1 \dots U_{j-1})}\right] \\
&= \mathbb{P}_{\mathrm{do}(A)}[U_j = \mathbf{z}_j \mid \mathrm{Pa}(U_1 \dots U_{j-1}) = \mathbf{z}_{\mathrm{Pa}(U_1 \dots U_j)}, \mathrm{Pa}(U_{j+1} \dots U_m) = \mathbf{z}_{\mathrm{Pa}(U_{j+1} \dots U_m)}, (U_1 \dots U_{j-1}) = \mathbf{z}_{(U_1 \dots U_{j-1})}] \\
&= \mathbb{P}_{\mathrm{do}(A)}\left[U_j = \mathbf{z}_j \mid \mathrm{Pa}(U_1 \dots U_{j-1}) = \mathbf{z}_{\mathrm{Pa}(U_1 \dots U_j)}, (U_1 \dots U_{j-1}) = \mathbf{z}_{(U_1 \dots U_{j-1})}\right] \\
&\qquad \text{(since } \mathrm{Pa}(\{U_1 \dots U_j\}) \cup \{U_1 \dots U_{j-1}\} \text{ d-separates } U_j \text{ from } \mathrm{Pa}(\{U_{j+1} \dots U_m\})\text{)} \\
&= \mathbb{P}_{\mathrm{do}(A)}[U_j = \mathbf{z}_j \mid \mathrm{Pa}'(j)] \qquad \text{(by definition of } \mathrm{Pa}'(j)\text{)}
\end{aligned}$$

Therefore,

$$\begin{aligned}
\mathcal{P}_{\mathbf{z}_{\mathrm{Pa}(C)}}(\mathbf{z}_C) &= \mathcal{P}_A\left(\mathbf{z}_C \mid \mathbf{z}_{\mathrm{Pa}(C)}\right) \\
&= \prod_{j \in C} \mathbb{P}_{\mathrm{do}(A)}\left[V_j = \mathbf{z}_j \mid \mathrm{Pa}'(j) = \mathbf{z}_{\mathrm{Pa}'(j)}\right] \\
&= \prod_{j \in C} \mathcal{P}_A\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}'(j)}\right)
\end{aligned}$$

This completes the proof of the lemma. ☐

Now, recall that the estimate $\widehat{\mu}(A)$ can be written as

$$\begin{aligned}
\widehat{\mu}(A) &= \sum_{\mathbf{z} \in Z(A)} \prod_{C_i \in \mathcal{C}(A)} \widehat{\mathcal{P}}_{\mathbf{z}_{\mathrm{Pa}(C_i)}}(\mathbf{z}_{C_i}) \\
&= \sum_{\mathbf{z} \in Z(A)} \prod_{i \in \mathcal{C}(A)} \left(\mathcal{P}_A\left(\mathbf{z}_{C_i} \mid \mathbf{z}_{\mathrm{Pa}(C_i)}\right) + \Delta\mathcal{P}_A\left(\mathbf{z}_{C_i} \mid \mathbf{z}_{\mathrm{Pa}(C_i)}\right)\right) \\
&= \mu(A) + \sum_{\mathbf{z} \in Z(A)} \Bigg(\sum_{C_i \in \mathcal{C}(A)} \Delta\mathcal{P}_A\left(\mathbf{z}_{C_i} \mid \mathbf{z}_{\mathrm{Pa}(C_i)}\right) \prod_{C_j \in \mathcal{C}(A), j \neq i} \mathcal{P}_A\left(\mathbf{z}_{C_j} \mid \mathbf{z}_{\mathrm{Pa}(C_j)}\right) + \\
&\quad \sum_{\substack{U \subseteq \mathcal{C}(A) \\ |U|=2}} \left(\prod_{C_i \in U} \Delta\mathcal{P}_A\left(\mathbf{z}_{C_i} \mid \mathbf{z}_{\mathrm{Pa}(C_i)}\right)\right)\left(\prod_{C_j \in \mathcal{C}(A) \setminus U} \mathcal{P}_A\left(\mathbf{z}_{C_j} \mid \mathbf{z}_{\mathrm{Pa}(C_j)}\right)\right) + \\
&\quad \sum_{\substack{U \subseteq \mathcal{C}(A) \\ |U|=3}} \left(\prod_{C_i \in U} \Delta\mathcal{P}_A\left(\mathbf{z}_{C_i} \mid \mathbf{z}_{\mathrm{Pa}(C_i)}\right)\right)\left(\prod_{C_j \in \mathcal{C}(A) \setminus U} \mathcal{P}_A\left(\mathbf{z}_{C_j} \mid \mathbf{z}_{\mathrm{Pa}(C_j)}\right)\right) + \cdots \Bigg) \quad \text{(expanding product terms)}
\end{aligned}$$

