A Causal Bandit Approach to Learning Good Atomic Interventions in Presence of Unobserved Confounders

Abstract

We study the problem of determining the best atomic intervention in a Causal Bayesian Network (CBN) specified only by its causal graph. We model this as a stochastic multi-armed bandit (MAB) problem with side-information, where interventions on CBN correspond to arms of the bandit instance. First, we propose a simple regret minimization algorithm that takes as input a causal graph with observable and unobservable nodes and in T exploration rounds achieves $\tilde{O}(\sqrt{m(\mathcal{C})/T})$ expected simple regret. Here $m(\mathcal{C})$ is a parameter dependent on the input CBN $\mathcal{C}$ and could be much smaller than the number of arms. We also show that this is almost optimal for CBNs whose causal graphs have an n-ary tree structure. Next, we propose a cumulative regret minimization algorithm that takes as input a causal graph with observable nodes and performs better than the optimal MAB algorithms that do not use causal side-information. We experimentally compare both our algorithms with the best known algorithms in the literature.

1 INTRODUCTION

Causal Bayesian Networks or CBNs [Pearl, 2000] have become the natural choice for modelling causal relationships in many real-world situations such as price-discovery [Haigh and Bessler, 2004], computational-advertising [Bottou et al., 2013], healthcare [Velikova et al., 2014], etc. A CBN has two components: a directed acyclic graph (DAG) called the causal graph, and conditional probability distributions of each node given its parents such that the joint distribution of all variables factorizes as a product of these conditionals. Edges in the causal graph represent direct causal relationships and therefore it captures the data generation process.

In its most general setup, only a subset of the variables appearing in the CBN are observable and the rest are unobserved (see Definition 1.3.1 in Pearl [2000]). CBNs enable modelers to simulate the effect of external manipulations via a process called *intervention*. An intervention forcibly fixes selected observable variables in the graph and breaks the edges coming into them. Data generated from the resulting model is the simulated outcome of the intervention. In the presence of an outcome variable of interest Y (assumed to be observable), a natural question (see epidemic prevention example below) is to find the variable X and a corresponding value x, such that the intervention setting X to x leads to the maximum expected value of Y i.e. $X = x$ has the highest causal impact on Y. Such an intervention which manipulates only a single variable is called an *atomic intervention*.

The problem of learning the best atomic intervention was formulated as a sequential decision making problem called *Causal Bandits* (CB) in Lattimore et al. [2016]. In CB, access to the underlying DAG of the CBN is assumed but the associated conditional probability distributions are unknown. The outcome variable Y is considered as a reward variable and the set of allowed atomic interventions are modelled as arms of a bandit instance. In addition, there is an *observational arm* corresponding to the empty intervention, and pulling the observational arm generates a sample from the joint distribution of all observable variables. Here, identifying the best atomic intervention is equivalent to the well-studied *best-arm identification* problem in a multi-armed bandit (MAB) instance. However, in CB, an algorithm while pulling an arm has access to *causal* side information derived from the causal graph associated with the input CBN. See Lattimore et al. [2016] and the references therein for a comparison of CB and MAB problems with other types of side-information.

In this work, we study CB for causal graphs with unobserved confounders. (UCs). These are unobserved variables that are parents of at least two observable variables. To the best of our knowledge, this is the first work that analyses the regret of causal bandit algorithms when input causal graphs contain UCs. Moreover, in the fully observable setting, i.e.

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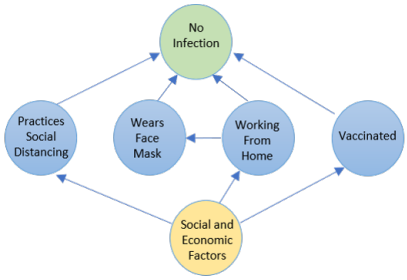

Figure 1: Causal Graph: Infection Prevention with Social and Economic Factors being an Unobserved Confounder

when all variables are observable, our algorithm does not assume any structural constraints on the input causal graph and hence can be applied quite generally. Before stating our contributions, we provide a motivating example where determining the best atomic intervention is important. Suppose a policy-maker is required to identify the best precautionary measure that should be enforced to reduce spread of a disease. The available measures are mandating social distancing, wearing of face mask, making people work from home and preventive vaccinations. Since the effect of each measure needs to be isolated while disrupting public life minimally, the policy-maker can enforce at most one of these measures at a given time. The policy-maker can conduct surveys to collect data from public about which measures were taken by them (other than the one enforced) and whether they got infected or not. The goal would then be to design a mechanism of implementing such enforcement one by one, during a time period and collecting the respective survey data to identify the best measure to enforce. Note that, using domain knowledge of health experts, policy makers can have access to an underlying causal graph such as the one in Fig. 1. They would want to use this graph to decide if and when a particular measure should be enforced.

1.1 OUR CONTRIBUTIONS

We study CB with respect to two standard objectives in MAB: simple and cumulative regret. Simple regret captures the best arm identification problem described above, whereas the cumulative regret is more natural when the goal is to maximize the cumulative reward at the end of T rounds instead of determining the best arm. We state our contributions below; meanings of the relevant terminologies are defined in Sec. 2.

Simple Regret Minimization: We propose a simple regret minimization algorithm called SRM−ALG. The input causal graph of the underlying CBN $\mathcal{C}$ is assumed to be (without loss of generality) a Semi-Markovian Causal Graph or SMCG (defined in Sec. 2) on observable nodes having both directed and bi-directed edges (representing presence of UCs) between the nodes. We assume that the input SMCG is identifiable with respect to a set of intervenable nodes $\mathbf{X}$, meaning that the interventional distributions arising from atomic interventions on variables in $\mathbf{X}$ can be consistently estimated from the observational data itself (see definition in Sec. 2). When the c-components (connected components of bi-directed edges, defined in Sec. 2) of the SMCG are bounded in size (by a constant) and the total in-degree of all vertices in the c-components are also bounded, given a time budget of T rounds, SRM−ALG attains $\tilde{O}(\sqrt{m(\mathcal{C})/T})$ expected simple regret (see Thm. 3.1). Here, $m(\mathcal{C})$ depends on the input CBN and is $\leq 2N$, where N is the number of intervenable nodes i.e. $N = |\mathbf{X}|$. In Sec. 3 we give examples of graphs, where $m(\mathcal{C}) \ll N$, and hence SRM−ALG performs better than standard bandit algorithms which achieve $\Omega(\sqrt{N/T})$ expected simple regret in the worst-case (Thm. 4 in Audibert et al. [2010]). SRM−ALG leverages the causal side-information available by deriving reward estimates for each arm from pulls of the observational arm. The quality of these derived estimates depends on the input CBN. The quantity $m(\mathcal{C})$ intuitively captures the trade-off between the number of arms with bad estimates, and the quality of estimates determined from intervening upon them explicitly.

We note that Lattimore et al. [2016] and Nair et al. [2021] propose algorithms in the fully observable setting, when the input causal graph is a parallel graph and a no-backdoor graph, respectively.[1] For these special classes of graphs, SRM−ALG recovers the regret guarantees given in Lattimore et al. [2016], Nair et al. [2021]. Hence, SRM−ALG can be viewed as a *significant* generalization of these algorithms to more general causal graphs with UCs. Further, Yabe et al. [2018] proposed a causal bandit algorithm for interventions which can simultaneously manipulate multiple variables. However, the input causal graph is assumed to have no UCs, and regret guarantee of their algorithm is $\tilde{O}(\sqrt{N/T})$ for atomic interventions. In particular, its performance is not better than optimal MAB algorithms that do not take causal side-information into account. In Sec. 6, we experimentally compare the regret guarantee of SRM−ALG with the algorithm in Yabe et al. [2018], as well as MAB algorithms that do not take causal side-information into account.