Here, $\Delta\mathcal{P}\,()$ denotes the error in the estimate of the conditional probabilities. Let $\mathcal{L}_{\mathbf{z}}$ represent all the product entries in the expansion that include more than one error term ($\Delta\mathcal{P}\,()$). Specifically,

$$\mathcal{L}_{\mathbf{z}} = \sum_{k=2}^{|\mathcal{C}(A)|} \sum_{\substack{U \subseteq \mathcal{C}(A)\\ |U|=k}} \left(\prod_{C_i \in U} \Delta\mathcal{P}_A\left(\mathbf{z}_{C_i} \mid \mathbf{z}_{\mathrm{Pa}(C_i)}\right)\right) \left(\prod_{C_j \in \mathcal{C}(A)\setminus U} \mathcal{P}_A\left(\mathbf{z}_{C_j} \mid \mathbf{z}_{\mathrm{Pa}(C_j)}\right)\right)$$

$$= \sum_{k=2}^{|\mathcal{C}(A)|} \sum_{\substack{U \subseteq \mathcal{C}(A)\\ |U|=k}} \left(\prod_{C_i \in U} \Delta\mathcal{P}_A\left(\mathbf{z}_{C_i} \mid \mathbf{z}_{\mathrm{Pa}(C_i)}\right)\right) \left(\prod_{\substack{C \in \mathcal{C}(A)\setminus C_i,\\ j \in C}} \mathcal{P}_A\left(\mathbf{z}_{j} \mid \mathbf{z}_{\mathrm{Pa}'(j)}\right)\right) \qquad \text{(via Lemma 6)}$$

We further represent all the entries with a single $\Delta\mathcal{P}\,()$ term as

$$\mathcal{H}_{\mathbf{z}} = \sum_{C_i \in \mathcal{C}(A)} \Delta\mathcal{P}_A\left(\mathbf{z}_{C_i} \mid \mathbf{z}_{\mathrm{Pa}(C_i)}\right) \prod_{\substack{C_k \in \mathcal{C}(A)\\ k \neq i}} \mathcal{P}_A\left(\mathbf{z}_{C_k} \mid \mathbf{z}_{\mathrm{Pa}(C_k)}\right)$$

$$= \sum_{C_i \in \mathcal{C}(A)} \Delta\mathcal{P}_A\left(\mathbf{z}_{C_i} \mid \mathbf{z}_{\mathrm{Pa}(C_i)}\right) \prod_{j \in \mathcal{V}(A)\setminus C_i} \mathcal{P}_A\left(\mathbf{z}_{j} \mid \mathbf{z}_{\mathrm{Pa}'(j)}\right) \tag{4}$$

Here, the last equality follows from Lemma 6. Hence, we have

$$\widehat{\mu}(A) - \mu(A) = \sum_{\mathbf{z} \in Z(A)} \left(\mathcal{H}_{\mathbf{z}} + \mathcal{L}_{\mathbf{z}}\right) \tag{5}$$

We will establish upper bounds on the sums of $\mathcal{L}_{\mathbf{z}}$s and $\mathcal{H}_{\mathbf{z}}$s in Lemma 8 and Lemma 9, respectively. These lemmas show that the sum of the $\mathcal{H}$ terms dominates the sum of $\mathcal{L}$ terms. Furthermore, these bounds imply that the estimated reward $\widehat{\mu}(A)$ is sufficiently close to the true expected reward $\mu(A)$ for each intervention $A \in \mathcal{A}$.

Lemma 7. *For estimates obtained via a covering intervention set $\mathcal{I}$, as in Algorithm 1, write $\mathcal{E}$ to denote the event that $|\Delta\mathcal{P}_{\mathbf{z}_{\mathrm{Pa}(C_i)}}(\mathbf{z}_{C_i})| \leq \sqrt{\frac{|\mathcal{I}|(\ell d+\ell+\log(NT))}{T}}$ for all c-components $C_i \in \mathcal{C}(A)$ and for all $A \in \mathcal{A}$. Then,* $\Pr\{\mathcal{E}\} \geq \left(1 - \frac{2}{T}\right)$.

Proof. Since $\mathcal{I}$ is a covering intervention set (see Defintion 2), for each distribution $\mathcal{P}_{\mathbf{z}_{\mathrm{Pa}(i)}}(\mathbf{z}_{C_i})$, we have at least $\frac{T}{|\mathcal{I}|}$ independent samples. Also, note that the total number of distributions to be estimated is at most $2^{(\ell d+\ell)}N$. This follows from the fact that each c-component—under any intervention—is a subset of a c-component in the original graph $\mathcal{G}$, and the number of c-components in $\mathcal{G}$ is at most N. Hence, the number of possible distinct c-components (across all intervention) is at most $N2^{\ell}$. Furthermore, each c-component can have at most ℓd parents with at most $2^{\ell d}$ distinct binary assignments to the parents.

With this count in hand, we invoke Lemma 1, with $\varepsilon = \sqrt{\frac{|\mathcal{I}|(\log(2^{\ell d+\ell}NT))}{T}}$ and apply the union bound over all $(\mathbf{z}_{C_i}, \mathbf{z}_{\mathrm{Pa}(C_i)})$ pairs. This gives us the desired probability bound and completes the proof of the lemma. □

Lemma 8. *For estimates obtained via a covering intervention set $\mathcal{I}$, the following event holds with probability at least $(1 - \frac{2}{T})$:*

$$\sum_{\mathbf{z} \in Z(A)} |\mathcal{L}_{\mathbf{z}}| \leq 4^{\ell}(N\eta)^2 \qquad \text{for all } A \in \mathcal{A}.$$

Here, parameter $\eta = \sqrt{\frac{|\mathcal{I}|(\ell d+\ell+\log(NT))}{T}}$ and T is moderately large.

Proof. We use the fact that each error term in $\mathcal{L}_{\mathbf{z}}$ satisfies the bound stated in Lemma 7. Moreover, we use the graph structure to marginalize variables that do not appear in the error terms. The idea is to split the sum $\sum_{\mathbf{z} \in Z(A)}$ into $\sum_{\mathbf{z}_{[1:x_1]}} \sum_{\mathbf{z}_{(x_1:x_2]}} \ldots \sum_{\mathbf{z}_{(x_k:N]}}$, where $\{x_1, x_2 \ldots, x_k\}$ denotes all the indices in $\mathcal{C}(A)$ that show up as $\Delta\mathcal{P}\,()$ in the expression for $\mathcal{L}_{\mathbf{z}}$.

$$\begin{aligned}
\sum_{\mathbf{z}\in Z(A)}|\mathcal{L}_{\mathbf{z}}| &\le \sum_{\mathbf{z}\in Z(A)}\sum_{k=2}^{|\mathcal{C}(A)|}\sum_{\substack{U\subseteq\mathcal{C}(A)\\|U|=k}}\left(\prod_{C_i\in U}\left|\Delta\mathcal{P}_A\left(\mathbf{z}_{C_i}\mid\mathbf{z}_{\mathrm{Pa}(C_i)}\right)\right|\right)\left(\prod_{C_j\in\mathcal{C}(A)\setminus U}\mathcal{P}_A\left(\mathbf{z}_{C_j}\mid\mathbf{z}_{\mathrm{Pa}(C_j)}\right)\right)\\
&=\sum_{k=2}^{|\mathcal{C}(A)|}\sum_{\mathbf{z}\in Z(A)}\sum_{\substack{U\subseteq\mathcal{C}(A)\\|U|=k}}\left(\prod_{C_i\in U}\left|\Delta\mathcal{P}_A\left(\mathbf{z}_{C_i}\mid\mathbf{z}_{\mathrm{Pa}(C_i)}\right)\right|\right)\left(\prod_{C_j\in\mathcal{C}(A)\setminus U}\mathcal{P}_A\left(\mathbf{z}_{C_j}\mid\mathbf{z}_{\mathrm{Pa}(C_j)}\right)\right)\\
&\le\sum_{k=2}^{|\mathcal{C}(A)|}\sum_{\substack{U\subseteq\mathcal{C}(A)\\|U|=k}}\sum_{\mathbf{z}\in Z(A)}\eta^k\left(\prod_{C_j\in\mathcal{C}(A)\setminus U}\mathcal{P}_A\left(\mathbf{z}_{C_j}\mid\mathbf{z}_{\mathrm{Pa}(C_j)}\right)\right)\quad\text{(via Lemma 7, }\left|\Delta\mathcal{P}_A\left(\mathbf{z}_{C_i}\mid\mathbf{z}_{\mathrm{Pa}(C_i)}\right)\right|\le\eta)
\end{aligned}$$