Lower Bound on Simple Regret: We also show that SRM−ALG is almost optimal for CBNs associated with a large and important class of causal graphs. Specifically, in Thm. 4.1, we show that for any causal graph $\mathcal{G}$ which is an n-ary tree on $N+1$ nodes[2], and any $M \in [1, N]$ there is a probability distribution $\mathbb{P}$ compatible with the the causal graph such that $m(\mathcal{C}) = M$, and the expected simple regret of any algorithm at the end of T rounds is $\Omega(\sqrt{M/T})$[3]. We remark that these graphs naturally capture important CBNs like causal trees [Greenewald et al., 2019]. Also, the class of

[1] These graphs have no backdoor paths from any $X \in \mathbf{X}$ to Y, implying $\mathbb{P}(Y \mid do(x)) = \mathbb{P}(Y \mid x)$.

[2] N nodes are intervenable and can causally effect node Y

[3] Here $\mathcal{C}$ is the CBN $(\mathcal{G}, \mathbb{P})$ and $m(\mathcal{C})$ is as described before

graphs considered in Thm. 4.1 subsumes the parallel graph model, and for them lower bound in Thm. 4.1 matches the lower bound given in Lattimore et al. [2016]. Importantly, Thm. 4.1 implies that the regret guarantee of SRM−ALG can be only improved by considering more nuanced structural restrictions on the causal graph, which could enable more causal information sharing between the interventions.

Cumulative Regret Minimization: We propose a cumulative regret minimization algorithm called CRM−ALG. All variables in the input causal graph are assumed to be observable. CRM−ALG achieves constant expected cumulative regret if the observational arm is optimal, and otherwise achieves better regret than the optimal MAB algorithm which does not take causal side-information into account (see Thm. 5.1). Cumulative regret minimization in general graphs were also studied by Lu et al. [2020] and Nair et al. [2021]. However, they crucially assume that distribution of parents of the reward node is known for every intervention. CRM−ALG does not make this assumption. The reason why we develop CRM−ALG in the fully observable setting (unlike SRM−ALG) is rather technical and is explained at the end of Sec. 5.

1.2 RELATED WORK

As noted before, causal bandits was introduced in Lattimore et al. [2016], where an almost optimal algorithm was proposed for CBNs associated with a parallel causal graph. Recently, a similar algorithm for simple regret minimization along with an algorithm for cumulative regret minimization was proposed for no-backdoor graphs in Nair et al. [2021], and the observation-intervention trade-off was studied when interventions are costlier than observations. An importance sampling based algorithm was proposed by Sen et al. [2017a] to minimize simple regret but only soft-interventions at a single node were considered. The cumulative regret minimization problem for general causal graphs was studied in Lu et al. [2020], Nair et al. [2021], but they assume the knowledge of the distributions of the the parents of the reward variable for every intervention. Recently Lu et al. [2021a] designed a cumulative regret minimization algorithm which only utilizes the side information that the underlying causal graph is a directed tree or a causal forest (and does not require the exact DAG). Assuming faithfulness and identifiability, their algorithm outperforms the standard MAB algorithms. Sen et al. [2017b] studied the contextual bandit problem where the observed context influences the reward via a latent confounder variable, and proposed an algorithm with better guarantee compared to standard contextual bandit. Lee and Bareinboim [2018, 2019] gave a procedure to compute the minimum possible intervention set by removing sub-optimal interventions identifiable from the input causal graph, and they empirically demonstrated that ignoring such information leads to huge regret. Recently, Lu et al. [2021b] introduced the causal Markov decision processes, where at each state a causal graph determines the action set, and gave algorithms that achieve better policy regret when the causal side-information is taken into account. Finally, in a related line of work Bareinboim et al. [2015] promote the use of observational data for bandit problems in the presence of UCs. We note that our proposed algorithms SRM−ALG and CRM−ALG both use observational samples to leverage side-information and hence achieve better regrets.

2 NOTATIONS AND PRELIMINARIES

Notations: For positive integers m, n with $m < n$, $[n]$ denotes the set $\{1, \ldots, n\}$ and $[m, n]$ denotes the set $\{m, m+1, \ldots, n\}$. Random variables are denoted using capital letters (e.g. X) and corresponding lower case letters (i.e. x) denote the assignment $X = x$. Unless otherwise specified, all random variables will be discrete with finite support. Sets of random variables are denoted by bold face letters (e.g. $\mathbf{X}$) and corresponding bold face lower case letter (i.e. $\mathbf{x}$) denotes the assignment $\mathbf{X} = \mathbf{x}$. We use $\mathbb{P}(\mathbf{X} = \mathbf{x})$ (equivalently $\mathbb{P}(\mathbf{x})$) to denote the probability of $\mathbf{X}$ taking the value $\mathbf{x}$. Conditional probability of $\mathbf{X} = \mathbf{x}$ given $\mathbf{Y} = \mathbf{y}$ is denoted by $\mathbb{P}(\mathbf{x} \mid \mathbf{y})$. Size of any set S is denoted by $|S|$.

Causal Bayesian Network: A Bayesian Network or BN is a tuple $(\mathcal{G}, \mathbb{P})$, where $\mathcal{G} = (\mathbf{V}, \mathbf{E})$ is a directed acyclic graph (DAG), and $\mathbf{V} = \{V_1, \ldots, V_n\}$ and $\mathbf{E}$ are the set of nodes and edges in $\mathcal{G}$ respectively. A node V_i is called the parent of V_j and V_j the child of V_i, if there is a directed edge from V_i to V_j in $\mathbf{E}$. The nodes in $\mathbf{V}$ are labelled by random variables, and $\mathbb{P}$ is the joint distribution of $\mathbf{V}$ that factorizes over $\mathcal{G}$, i.e. $\mathbb{P}(\mathbf{V}) = \prod_{i=1}^{n} \mathbb{P}(V_i \mid \mathbf{Pa}(V_i))$, where $\mathbf{Pa}(V_i)$ is the set of parents of V_i. Sometimes, in a BN, certain nodes are not observable and are termed unobserved variables. In this situation, for each node $V_i \in \mathbf{V}$, $\mathbf{Pa}(V_i)$ will denote the set of *observable* parents of V_i. A **Causal Bayesian Network** or CBN is a BN where each edge denotes an immediate causal relationship. The graph $\mathcal{G}$ (called the **Causal Graph**) corresponding to a CBN describes the data generation process not just of the observational distribution $\mathbb{P}$ but also of interventional distributions that can be derived from it. An intervention on an observable node $X \in \mathbf{V}$ is denoted as $do(X = x)$, where X is set to value x and all the edges coming in to X are removed. The resulting graph defines a probability distribution $\mathbb{P}(\mathbf{V} \setminus \{X\} \mid do(X = x))$ over $\mathbf{V} \setminus \{X\}$, called an interventional distribution. In the presence of unobserved variables it is convenient to assume (without loss of generality) [Tian and Pearl, 2002b, Verma and Pearl, 1988] that the underlying graph $\mathcal{G}$ of the CBN is semi-markovian. Formally, a **Semi-Markovian Causal Graph** or an SMCG is a DAG, where every unobserved variable is a root and has exactly two observable children [Tian and Pearl, 2002b, Acharya et al., 2018]. These unobserved variables are called **Unobserved Confounders** or UCs in the rest of the paper. It is convenient to represent SMCGs

with observable vertices only by adding a bi-directed edge between two observable vertices if they have a common unobserved parent and removing the unobserved parent from the graph [Tian and Pearl, 2002b]. Such graphs thus comprise of both directed and bi-directed edges with all vertices $\mathbf{V} = \{V_1, \ldots, V_n\}$[4] observable. The bi-directed edges can be used to partition the observable vertices into what are called **c-components**[5] [Tian and Pearl, 2002b]. Two observable vertices are said to be in the same c-component if and only if they are connected by a path of bi-directed edges. Let $\mathbf{X} = \{X_1, \ldots, X_N\} \subset \mathbf{V}$ denote the set of intervenable nodes. The c-component containing the node X_i is denoted by S_i and its size is denoted by k_i i.e. $k_i = |S_i|$. The number of observable parents of X_i is denoted by d_i, i.e. $d_i = |\mathbf{Pa}(X_i)|$. We define $\mathbf{Pa}^+(S_i) = S_i \cup \bigcup_{V \in S_i} \mathbf{Pa}(V)$, and $\mathbf{Pa}^c(X_i) = \mathbf{Pa}^+(S_i) \setminus \{X_i\}$. For more details on these definitions we refer the reader to Tian and Pearl [2002b], Verma and Pearl [1988], Acharya et al. [2018]. An important question that arises in the context of SMCGs is that of **identifiability**, which asks whether the interventional distributions $\mathbb{P}(\mathbf{V} \setminus \{X\} \mid do(X = x))$ can be estimated consistently using observational data sampled from $\mathbb{P}(\mathbf{V})$. In the case of atomic interventions, Tian and Pearl [2002a] provided a necessary and sufficient condition for this to happen. They show that (Thm. 3 in Tian and Pearl [2002a]) $\mathbb{P}(\mathbf{V} \setminus \{X\} \mid do(X = x))$ is identifiable if and only if there is no bi-directed path connecting X to any of its children. For this work, we say that an "SMCG is identifiable with respect to variables in $\mathbf{X}$" if the identifiability condition mentioned above holds for all intervenable nodes in $\mathbf{X}$. Note that, when all variables are observable, there are no bi-directed paths and the interventional probabilities are always identifiable. Moreover, in the observable setting one can use the *backdoor criterion* [Pearl, 2009] for estimating the interventional probabilities from observational samples. In the general setting, Bhattacharyya et al. [2020] provides an efficient procedure (based on construction in Tian and Pearl [2002a]) to estimate the interventional distribution using observational samples which we use in Sec. 3.

Causal Bandits: A causal bandit algorithm receives as input a causal graph $\mathcal{G} = (\mathbf{V}, \mathbf{E})$ (corresponding to some CBN $\mathcal{C}$), the associated set of (binary) intervenable nodes $\mathbf{X} \subseteq \mathbf{V}$ and the designated (observable) reward node $Y \in \mathbf{V}$. We assume there are N intervenable nodes $\mathbf{X} = \{X_1, \ldots, X_N\}$, and there are $2N$ interventions denoted $a_{i,x} = do(X_i = x)$ for $i \in [N]$ and $x \in \{0, 1\}$. The empty intervention $do()$, which corresponds to the observational distribution is denoted as a_0. These $2N + 1$ interventions constitute the arms $\mathcal{A} = \{a_{i,x} \mid i \in [N], x \in \{0, 1\}\} \cup \{a_0\}$ of the bandit instance. A causal bandit algorithm is a sequential decision making process that at each time t, makes an intervention $a_t \in \mathcal{A}$, and observes the sampled values of the nodes in $\mathbf{V}$ including the value of the node Y. The values of nodes $V \in \mathbf{V}$, $X \in \mathbf{X}$ and Y sampled at time t are denoted as $V(t), X(t)$, and $Y(t)$ respectively. Throughout the paper we use i, x, and a to index the sets $[N]$, $\{0, 1\}$, and $\mathcal{A}$ respectively. The expected reward corresponding to intervention $a_{i,x} \in \mathcal{A}$ and $a_0 \in \mathcal{A}$ is denoted as $\mu_{i,x} = \mathbb{E}[Y \mid do(X_i = x)]$ and $\mu_0 = E[Y]$. We study the causal bandit problem with respect two standard objectives in bandit literature: simple and cumulative regret.

Simple Regret: The expected simple regret of an algorithm $\texttt{ALG}$ that outputs arm a_T at the end of T rounds is defined as $r_{\texttt{ALG}}(T) = \max_{a \in \mathcal{A}} \mu_a - \mu_{a_T}$.

Cumulative Regret: Let $\texttt{ALG}$ be an algorithm that plays arm a_t at time $t \in [T]$. Then the expected cumulative regret of $\texttt{ALG}$ at the end of T rounds is defined as $R_{\texttt{ALG}}(T) = \max_{a \in \mathcal{A}} \mu_a \cdot T - \sum_{t \in [T]} \mu_{a_t}$.

Throughout this paper, we assume that the intervenable nodes are binary, distribution of any intervenable node X_i conditioned on its parents $\mathbf{Pa}(X_i)$ is Bernoulli. We assume without loss of generality that $X_i \prec Y$ where $\prec$ is a topological order on $\mathcal{G}$. In $\texttt{SRM-ALG}$ (Sec. 3) we assume that the input is an SMCG that is identifiable with respect to the intervenable variables $\mathbf{X}$ and in $\texttt{CRM-ALG}$ (Sec. 5), we assume the input causal graph has no UCs and the underlying distribution $\mathbb{P}$ is strictly positive i.e. $\mathbb{P}(\mathbf{v}) > 0$ for all $\mathbf{v}$.

Other than the above, our algorithms do not make any other structural assumptions and are therefore significantly general compared to the previous works [Lattimore et al., 2016, Lu et al., 2020, Nair et al., 2021, Lu et al., 2021a]. However, we would like to note that the results in our main theorems i.e. Thms. 3.1, 4.1, 4.2, 5.1 are stated assuming that all the c-components have bounded size implying that $k_i = O(1)$ for all $i \in [N]$ and that the total number of observable parents of nodes in c-component S_i, i.e. $|\cup_{V \in S_i} \mathbf{Pa}(V)|$ is also bounded above by a constant. Note that this clearly implies that the indegree $d_i = |\mathbf{Pa}(X_i)|$ is also $O(1)$. These help us describe the results more cleanly highlighting the main parameters of importance for this work. But our algorithms work even without these assumptions. We note that these assumptions are common in the causal inference literature [Acharya et al., 2018, Bhattacharyya et al., 2020].

3 SIMPLE REGRET MINIMIZATION

In this section, we state and analyze our simple regret minimization algorithm called $\texttt{SRM-ALG}$ which takes as input an SMCG which is identifiable with respect to intervenable variables $\mathbf{X}$ (See Sec. 2 for definition). Our proposed algorithm repeatedly plays the observational arm a_0 for the first $T/2$ rounds. Using this observational data, it determines a small set of arms to pull (i.e. perform interventions) in

[4] By abuse of notation we denote the set of observable vertices by $\mathbf{V}$ from here on wards.

[5] If a node is not incident by any bi-directed edge then its c-component is itself.

the next $T/2$ rounds and estimates their rewards using the interventional samples thus obtained. Finally, for the arms it does not pull, it uses the collected observational samples (from the initial $T/2$ pulls of a_0) to estimate their rewards by adapting a procedure from Bhattacharyya et al. [2020] which efficiently estimates distributions resulting from an atomic intervention using observational samples. We remark that previous works in Lattimore et al. [2016] and Nair et al. [2021] imposed structural restrictions on the input causal graphs which allowed observational samples to be directly used for estimating rewards corresponding to interventions[6]. SRM-ALG, on the other hand, can work with more general identifiable SMCGs and still estimate rewards of multiple arms simultaneously using the observational arm pulls. SRM-ALG is presented in Algorithm 1. We explain each step below.

Algorithm 1 SRM-ALG

INPUT: Causal Graph $\mathcal{G} = (\mathbf{V}, \mathbf{E})$, set of intervenable nodes $\mathbf{X} \subseteq \mathbf{V}$ and time horizon T.

1: $\mathsf{His} = \{\}$ /* His would be used to keep the history of sampled values in the first $T/2$ rounds. */
2: **for** $t \in [1, \ldots, T/2]$ **do**
3: Play arm a_0 and let $\mathsf{His} = \mathsf{His} \cup \{\mathbf{V}(\mathbf{t}) \setminus \mathbf{U}(t), Y(t)\}$.
4: For each $i \in [n]$, compute $\widehat{q}_i$ (as defined in Equation 2) and $\widehat{m}$ (as an estimate of m) by plugging in $\widehat{q}_i$ in place of q_i in Equation 1. Let $\mathcal{Q} = \{a_{i,x} \in \mathcal{A} : \widehat{q}_i^{k_i} < 1/\widehat{m}\}$.
5: **for** $a_{i,x} \in \mathcal{Q}$ **do**
6: Play arm $a_{i,x}$ and observe Y for $\frac{T}{2|\mathcal{Q}|}$ rounds.
7: Estimate reward as $\widehat{\mu}_{i,x} = \frac{2|\mathcal{Q}|}{T} \sum_{t=1}^{T/2|\mathcal{Q}|} Y(t)$.
8: **for** $a_{i,x} \notin \mathcal{Q}$ **do**
9: For each $i \in [n], x \in \{0, 1\}$, use Algorithm 3 in App. C with inputs $\mathcal{G}$, His to get reward estimate $\widehat{\mu}_{i,x}$.
10: Return estimated optimal $a_T^* \in \arg\text{-}\max_{a \in \mathcal{A}} \widehat{\mu}_a$.