First, we upper bound each term considered in the outer-most sum. Towards this, let U denote the set of c-components that show up as $\Delta\mathcal{P}\left(\right)$, we define $X \coloneqq \cup_{C_i\in U}C_i=\{x_1,x_2,\cdots,x_m\}$ where x_i denotes the vertex $V_{x_i}\in\mathcal{V}(A)$. Note that since c-components are at most of size ℓ and for $|U|=k$, we have $|X|\le\ell k$. Now, using Lemma 6, we obtain

$$\begin{aligned}
&\sum_{\substack{U\subseteq\mathcal{C}(A)\\|U|=k}}\sum_{\mathbf{z}\in Z(A)}\eta^k\left(\prod_{C_j\in\mathcal{C}(A)\setminus U}\mathcal{P}_A\left(\mathbf{z}_{C_j}\mid\mathbf{z}_{\mathrm{Pa}(C_j)}\right)\right)\\
&=\sum_{\substack{U\subseteq\mathcal{C}(A)\\|U|=k}}\sum_{\mathbf{z}\in Z(A)}\eta^k\left(\prod_{j\in\mathcal{V}(A)\setminus X}\mathcal{P}_A\left(\mathbf{z}_j\mid\mathbf{z}_{\mathrm{Pa}'(j)}\right)\right)\\
&=\sum_{\substack{U\subseteq\mathcal{C}(A)\\|U|=k}}\eta^k\sum_{\mathbf{z}_{[1:\mathbf{x}_1]}\in Z_{[1:\mathbf{x}_1]}(A)}\left(\prod_{j\in\mathcal{V}_{[1:x_1)}(A)}\mathcal{P}_A\left(\mathbf{z}_j\mid\mathbf{z}_{\mathrm{Pa}'(j)}\right)\right)\sum_{\mathbf{z}_{(x_1:\mathbf{x}_2]}\in Z_{(x_1:x_1]}(A)}\left(\prod_{j\in\mathcal{V}_{(x_1:x_2)}(A)}\mathcal{P}_A\left(\mathbf{z}_j\mid\mathbf{z}_{\mathrm{Pa}'(j)}\right)\right)\dots\\
&\sum_{\mathbf{z}\in Z_{(x_i:x_{i+1}]}(A)}\left(\prod_{i\in\mathcal{V}_{(x_i:x_{i+1})}(A)}\mathcal{P}_A\left(\mathbf{z}_j\mid\mathbf{z}_{\mathrm{Pa}'(j)}\right)\right)\dots\sum_{\mathbf{z}_{(x_k:N]}\in Z_{(x_k:N]}(A)}\left(\prod_{j\in\mathcal{V}_{(x_k:N]}(A)}\mathcal{P}_A\left(\mathbf{z}_j\mid\mathbf{z}_{\mathrm{Pa}'(j)}\right)\right)
\end{aligned}\tag{6}$$

The last term in the above expression can be bounded as follows

$$\begin{aligned}
\sum_{\mathbf{z}_{(x_k:N]}\in Z_{(x_k:N]}(A)}\left(\prod_{i\in\mathcal{V}_{(x_k:N]}(A)}\mathcal{P}_A\left(\mathbf{z}_j\mid\mathbf{z}_{\mathrm{Pa}'(j)}\right)\right)&=\sum_{\mathbf{z}_{(x_k:N]}\in Z_{(x_k:N]}(A)}\mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{(x_k:N]}(A)=\mathbf{z}_{(x_k:N]}|\mathrm{Pa}'(\mathcal{V}_{(x_k:N]}(A))\right]\\
&=\mathbb{P}_{\mathrm{do}(A)}\left[V_N=1|\mathrm{Pa}'\left(\mathcal{V}_{(x_k:N]}(A)\right)\right]\le 1.
\end{aligned}$$

For all the other terms, we have the following bound

$$\begin{aligned}
&\sum_{\mathbf{z}\in Z_{(x_i:x_{i+1}]}(A)}\left(\prod_{i\in\mathcal{V}_{(x_i:x_{i+1})}(A)}\mathcal{P}_A\left(\mathbf{z}_j\mid\mathbf{z}_{\mathrm{Pa}'(j)}\right)\right)\\
&\qquad=\sum_{\mathbf{z}_{x_{i+1}}\in\{0,1\}}\sum_{\mathbf{z}_{(x_i:x_{i+1})}\in Z_{(x_i:x_{i+1})}(A)}\left(\prod_{i\in\mathcal{V}_{(x_i:x_{i+1})}(A)}\mathcal{P}_A\left(\mathbf{z}_j\mid\mathbf{z}_{\mathrm{Pa}'(j)}\right)\right)\\
&\qquad=\sum_{\mathbf{z}_{x_{i+1}}\in\{0,1\}}\sum_{\mathbf{z}_{(x_i:x_{i+1})}\in Z_{(x_i:x_{i+1})}(A)}\mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{(x_i:x_{i+1})}(A)=\mathbf{z}_{(x_i:x_{i+1})}|\mathrm{Pa}'\left(\mathcal{V}_{(x_i:x_{i+1})}(A)\right)\right]\\
&\qquad\le\sum_{\mathbf{z}_{x_{i+1}}\in\{0,1\}}1\\
&\qquad=2.
\end{aligned}$$