Steps 1–4: At Steps $1-3$, SRM-ALG collects $T/2$ observational samples from pulls of a_0 and at Step 4 it identifies a set of arms $\mathcal{Q}$ whose reward estimates (when computed using the collected observational samples) will be bad[7]. This is done using a quantity $m(\mathcal{C})$ defined next; the meaning of relevant notations can be found in Sec. 2. Let $q_i = \min_{\mathbf{z},x} \mathbb{P}(X_i = x, \mathbf{Pa}^c(X_i) = \mathbf{z})$. For each $\tau \in [2, 2N]$, let $I_\tau = \{i : q_i^{k_i} < 1/\tau\}$[8]. We define,

$$m(\mathcal{C}) = \min\{\tau : |I_\tau| \leq \tau\}. \tag{1}$$

The observational samples that were collected are used to first compute estimates $\widehat{q}_i$ of q_i given as:

$$\widehat{q}_i = \left(\frac{2}{T}\right) \cdot \min_{\mathbf{z},x} \left\{ \sum_{t=1}^{T/2} \mathbb{1}\{X_i(t) = x, \mathbf{Pa}^c(X_i)(t) = \mathbf{z}\} \right\} \tag{2}$$

These estimates are then plugged into the above definition of $m(\mathcal{C})$ to obtain it's estimate $\widehat{m}$. Finally the set of arms $\mathcal{Q}$ is defined as $\mathcal{Q} = \{a_{i,x} \in \mathcal{A} : \widehat{q}_i^{k_i} < 1/\widehat{m}\}$.

Steps 5–10: Since, using observational samples reward estimates of arms in $\mathcal{Q}$ will be bad, in Steps $5-7$, we pull these arms equal number of times by performing the corresponding interventions and estimate their rewards directly from the interventional samples. The observational samples collected in first $T/2$ rounds are used to compute the estimates for each arm $a_{i,x} \notin \mathcal{Q}$ at Steps $8, 9$. Reward estimates of these arms are computed using Algorithm 3, App. C. Finally in Step 10, we return arm $a_{i,x}$ with the best reward estimate. Even though Algorithm 3 uses Bhattacharyya et al. [2020], which assumes strong positivity, we do not need to explicitly make this assumption since low probability arms $a_{i,x}$ get pulled (by intervention) in Step 6 and only high probability arms are estimated using Algorithm 3.

Some remarks about $m(\mathcal{C})$: Our definition of $m(\mathcal{C})$ above is a novel extension of a similar quantity m defined in Lattimore et al. [2016] and reduces to $\Theta(m)$ for parallel graphs [Lattimore et al., 2016] and no-backdoor graphs [Nair et al., 2021]. As a result, the regret guarantee of SRM-ALG for these special classes of graphs matches those of the respective algorithms in these works. Operationally, $m(\mathcal{C})$ determines for us the optimal number of arms to be pulled in Steps $5-7$, in order to minimize expected regret. In particular, $I_{m(\mathcal{C})}$ is a set of arms such that the best arm in it (found using $T/2$ rounds of interventions) and the best arm in its complement $I^c_{m(\mathcal{C})}$ (found using $T/2$ rounds of observations) have reward estimates of similar quality.

We show that the expected simple regret of SRM-ALG in Theorem 3.1 stated below is $\tilde{O}(\sqrt{m(\mathcal{C})/T})$, which is an instance-dependent regret guarantee as $m(\mathcal{C})$ depends on the input CBN. If $m(\mathcal{C}) \ll N$ then SRM-ALG performs better than the optimal MAB algorithm. In particular, SRM-ALG explores only at most $2\widehat{m}+1$ arms compared to the $2N$ arms that must be explored by a standard best-arm identification MAB algorithm which achieves $\Omega(\sqrt{N/T})$ expected worst-case simple regret [Audibert et al., 2010]. It is easy to see that there are CBNs $\mathcal{C}$ with $m(\mathcal{C}) \ll N$ as illustrated in App. B. The proof of Theorem 3.1 is given in App. D.

Theorem 3.1
The expected simple regret of SRM-ALG at the end of T rounds is $r_{\textsc{srm-alg}}(T) = O\left(\sqrt{\frac{m(\mathcal{C})}{T} \log \frac{NT}{m(\mathcal{C})}}\right)$.

Remark: The constant involved in the regret expression

[6]The restrictions ensured that the conditional distributions are equal to the corresponding interventional distributions

[7]Can be seen easily using Lemma D.3.

[8]Recall from Sec. 2 that k_i is size of the c-component of X_i.

is exponential in $\max_i\{k_i\}$ and $\max_i\{|\mathbf{Pa}^c(X_i)|\}$. Recall that these are constant as per our assumptions in Sec. 2.

4 SIMPLE REGRET LOWER BOUND

A closer inspection of SRM−ALG given in Sec. 3 reveals that the algorithm only leverages causal side-information while pulling the observational arm. Hence, there remains a possibility that a better algorithm could be designed which uses the information shared between any two interventions. In this section, we show that this is not possible for a large and important class of causal graphs that we call tree-graphs and denote it as T. Each graph in T is an n-ary tree, where each node can have 2 to n children. Additionally, all the leaves are connected to the outcome node Y. We also assume that all nodes of any graph in T are observable. Note that a causal bandit algorithm receives as input a causal graph $\mathcal{G}$ (corresponding to some CBN $\mathcal{C} = (\mathcal{G}, \mathbb{P})$) but the associated distribution $\mathbb{P}$ is unknown to the algorithm. Since there are multiple probability distributions that are compatible with a given $\mathcal{G}$ the algorithm is required to learn the unknown $\mathbb{P}$ through the arm pulls. We show in Thm. 4.1 that for any causal graph $\mathcal{G}$ in T and any positive integer $M \leq N$, there exists a distribution $\mathbb{P}$ such that $M = m(\mathcal{C})$, where $\mathcal{C}$ is CBN $(\mathcal{G}, \mathbb{P})$, and, any algorithm must explore at least $\Omega(M)$ arms to minimize the worst-case expected simple regret.

Theorem 4.1
Corresponding to every causal graph $\mathcal{G} \in \mathsf{T}$, with N intervenable nodes and any positive integer $M \leq N$, there exists a probability measure $\mathbb{P}$ and CBN $\mathcal{C} = (\mathcal{G}, \mathbb{P})$ such that $m(\mathcal{C}) = M$ and the expected simple regret of any causal bandit algorithm ALG is $r_{\texttt{ALG}}(T) = \Omega\big(\sqrt{m(\mathcal{C})/T}\big)$.

The proof of Thm. 4.1 is in App. E. Recall, from Sec. 3 that $m(\mathcal{C})$ is completely defined by $\mathbf{q} = (q_1, \ldots, q_N)$ and $\mathcal{G}$; in particular the definition of $m(\mathcal{C})$ does not depend on the entire probability distribution corresponding to CBN $\mathcal{C}$. We conclude this section by showing in Thm. 4.2 that the dependence of the regret on $\mathbf{q}$ in the definition of $m(\mathcal{C})$ is optimal for certain graphs. In Thm. 4.2, a $\mathbf{q}$ is valid if there exists a probability measure $\mathbb{P}$ for the graph $\mathcal{G}$, which results in the given $\mathbf{q}$. The proof of Thm. 4.2 is in App. F.