Substituting in (6), we get

$$\sum_{\substack{U\subseteq\mathcal{C}(A)\\|U|=k}}\sum_{\mathbf{z}\in Z(A)}\eta^k\left(\prod_{C_j\in\mathcal{C}(A)\setminus U}\mathcal{P}_A\left(\mathbf{z}_{C_j}\mid\mathbf{z}_{\mathrm{Pa}(C_j)}\right)\right)\le\sum_{\substack{U\subseteq\mathcal{C}(A)\\|U|=k}}\eta^k\,2^{\ell k}\qquad\text{(since }|X|\le\ell k\text{)}$$
$$=\binom{N}{k}\left(2^\ell\eta\right)^k$$

Therefore, the sum $\sum_{\mathbf{z}\in Z(A)}|\mathcal{L}_{\mathbf{z}}|$ satisfies

$$\begin{aligned}\sum_{\mathbf{z}\in Z(A)}|\mathcal{L}_{\mathbf{z}}|&\le\sum_{k=2}^{N}\binom{N}{k}\left(2^\ell\eta\right)^k\\&=\sum_{k=0}^{N}\binom{N}{k}\left(2^\ell\eta\right)^k-2^\ell N\eta-1\\&=(1+2^\ell\eta)^N-2^\ell N\eta-1\\&\le e^{2^\ell N\eta}-2^\ell N\eta-1\\&\le 1+2^\ell N\eta+(2^\ell N\eta)^2-2^\ell N\eta-1\qquad\text{(with }\eta\le\tfrac{1}{2^\ell N}\text{)}\\&\le 4^\ell N^2\eta^2\end{aligned}$$

The lemma stands proved. ☐

Lemma 9. *For estimates obtained via a covering intervention set $\mathcal{I}$, the following event holds with probability at least $1-\frac{2}{T}$:*

$$\left|\sum_{\mathbf{z}\in Z(A)}\mathcal{H}_{\mathbf{z}}\right|\le\sqrt{\frac{N\,4^\ell\,2^d\,|\mathcal{I}|\log\left(|\mathcal{A}|T\right)}{T}}\qquad\textit{for all } A\in\mathcal{A}.$$

Proof. Equation (4) gives us

$$\left|\sum_{\mathbf{z}\in Z(A)}\mathcal{H}_{\mathbf{z}}\right|=\left|\sum_{C_i\in\mathcal{C}(A)}\sum_{\mathbf{z}\in Z(A)}\Delta\mathcal{P}_A\left(\mathbf{z}_{C_i}\mid\mathbf{z}_{\mathrm{Pa}(C_i)}\right)\prod_{j\in\mathcal{V}(A)\setminus C_i}\mathcal{P}_A\left(\mathbf{z}_j\mid\mathbf{z}_{\mathrm{Pa}'(j)}\right)\right|.$$

Let $X\coloneqq\{x_1,x_2\cdots x_m\}$ be the vertices in a c-component C_i considered in the outer summation. Furthermore, for ease of exposition, write $(x_k:x_{k+1})'\coloneqq(x_k:x_{k+1})\setminus\mathrm{Pa}(C_i)$, i.e., the set $(x_k:x_{k+1})'$ excludes the parents of the c-component C_i. We have

$$\begin{aligned}&\left|\sum_{\mathbf{z}\in Z(A)}\mathcal{H}_{\mathbf{z}}\right|\\&=\Bigg|\sum_{C_i\in\mathcal{C}(A)}\sum_{\substack{\mathbf{z}_{\mathrm{Pa}(C_i)}\in\\ Z_{\mathrm{Pa}(C_i)}(A)}}\sum_{\substack{\mathbf{z}_{C_i}\in\\ Z_{C_i}(A)}}\Delta\mathcal{P}_A\left(\mathbf{z}_{C_i}\mid\mathbf{z}_{\mathrm{Pa}(C_i)}\right)\sum_{\substack{\mathbf{z}_{[1:x_1)'}\in\\ Z_{[1:x_1)'}(A)}}\prod_{j_1\in\mathcal{V}_{[1:x_1)}(A)}\mathcal{P}\left(\mathbf{z}_{j_1}\mid\mathbf{z}_{\mathrm{Pa}'(j_1)}\right)\\&\quad\sum_{\substack{\mathbf{z}_{(x_1:x_2)'}\in\\ Z_{(x_1:x_2)'}(A)}}\prod_{j_2\in\mathcal{V}_{(x_1:x_2)}(A)}\mathcal{P}_A\left(\mathbf{z}_{j_2}\mid\mathbf{z}_{\mathrm{Pa}'(j_2)}\right)\dots\sum_{\substack{\mathbf{z}_{(x_k:x_k+1)'}\in\\ Z_{(x_k:x_{k+1})'}(A)}}\prod_{j_2\in\mathcal{V}_{(x_k:x_{k+1})}(A)}\mathcal{P}_A\left(\mathbf{z}_{j_k}\mid\mathbf{z}_{\mathrm{Pa}'(j_k)}\right)\dots\Bigg|\\&=\left|\sum_{C_i\in\mathcal{C}(A)}\sum_{\substack{\mathbf{z}_{\mathrm{Pa}(C_i)}\in\\ Z_{\mathrm{Pa}(C_i)}(A)}}\sum_{\substack{\mathbf{z}_{C_i}\in\\ Z_{C_i}(A)}}\Delta\mathcal{P}_A\left(\mathbf{z}_{C_i}\mid\mathbf{z}_{\mathrm{Pa}(C_i)}\right)c_i\left(\mathbf{z}_{C_i},\mathbf{z}_{\mathrm{Pa}(C_i)}\right)\right|.\end{aligned}$$