Theorem 4.2
There exists a fully observable causal graph $\mathcal{G}$ with $N \geq 3$ nodes such that given any valid $\mathbf{q}$ corresponding to $\mathcal{G}$, there is a probability measure $\mathbb{P}$ conforming with $\mathbf{q}$ and CBN $\mathcal{C} = (\mathcal{G}, \mathbb{P})$ for which expected simple regret of any causal bandit algorithm is $\Omega\big(\sqrt{m(\mathcal{C})/T}\big)$.

5 CUMULATIVE REGRET MINIMIZATION

In this section, we propose CRM−ALG, an algorithm based on the well-known UCB algorithm [Auer et al., 2002], that sequentially performs (atomic) interventions and minimizes the cumulative regret incurred over the time horizon T. Unlike SRM−ALG, here we assume all nodes in the input graph $\mathcal{G}$ are observable and the joint distribution $\mathbb{P}$ is strictly positive[9]. Similar to the UCB family of algorithms CRM−ALG maintains UCB estimates at each round and pulls the arm with the highest UCB estimate. CRM−ALG performs better than the standard UCB algorithm [Auer et al., 2002] by leveraging (via *backdoor criterion* [Pearl, 2009]) the available causal side-information. In particular, CRM−ALG uses the samples from the observational arm pulls in addition to the samples from the arm pulls of $a_{i,x}$ to compute UCB estimates of $a_{i,x}$. Note that even though the observational arm may not be reward optimal, pulling it gives a simultaneous causal side-information about all the arms. CRM−ALG ensures a good trade-off between such a simultaneous exploration and the possible loss in reward by ensuring that a_0 is pulled at least a pre-specified (carefully chosen) number of times. We note that CRM−NB−ALG proposed for no-backdoor graphs in Nair et al. [2021], also ensures that the observational arm a_0 is pulled a pre-specified number of times, but CRM−ALG differs from CRM−NB−ALG on how the UCB estimates for the arms are computed at the end of each round. Next, we present the details of CRM−ALG.

Algorithm 2 CRM−ALG (Minimizing cumulative regret in general causal graph)

INPUT: Causal graph $\mathcal{G}$ and the set of intervenable nodes
1: Pull each arm once and set $t = 2N + 2$
2: Let $\beta = 1$
3: **for** $t = 2N + 2, 2N + 3, \ldots$ **do**
4: **if** $N^0_{t-1} < \beta^2 \log t$ **then**
5: Pull $a_t = a_0$
6: **else**
7: Pull $a_t = \arg\text{-}\max_{a \in A} \bar{\mu}_a(t-1)$
8: $N^a_t = N^a_{t-1} + \mathbb{1}\{a_t = a\}$
9: Update $\widehat{\mu}_a(t)$ and $\bar{\mu}_a(t)$ for all $a \in A$ according to Equations 3, 5, 6 and 7.
10: Let $\widehat{\mu}^* = \max_a \widehat{\mu}_a(t)$
11: **if** $\widehat{\mu}_0(t) < \widehat{\mu}^*$ **then**
12: Set $\beta = \min\{\frac{2\sqrt{2}}{\widehat{\mu}^* - \widehat{\mu}_0(t)}, \sqrt{\log t}\}$
13: $t = t + 1$

We use $N^{i,x}_t$ and N^0_t to denote the number of times arms $a_{i,x}$ and a_0 have been played at the end of t rounds respectively, and further let a_t denote the arm pulled at round t. Also, $\widehat{\mu}_{i,x}(t)$ and $\bar{\mu}_{i,x}(t)$ (respectively $\widehat{\mu}_0(t)$ and $\bar{\mu}_0(t)$) denotes the empirical and UCB estimates of the arm $a_{i,x}$ (respectively arm a_0) computed at the end of round t. At Step 4 CRM−ALG checks if the observational arm is pulled at least $\beta^2 \log t$ times, and accordingly either plays the ob-

[9] Strict positivity of the joint distribution is often assumed in the causality literature [Hauser and Bühlmann, 2012]

servational arm or the arm with the highest UCB estimate. Here the value of β is updated as in Steps 11-12 . As noted before, the chosen update for β and the corresponding pre-specified number of pulls for arm a_0 delicately balances the exploration-exploitation trade-off in expectation. The empirical estimate for arm a_0 at Step 9 is computed as follows

$$\widehat{\mu}_0(t) = \frac{1}{N_t^0} \sum_{s=1}^{t} \mathbb{1}\{Y(s) = 1, a_s = a_0\} \ . \tag{3}$$

The empirical estimate for arm $a_{i,x}$ is involved, and as mentioned before is done by leveraging the following backdoor criterion (see Thm. 3.3.2 in Pearl [2009]).

$$\mathbb{P}(Y = 1 \mid do(X_i = x)) = \tag{4}$$
$$\sum_{\mathbf{z}} \mathbb{P}(Y = 1 \mid X_i = x, \mathbf{Pa}(X_i) = z)\mathbb{P}(\mathbf{Pa}(X_i) = \mathbf{z})$$

Let the set of time steps $s \leq t$ at which arm a_0 is pulled be denoted by $S_t = \{t_1, \ldots, t_{N_t^0}\}$. Partition S_t into two parts O_t containing all the time steps with odd indices (i.e. t_1, t_3, etc.) and E_t containing all the time steps with even indices (i.e. t_2, t_4, etc.). We will now define some sets and intermediate estimators in order to describe the final estimator. Since X_i is clear from the context, we do not use i to index these intermediate estimators. In general these sets and estimators will be different for different i. We use time steps in O_t to estimate $\mathbb{P}(Y = 1 \mid X_i = x,\ \mathbf{Pa}(X_i) = \mathbf{z})$, and those in E_t to estimate $\mathbb{P}(\mathbf{Pa}(X_i) = \mathbf{z})$. These probabilities are estimated on disjoint sets of time steps to make the estimators independent of each other which we require while showing that the estimator is unbiased (Lemma G.1 in App. G). To estimate the above mentioned probabilities, we focus on the subsets

$$O_t^{x,z} = \{s \in O_t \mid X_i(s) = x, \mathbf{Pa}(X_i)(s) = \mathbf{z}\} \subseteq O_t$$

Let C_t^x be the minimum value of $|O_t^{x,z}|$ (as $\mathbf{z}$ is varied). To use time steps in E_t for estimating $\mathbb{P}(\mathbf{Pa}(X_i) = \mathbf{z})$, we partition this set into C_t^x many parts[10], say $E_t = E_{t,1} \cup \ldots \cup E_{t,C_t^x}$. For each part $E_{t,c}$, $c \in [C_t^x]$, we create an estimator of the probability $\mathbb{P}(\mathbf{Pa}(X_i) = \mathbf{z})$ as follows:

$$\widehat{p}_{t,c}^{\,\mathbf{z}} = \sum_{s \in E_{t,c}} \frac{\mathbb{1}\{\mathbf{Pa}(X_i)(s) = \mathbf{z}\}}{|E_{t,c}|}$$

Now we are ready to build an estimator using Equation 4. Let $s_1, \ldots, s_{C_t^x}$ be any distinct elements[11] of set $O_t^{x,z}$. For each $c \in [C_t^x]$, we define a variable Y_c^x as follows:

$$Y_c^x = \sum_{\mathbf{z}} \mathbb{1}\{Y(s_c) = 1\}\widehat{p}_{t,c}^{\,\mathbf{z}}$$

[10]Each part has at least $\lfloor |E_t|/C_t^x \rfloor$ elements. Choice of C_t^x helps in bounding regret (Lemma G.2 in App. G)

[11]They exist since $|O_t^{x,z}| \geq C_t^x$.