Here,

$$c_i(\mathbf{z}_{C_i}, \mathbf{z}_{\mathrm{Pa}(C_i)}) \coloneqq \sum_{\substack{\mathbf{z}_{[1:x_1)'} \in \\ Z_{[1:x_1)'}(A)}} \prod_{j_1 \in \mathcal{V}_{[1:x_1)}(A)} \mathcal{P}_A\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}'(j_1)}\right) \sum_{\substack{\mathbf{z}_{(x_1:x_2)'} \in \\ Z_{(x_1:x_2)'}(A)}} \prod_{j_2 \in \mathcal{V}_{(x_1:x_2)}(A)} \mathcal{P}_A\left(\mathbf{z}_{j_2} \mid \mathbf{z}_{\mathrm{Pa}'(j_2)}\right) \cdots$$
$$\sum_{\substack{\mathbf{z}_{(x_k:x_k+1)'} \in \\ Z_{(x_k:x_{k+1})'}(A)}} \prod_{j_k \in \mathcal{V}_{(x_k:x_{k+1})}(A)} \mathcal{P}_A\left(\mathbf{z}_{j_k} \mid \mathbf{z}_{\mathrm{Pa}'(j_k)}\right) \cdots \sum_{\substack{\mathbf{z}_{(x_m:N]'} \in \\ Z_{(x_m:N]'}(A)}} \prod_{j_m \in \mathcal{V}_{(x_k:x_{k+1})}(A)} \mathcal{P}_A\left(\mathbf{z}_{j_m} \mid \mathbf{z}_{\mathrm{Pa}'(j_m)}\right)$$

We show in Claim 10 (proved below) that $c_i(z_{C_i}, \mathbf{z}_{\mathrm{Pa}(C_i)}) \leq 1$. Therefore,

$$\left|\sum_{\mathbf{z} \in Z(A)} \mathcal{H}_{\mathbf{z}}\right| \leq \left|\sum_{C_i \in \mathcal{C}(A)} \sum_{\substack{\mathbf{z}_{\mathrm{Pa}(C_i)} \in \\ Z_{\mathrm{Pa}(C_i)}(A)}} \sum_{\substack{\mathbf{z}_{C_i} \in \\ Z_{C_i}(A)}} \Delta\mathcal{P}\left(\mathbf{z}_{C_i} \mid \mathbf{z}_{\mathrm{Pa}(C_i)}\right)\right| \tag{7}$$

Since $\mathcal{I}$ is a covering intervention set, for each pair $(C_i, \mathbf{z}_{\mathrm{Pa}(C_i)})$, there exits an intervention $I \in \mathcal{I}$ such that intervening $\mathrm{do}(I)$ provides a sample for the distribution $\mathbb{P}[\mathcal{V}_{C_i} \mid \mathrm{do}(\mathrm{Pa}(C_i) = \mathbf{z}_{\mathrm{Pa}(C_i)})]$. Hence, we have at least $\frac{T}{|\mathcal{I}|}$ samples for the distribution $\mathbb{P}[\mathcal{V}_{C_i} \mid \mathrm{do}(\mathrm{Pa}(C_i) = \mathbf{z}_{\mathrm{Pa}(C_i)})]$. We represent the s^{th} sample for the distribution by indicator random variable $Y_s(\mathbf{z}_{C_i}, \mathbf{z}_{\mathrm{Pa}(C_i)})$ which takes value one when $\mathcal{V}_{C_i} = \mathbf{z}_{C_i}$, else its zero. Hence, inequality (7) reduces to

$$\left|\sum_{\mathbf{z} \in Z(A)} \mathcal{H}_{\mathbf{z}}\right| \leq \left|\sum_{C_i \in \mathcal{V}(A)} \sum_{\substack{\mathbf{z}_{\mathrm{Pa}(C_i)} \in \\ Z_{\mathrm{Pa}(C_i)}(A)}} \frac{|\mathcal{I}|}{T} \sum_{s=1}^{T/|\mathcal{I}|} \left(\sum_{\mathbf{z}_{C_i} \in Z_{C_i}(A)} Y_s(\mathbf{z}_{C_i}, \mathbf{z}_{\mathrm{Pa}(C_i)}) - \mathcal{P}_A\left(\mathbf{z}_{C_i} \mid \mathbf{z}_{\mathrm{Pa}(C_i)}\right)\right)\right|$$