Let $S_t^{i,x}$ be the set of timestamps $s \leq t$, when arm $a_{i,x}$ is pulled. Our final empirical estimator $\widehat{\mu}_{i,x}(t)$ of arm $a_{i,x}$ is:

$$\widehat{\mu}_{i,x}(t) = \frac{\sum_{s \in S_t^{i,x}} \mathbb{1}\{Y(s) = 1\} + \sum_{c \in [C_t^x]} Y_c^x}{N_t^{i,x} + C_t^x} \tag{5}$$

It is easy to see that $\mathbb{E}[\widehat{\mu}_0(t)] = \mu_0$, and in Lemma G.1 (App. G) using backdoor criterion (Sec. 3.3.1 in Pearl [2009]) we show that $\mathbb{E}[\widehat{\mu}_{i,x}(t)] = \mu_{i,x}$ for every i, x. Finally, CRM-ALG uses Equations 3 and 5 to compute the UCB estimates $\bar{\mu}_{i,x}(t)$ and $\bar{\mu}_0(t)$ of arms $a_{i,x}$ and arm a_0 respectively

$$\bar{\mu}_{i,x}(t) = \widehat{\mu}_{i,x}(t) + \sqrt{\frac{2 \ln t}{N_t^{i,x} + C_t^x}} \tag{6}$$

$$\bar{\mu}_0(t) = \widehat{\mu}_0(t) + \sqrt{\frac{2 \ln t}{N_t^0}} \tag{7}$$

We bound the expected cumulative regret of CRM-ALG in Thm. 5.1, where $a^* = \arg\text{-}\max_{a \in A} \mu_a$ and, for $a \in \mathcal{A}$, $\Delta_a = \mu_{a*} - \mu_a$, $p_{\mathbf{z}}^{i,x} = \mathbb{P}(X_i = x, \mathbf{Pa}(X_i) = \mathbf{z})$, $p_{i,x} = \min_{\mathbf{z}} p_{\mathbf{z}}^{i,x}$. Additionally, $\eta_T^{i,x}$ denotes the probability that the empirical estimate of $p_{i,x}$ at time T is large (See Observation G.6 in App. G) and is defined as $\eta_T^{i,x} = \max\left\{0, \left(1 - Z_i T^{-\frac{p_{i,x}^2}{4}}\right)\right\}$, where Z_i is the size of the domain of $\mathbf{Pa}(X_i)$.

Theorem 5.1
If $a^* = a_0$, then at the end of T rounds the expected cumulative regret is $O(1)$. Otherwise, the expected cumulative regret is of the order $\frac{58 \ln T}{\Delta_0} + \Delta_0 + \sum_{\Delta_{i,x} > 0} \Delta_{i,x} \max\left\{0, 1 + 8 \ln T \left(\frac{1}{\Delta_{i,x}^2} - \frac{p_{i,x} \cdot \eta_T^{i,x}}{36 \Delta_0^2}\right)\right\} + \sum_{\Delta_a > 0} \Delta_a \frac{\pi^2}{3}$.

The proof of Thm. 5.1 is given in App. G. Notice that the regret guarantee in Thm. 5.1 is an instance dependent constant if a_0 is optimal and otherwise slightly better than the UCB family of algorithms. Also, it is easy to construct examples of CBNs where the observational arm is optimal, for example see Experiment 2 in Sec. 6.

No unobserved variable assumption: As mentioned, in CRM-ALG we work in the fully observable setting unlike SRM-ALG (Sec. 3). A natural question is whether Algorithm 3 (App. C) can also be used in CRM-ALG in the presence of unobserved confounders. We believe there is no straightforward way to accomplish this due to a rather technical reason. Our estimator (Equation 5) cleverly interprets observational samples as C_t^x many interventional samples and can be shown to be unbiased (Lemma G.1, App. G). The technique in Algorithm 3 does not enable the same interpretation of observational samples, and hence cannot be easily used to create an estimator with similar properties.

6 EXPERIMENTS

In this section, we validate our results empirically. In Exp. 1, we compare the simple regret of our proposed algorithm SRM−ALG to two baseline MAB algorithms: uniform exploration (UE) and successive rejects (SR) [Audibert et al., 2010]. In Exp. 2, we compare the expected cumulative regret of CRM−ALG and UCB when the observational arm is the best arm (i.e. $a^* = a_0$) to validate the first part of Thm. 5.1. We conduct additional experiments which are presented in App. H due to lack of space. In Exp. 3 (App. H), we compare the simple regret of SRM−ALG with baselines UE and SR as m increases. In Exp. 4 (App. H), we compare SRM−ALG with the simple regret minimization algorithm (Alg. 3) in Yabe et al. [2018]. Since their algorithm runs in time exponential in the in-degree of Y (whereas our SRM−ALG takes polynomial time in in-degree of Y), a comparison with them is feasible only on smaller simpler instances. In Exp. 5 (App. H), we compare expected cumulative regret of CRM−ALG and UCB on random CBN instances without the assumption of $a^* = a_0$ to validate second part of Thm. 5.1.

Experiment 1 **(Simple Regret vs. T):** This experiment compares the expected simple regret of SRM−ALG with UE and SR as T increases. We run the algorithms on 50 CBNs, where every constructed CBN C, has 100 intervenable nodes with $m(\mathcal{C}) = 9$. The CBNs are constructed as follows: a) randomly generate 50 DAGs on 101 nodes $X_1, \ldots, X_{100}, Y$ such that $X_1 \prec \ldots \prec X_{100} \prec Y$ is a topological order in each such DAG, b) $\mathbf{Pa}(X_i)$ contains ≤ 2 nodes chosen uniformly at random from $X_1, \ldots, X_{i-1}$, and $\mathbf{Pa}(Y)$ equals the set of all X_is, c) $\mathbb{P}(X_i \mid \mathbf{Pa}(X_i)) = 0.5$ for $i \in [91]$ and $\mathbb{P}(X_i|\mathbf{Pa}(X_i)) = 1/18$ for $i \in [92, 100]$, d) uniformly at random choose a $j \in \{92, \ldots, 100\}$ and set $P(Y|X_1, \ldots, X_j = 1, \ldots, X_{100}) = 0.5 + \epsilon$ and $P(Y|X_1, \ldots, X_j = 0, \ldots, X_{100}) = 0.5 - \epsilon'$ where $\epsilon = 0.3$ and $\epsilon' = q\epsilon/(1-q)$ for $q = 1/18$. The choice of the conditional probability distributions in (c) ensures $m(\mathcal{C}) = 9$ for every generated CBN $\mathcal{C}$. We note that the above strategy to generate CBNs is a generalization of the one used in Lattimore et al. [2016]. For each of the 50 random CBN, we run SRM−ALG, MAB, SR for multiple values of the time horizon T in $[500, 2500]$ and average the regret over 100 independent runs. Finally, we calculate the mean regret over all the 50 random CBNs and plot mean regret vs. T in Fig. 2. Since $m \ll N$, as seen in Fig. 2, SRM−ALG has a much lower regret as compared to UE and SR which is in accordance with Thm. 3.1.

Experiment 2 **(Cumulative Regret vs. T):** In this experiment, we compare the cumulative regret of CRM−ALG with UCB for CBN on four nodes X_1, X_2, X_3, and Y. Variable X_1 has no parents and is the only parent of X_2, X_3. Parents of Y are X_2, X_3. We choose CPDs: $\mathbb{P}(X_1 = 1) = 0.5$, $\mathbb{P}(X_2 = 1|X_1)$ and $\mathbb{P}(X_3 = 1|X_1)$ are equal to $0.75X_1 + 0.25(1 - X_1)$ and $P(Y = 1|X_2, X_3) = \mathbb{1}_{X_2 = X_3}$.

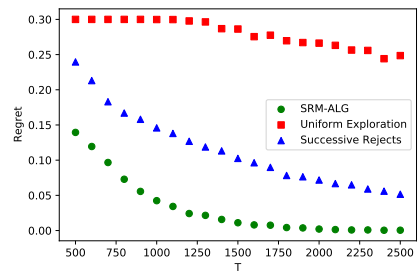

Figure 2: Simple Regret vs Horizon

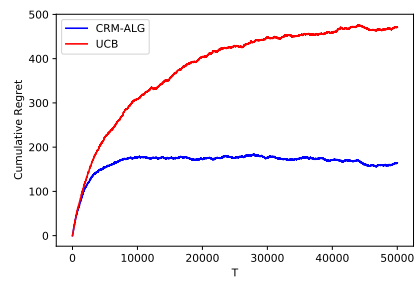

Figure 3: Cumulative Regret vs Horizon

For this instance, it is easy to see that $\mathbb{P}(Y = 1|do(X_2 = x)) = P(Y = 1|do(X_3 = x)) = 0.5$ for $x \in \{0, 1\}$ and $P(Y = 1|do()) = 5/8$, implying that observational arm is the best arm. We run CRM−ALG and UCB for a sufficient time T and average the cumulative regrets over 30 independent runs. Fig. 3 demonstrates that while cumulative regret of UCB increases, that of CRM−ALG becomes constant for large enough T as expected by result in Thm. 5.1.

7 CONCLUSION

We proposed two algorithms SRM−ALG and CRM−ALG that take as input causal graphs, pull observational/interventional arms, and minimize simple and cumulative regret respectively. While SRM−ALG works over SMCGs and can handle unobserved variables, CRM−ALG works in the fully observable setting. We theoretically and empirically show that our algorithms are better than standard MAB algorithms that do not take causal side-information into account. Further, we show that SRM−ALG is almost optimal for causal graphs having an n-ary tree structure. In the fully observable setting, our algorithms do not put any restrictions on the graph structure and subsume previous results which imposed strong structural restrictions. We plan to explore cumulative regret minimization in the presence of UCs in a future work. Another interesting direction is to identify graphs where better simple regret guarantee than SRM−ALG can be attained. Finally, obtaining regret guarantees when interventions are non-atomic will be a nice extension to our work.

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A PRELIMINARY LEMMAS

We state some standard concentration bounds that are used in our proofs. Their proofs can be found in the citations provided.

Lemma A.1 (Chernoff Bounds, Section 4.2 in Mitzenmacher and Upfal [2005])
Let Z be any random variable. Then for any $t > 0$,

1. $\mathbb{P}(Z \geq \mathbb{E}[Z] + t) \leq \min_{\lambda > 0} \mathbb{E}[e^{\lambda(Z - \mathbb{E}[Z])}]e^{-\lambda t}$
2. $\mathbb{P}(Z \leq \mathbb{E}[Z] - t) \leq \min_{\lambda > 0} \mathbb{E}[e^{\lambda(\mathbb{E}[Z] - Z)}]e^{-\lambda t}$

Lemma A.2 (Hoeffding's Lemma, Lemma 2.6 in Massart and Picard [2007])
Let Z be a bounded random variable with $Z \in [a, b]$. Then,

$$\mathbb{E}[\exp(\lambda(Z - \mathbb{E}[Z])] \leq \exp\Big(\frac{\lambda^2(b-a)^2}{8}\Big)$$

for all $\lambda \in \mathbb{R}$.

Lemma A.3 (Chernoff-Hoeffeding inequality, Chernoff [1952], Hoeffding [1963])
Suppose $X_1, \ldots, X_T$ are independent random variables taking values in the interval $[0, 1]$, and let $X = \sum_{t \in [T]} X_t$ and $\overline{X} = \frac{1}{T}(\sum_{t \in [T]} X_t)$. Then for any $\varepsilon \geq 0$ the following holds:

1. $\mathbb{P}(\overline{X} - \mathbb{E}[\overline{X}] \geq \varepsilon) \leq e^{-2\varepsilon^2 T}$
2. $\mathbb{P}(\overline{X} - \mathbb{E}[\overline{X}] \leq -\varepsilon) \leq e^{-2\varepsilon^2 T}$

B EXAMPLE OF CBN WITH $m(\mathcal{C}) \ll N$

Consider a CBN $\mathcal{C} = (\mathcal{G}, \mathbb{P})$ with N intervenable nodes and in-degree at most $k-1$, and let k be such that $2^k \ll N$. Further, let $\mathbb{P}$ be such that for at most 2^k nodes, chosen in the reverse topological order, the conditional probability of a node given its parents is Bernoulli with parameter $1/2^{k+1}$, and for the remaining nodes the conditional probability of a node given its parents is Bernoulli with parameter $1/2$. Now, using the definition of $m(\mathcal{C})$ provided in Section 3, it is easy to see that $m(\mathcal{C}) \leq 2^k \ll N$.

C ESTIMATION OF REWARD FROM OBSERVATION

In Algorithm 3 below we explain our strategy (derived from Bhattacharyya et al. [2020]) for estimating the reward of the interventional arms $a_{i,x}$ using $T/2$ observational samples collected by playing the observational arm a_0. This is followed by details on each of the steps involved. Recall, N is the number of intervenable nodes.

Algorithm 3 Estimating Rewards from Observational Samples

INPUT: His containing the $T/2$ observational samples collected by playing arm a_0, and $\mathcal{G}$

1: For each $i \in [N]$, reduce the input ADMG $\mathcal{G}$ to ADMG $\mathcal{H}_i$ as outlined in Algorithm 4.
2: Next, for each $i \in [N]$ and $x \in \{0, 1\}$, construct the Bayes net $D_{i,x}$ which simulates the causal effect of intervention $do(X_i = x)$ on the reduced graph $\mathcal{H}_i$.
3: Using Algorithm 5 on the input samples, estimate the distributions of all $D_{i,x}$. Then, using learned $D_{i,x}$, generate samples to estimate marginal of Y and return them as estimated rewards.

Step 1 **:** This step executes Algorithm 4 based on the reduction algorithm from Bhattacharyya et al. [2020].

Algorithm 4 Reducing $\mathcal{G}$ to $\mathcal{H}_i$

INPUT: ADMG $\mathcal{G}$ and index $i \in [N]$.

1: Let $\mathbf{W} = Y \cup X_i \cup \mathbf{Pa}^c(X_i)$, and $\mathcal{G}'_i$ be the graph obtained by considering $\mathbf{V} \backslash \mathbf{W}$ as hidden variables. Let $\mathbf{V}_i$ denote the nodes in $\mathcal{G}'_i$

2: **Projection Algorithm:** It reduces $\mathcal{G}'_i$ to $\mathcal{H}_i$ as follows:

1. Add all observable variables in $\mathcal{G}'_i$ to $\mathcal{H}_i$.
2. For every pair of observable variable $V^i_j, V^i_k \in \mathbf{V}_i$, add a directed edge from V^i_j to V^i_k in $\mathcal{H}_i$, if (a) there exists a directed edge from V^i_j to V^i_k in $\mathcal{G}'_i$, or if (b) there exists a directed path from V^i_j to V^i_k in $\mathcal{G}'_i$ which contains only unobservable variables.
3. For every pair of observable variable $V^i_j, V^i_k \in \mathbf{V}_i$, add a bi-directed edge between V^i_j and V^i_k in $\mathcal{H}_i$, if (a) there exists an unobserved variable U with two directed paths in $\mathcal{G}'_i$ going from U to V^i_j and U to V^i_k and containing only unobservable variables.

3: Return $\mathcal{H}_i$.

Algorithm 5 Estimating distributions of $D_{i,x}$

INPUT: ADMG $\mathcal{H}_i$ and $x \in \{0, 1\}$.

for every $V_j \in S_1$ **do**
  for every assignment $V_j = v$ and $\mathbf{Z_j} = \mathbf{z}$ where $\mathbf{Z_j}$ are effective parents of V_j in $\mathcal{H}_i$ **do**
    $N_j \leftarrow$ the number of samples with $\mathbf{Z_j} = \mathbf{z}$
    $N_{j,v} \leftarrow$ the number of samples with $\mathbf{Z_j} = \mathbf{z}$ and $V_j = v$
    $\widehat{D}_{i,x}(V_j = v | \mathbf{Z_i} = \mathbf{z}) \leftarrow \frac{N_{j,v}+1}{N_j+2}$
for every $V_j \in \mathbf{V_i} \backslash \mathbf{S_1}$ **do**
  for every $V_j = v$ and $\mathbf{Z_j} \backslash X_i = \mathbf{z}$, where $\mathbf{Z_j}$ are effective parents of V_j in $\mathcal{H}_i$ **do**
    if $X \in \mathbf{Z_i}$ **then**
      $N_j \leftarrow$ the number of samples with $\mathbf{Z_j} \backslash X_i = \mathbf{z}$ and $X_i = x$
      $N_{j,v} \leftarrow$ the number of samples with $V_j = v$, $\mathbf{Z_j} \backslash X_i = \mathbf{z}$ and $X_i = x$
      if $N_j \geq t$ **then**
        $\widehat{D}_{i,x}(V_j = v | \mathbf{Z_i} = \mathbf{z}) \leftarrow \frac{N_{j,v}+1}{N_j+2}$
      else
        $\widehat{D}_{i,x}(V_j = v | \mathbf{Z_j} - \{X_i\} = \mathbf{z}, X_i = x) \leftarrow \frac{1}{2}$
    else
      $N_j \leftarrow$ the number of samples with $\mathbf{Z_j} = \mathbf{z}$
      $N_{j,v} \leftarrow$ the number of samples with $V_j = v$ and $\mathbf{Z_j} = \mathbf{z}$
      if $N_j \geq t$ **then**
        $\widehat{D}_{i,x}(V_j = v | \mathbf{Z_i} = \mathbf{z}) \leftarrow \frac{N_{j,v}+1}{N_j+2}$
      else
        $\widehat{D}_{i,x}(V_j = v | \mathbf{Z_j} = \mathbf{z}) \leftarrow \frac{1}{2}$
Return $\widehat{D}_{i,x}$.