In the above expression, the term $\sum_{\mathbf{z}_{C_i} \in Z_{C_i}(A)} Y_s(\mathbf{z}_{C_i}, \mathbf{z}_{\mathrm{Pa}(C_i)}) - \mathcal{P}_A\left(\mathbf{z}_{C_i} \mid \mathbf{z}_{\mathrm{Pa}(C_i)}\right)$ is an independent random quantity bounded between $[-2^{|C_i|}, 2^{|C_i|}]$. We now apply Heoffding's inequality (Lemma 1)

$$\mathbb{P}_{\mathrm{do}(A)}\left[\left|\sum_{\mathbf{z} \in Z(A)} \mathcal{H}_{\mathbf{z}}\right| \geq \varepsilon\right] \leq 2\exp\left(\frac{-T\varepsilon^2}{2|\mathcal{I}| \sum_{C_i \in \mathcal{C}(A)} \sum_{\mathbf{z}_{\mathrm{Pa}(i)} \in \mathbf{z}_{\mathrm{Pa}(i)}} 2^{2|C_i|}}\right)$$
$$\leq 2\exp\left(\frac{-T\varepsilon^2}{2|\mathcal{I}| \sum_{C_i \in \mathcal{C}(A)} \sum_{\mathbf{z}_{\mathrm{Pa}(i)} \in \mathbf{z}_{\mathrm{Pa}(i)}} 2^{2\ell}}\right) \leq 2\exp\left(\frac{-T\varepsilon^2}{2|\mathcal{I}| N 2^{\ell d} \cdot 2^{2\ell}}\right)$$

Setting $\varepsilon = \sqrt{\frac{2N\ |\mathcal{I}|\ 2^{\ell d}\ 4^{\ell} \log(|\mathcal{A}| \cdot T)}{T}}$ and taking union bound over all of $A \in \mathcal{A}$, gives us the required probability bound. This completes the proof of the lemma. □

We next establish the claim used in the proof of Lemma 9.

Claim 10.

$$c_i(\mathbf{z}_{C_i}, \mathbf{z}_{\mathrm{Pa}(C_i)}) \leq 1.$$

Proof. It holds that

$$c_i(\mathbf{z}_{C_i}, \mathbf{z}_{\mathrm{Pa}(C_i)}) = \sum_{\substack{\mathbf{z}_{[1:x_1)'} \in \\ Z_{[1:x_1)'}(A)}} \prod_{j_1 \in \mathcal{V}_{[1:x_1)}(A)} \mathcal{P}_A\left(\mathbf{z}_j \mid \mathbf{z}_{\mathrm{Pa}'(j)}\right) \sum_{\substack{\mathbf{z}_{(x_1:x_2)'} \in \\ Z_{(x_1:x_2)'}(A)}} \prod_{j_2 \in \mathcal{V}_{(x_1:x_2)}(A)} \mathcal{P}_A\left(\mathbf{z}_{j_2} \mid \mathbf{z}_{\mathrm{Pa}'(j_2)}\right) \cdots$$
$$\sum_{\substack{\mathbf{z}_{(x_k:x_k+1)'} \in \\ Z_{(x_k:x_{k+1})'}(A)}} \prod_{j_k \in \mathcal{V}_{(x_k:x_{k+1})}(A)} \mathcal{P}_A\left(\mathbf{z}_{j_k} \mid \mathbf{z}_{\mathrm{Pa}'(j_k)}\right) \cdots \sum_{\substack{\mathbf{z}_{(x_m:N]'} \in \\ Z_{(x_m:N]'}(A)}} \prod_{j_k \in \mathcal{V}_{(x_k:x_{k+1})}(A)} \mathcal{P}_A\left(\mathbf{z}_{j_k} \mid \mathbf{z}_{\mathrm{Pa}'(j_k)}\right)$$

We can upper bound each term in the above expression as shown below,

$$
\begin{aligned}
&\sum_{\substack{\mathbf{z}_{(x_k:x_k+1)'} \in \\ Z_{(x_k:x_{k+1})'}(A)}} \prod_{j_k \in \mathcal{V}_{(x_k:x_{k+1})}(A)} \mathcal{P}_A\left(\mathbf{z}_{j_k} \mid \mathbf{z}_{\mathrm{Pa}'(j_k)}\right) \\
&= \sum_{\substack{\mathbf{z}_{(x_k:x_k+1)'} \in \\ Z_{(x_k:x_{k+1})}(A)}} \mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{(x_k:x_{k+1})}(A) = \mathbf{z}_{(x_k:x_k+1)} | \mathrm{Pa}'(x_k : x_{k+1})\right] \\
&= \mathbb{P}_{\mathrm{do}(A)}\left[\mathcal{V}_{(x_k:x_{k+1}) \cap \mathrm{Pa}(C_i)}(A) = \mathbf{z}_{(x_k:x_k+1) \cap \mathrm{Pa}(C_i)} | \mathrm{Pa}'(x_k : x_{k+1})\right] \\
&\leq 1
\end{aligned}
$$

Substituting this in the expression for $c_i(\mathbf{z}_{C_i}, \mathbf{z}_{\mathrm{Pa}(C_i)})$, we get the required bound. □

Next, we restate and prove Theorem 2.

Theorem 1. *Let $\mathcal{G}$ be any given causal graph over N vertices and with c-components of size at most ℓ. Also, let the in-degree of the vertices in $\mathcal{G}$ be at most d. Then, for any (moderately large) time horizon T and given any covering intervention set $\mathcal{I}$ of $\mathcal{G}$, Algorithm 1 achieves simple regret*

$$
\mathrm{R}_T = O\left(\sqrt{\frac{N\, 2^d\, 4^\ell\, |\mathcal{I}| \log\left(|\mathcal{A}| T\right)}{T}}\right).
$$

Hence, using Lemma 5, we obtain the following bound on the simple regret

$$
\mathrm{R}_T = O\left(\sqrt{\frac{N\, (3d\, 8^d)^\ell\, \log |\mathcal{A}|}{T}} \log T\right).
$$

Proof. Lemma 5 implies that, with probability at least $\left(1 - \frac{1}{T}\right)$, the set $\mathcal{I}$ is indeed a covering intervention set for the graph $\mathcal{G}$. We combine this guarantee with Lemmas 8 and 9. In particular, with probability at least $\left(1 - \frac{5}{T}\right)$, we have, for all $A \in \mathcal{A}$:

$$
\begin{aligned}
|\mu(A) - \widehat{\mu}(A)| &= \left| \sum_{\mathbf{z} \in Z(A)} \left(\mathcal{H}_{\mathbf{z}} + \mathcal{L}_{\mathbf{z}}\right) \right| \\
&\leq \sqrt{\frac{N\, 4^\ell\, 2^d\, |\mathcal{I}| \log\left(|\mathcal{A}| T\right)}{T}} + \frac{4^\ell N^2 |\mathcal{I}| (\ell d + \ell + \log\left(NT\right))}{T} \\
&\leq 2\sqrt{\frac{N\, 4^\ell\, 2^d\, |\mathcal{I}| \log(|\mathcal{A}| T)}{T}} && \text{(For } T \gtrsim N^3\text{)}
\end{aligned}
$$

Let A_T be the output after T rounds of interventions, i.e., $A_T = \arg\max_{A \in \mathcal{A}}\ \widehat{\mu}(A)$. In addition, let $A^* = \arg\max_{A \in \mathcal{A}}\ \mu(A)$ be the optimal intervention. Hence, with probability at least $1 - \frac{5}{T}$ we have,

$$
\mu(A^*) - \mu(A_T) \leq 4\sqrt{\frac{N\, 4^\ell\, 2^d\, |\mathcal{I}| \log(|\mathcal{A}| T)}{T}} \tag{8}
$$

This gives the desired upper bound on the simple regret, R_T:

$$
R_T = \mathbb{E}\left[\mu(A^*) - \mu(A_T)\right] \leq \left(4\sqrt{\frac{N\, 4^\ell\, 2^d\, |\mathcal{I}| \log(|\mathcal{A}| T)}{T}}\right)\left(1 - \frac{5}{T}\right) + \frac{5}{T} \leq 5\sqrt{\frac{N\, 4^\ell\, 2^d\, |\mathcal{I}| \log(|\mathcal{A}| T)}{T}}.
$$

For SMBNs, since the size of the covering intervention set satisfies $|\mathcal{I}| = (3d)^\ell \cdot 2^{\ell d}(\log N + 2\ell d + \log T)$ (see Lemma 5), we also have the following explicit form of the simple regret bound

$$
\mathrm{R}_T = O\left(\sqrt{\frac{N\, (3d\, 8^d)^\ell\, \log |\mathcal{A}|}{T}} \log T\right).
$$

The theorem stands proved. □

References

Judea Pearl. *Causality*. Cambridge university press, 2009.