Step 2 **:** Construction of $D_{i,x}$ is done using the method described in Section 4.1 of Bhattacharyya et al. [2020]. Without loss of generality let $\mathbf{S_1}$ be the c-component containing X_i. To construct $D_{i,x}$, we start with $\mathcal{H}_i$. Then, for each $V \notin \mathbf{S_1}$ such that X_i is in the set $\mathbf{Z_i}$ of "effective parents" (Section 4, Bhattacharyya et al. [2020]) of V, we create a clone of X_i and fix its value to x (i.e. the clone has no parents). Then we remove all the outgoing edges from the original X_i. Note that, for any assignment $\boldsymbol{v}$ of all variables except X_i in $\mathcal{H}_i$, the causal effect $\mathbb{P}_{\mathcal{H}_i}(\boldsymbol{v}|do(X_i = x)) = \sum_x \mathbb{P}_{D_{i,x}}(\boldsymbol{v}, X_i = x)$.

Step 3 **:** In this step, we estimate the distributions of all $D_{i,x}$ using the $T/2$ samples that were provided as input. Details are described in Algorithm 5. Using this estimated distribution, we get $O(T)$ samples and compute an empirical estimate $\widehat{\mu}_{i,x}$ of the reward $\mu_{i,x} = \mathbb{P}_{\mathcal{G}}(Y = 1|do(X_i = x))$. This follows from the construction of $D_{i,x}$ in Step 2 which implies,

$$\mu_{i,x} = \mathbb{P}_{\mathcal{G}}(Y = 1|do(X_i = x)) = \mathbb{P}_{\mathcal{H}_i}(Y = 1|do(X_i = x)) = \sum_{x,\boldsymbol{v}'} \mathbb{P}_{D_{i,x}}(Y = 1, \boldsymbol{v}', X_i = x)$$

where $\boldsymbol{v}'$ is an assignment of nodes in $D_{i,x}$ other than X_i and Y.

D PROOF OF THEOREM 3.1

For the sake of analysis, we assume without loss of generality that $q_1, q_2, \ldots, q_N$ are arranged such that their corresponding c-component sizes $k_1, k_2, \ldots, k_N$ satisfy the following relation: $(q_1)^{k_1} \leq (q_2)^{k_2} \leq \ldots \leq (q_N)^{k_N}$. Also, let $q = \min_{i\{q_i>0\}} q_i$ (if $q_i = 0$ for all $i \in [N]$ then $q = \frac{1}{N+1}$), $k = \max_i k_i$, and $p_{\mathbf{z}}^{i,x} = \mathbb{P}(X_i = x, \mathbf{Pa}^c(X_i) = \mathbf{z})$. We remark that $p_{\mathbf{z}}^{i,x}$ is different from $p_{\mathbf{z}}^{i,x}$ used in Section 5 to denote $\mathbb{P}(X_i = x, \mathbf{Pa}(X_i) = \mathbf{z})$; note that $\mathbf{Pa}(X_i) \subseteq \mathbf{Pa}^c(X_i)$. Let d be the maximum indegree of any node in S_i for $i \in [N]$. Finally, let Z_i be the size of the domain from which $\mathbf{Pa}^c(X_i)$ takes values, and note that $Z_i \leq 2^{k_i d + k_i}$ and let $Z = \max_i Z_i$. Note that, by our assumption Z is $O(1)$. Also, in this section, let $m(\mathcal{C})$ be denoted by m.

We begin by proving Lemmas D.1, D.2, and D.3 which would be used to prove Theorem 3.1. The following lemma bounds the probability of making a bad estimate of q_i for any $i \in [N]$, at the end of $T/2$ rounds.

Lemma D.1
Let $F = \mathbb{1}\{$At the end of $T/2$ rounds, there exists i such that $|\widehat{q}_i - q_i| \geq \frac{1}{4}(1 - 2^{-1/k})q\}$. Then $\mathbb{P}(F = 1) \leq 4NZe^{-\frac{1}{16}(1-2^{-1/k})^2 q^2 T}$.

Proof. Let $F_{i,x} = \mathbb{1}\{$At the end of $T/2$ rounds there exists $\mathbf{z}$ such that $|\widehat{p}_{\mathbf{z}}^{i,x} - p_{\mathbf{z}}^{i,x}| \geq \frac{1}{4}(1 - 2^{-1/k})q\}$. From Lemma A.3, it follows that,

$$\mathbb{P}\Big(|\widehat{p}_{\mathbf{z}}^{i,x} - p_{\mathbf{z}}^{i,x}| \geq \frac{1}{4}(1 - 2^{-1/k})q\Big) \leq 2e^{-2\frac{1}{16}(1-2^{-1/k})^2 q^2 \frac{T}{2}}$$

By union bound,

$$\mathbb{P}(F_{i,x} = 1) \leq 2Z_i e^{-\frac{1}{16}(1-2^{-1/k})^2 q^2 T}$$

By definition $q_i = \min_{x,\mathbf{z}} p_{\mathbf{z}}^{i,x}$ and $\widehat{q}_i = \min_{x,\mathbf{z}} \widehat{p}_{\mathbf{z}}^{i,x}$. Hence,

$$\mathbb{P}\Big(|\widehat{q}_i - q_i| \geq \frac{1}{4}(1 - 2^{-1/k})q\Big) \leq 2P(F_{i,x} = 1) \leq 4Z_i e^{-\frac{1}{16}(1-2^{-1/k})^2 q^2 T}$$

Taking union bound, we get $\mathbb{P}(F = 1) \leq 4NZe^{-\frac{1}{16}(1-2^{-1/k})^2 q^2 T}$. □

The next lemma shows that with high probability the estimate of m at Step 6 of `SRM-ALG` is good.

Lemma D.2
Let F be as defined in Lemma D.1 and let $J = \mathbb{1}\{$At the end of $T/2$ rounds the following holds $\widehat{m} \leq 2m$. Then $F = 0$ implies $J = 1$, and in particular, $\mathbb{P}(J = 1) \geq 1 - 4NZe^{-\frac{1}{16}(1-2^{-1/k})^2 q^2 T}$.

Proof. Note that if $q_i = 0$ for all $i \in [N]$, then our proposition is trivially true. $F = 0$ implies after $T/2$ rounds for all $i \in [N]$, $|\widehat{q}_i - q_i| \leq \frac{1}{4}(1 - 2^{-1/k})q$. Now from definition of m we know that there is an $l \leq m$ such that for $i > l$, $(q_i)^{k_i} \geq (\frac{1}{m})$. Hence, for $i > l$, since $q \leq q_i$ by definition

$$(\widehat{q}_i)^{k_i} \geq \Big(q_i - \frac{1}{4}(1 - 2^{-1/k})q\Big)^{k_i} \geq \Big(q_i - (1 - 2^{-1/k})q_i\Big)^{k_i} \geq \frac{1}{2^{k_i/k}m} \geq \frac{1}{2m}$$

Since, $l \leq m$, we have $|\{j \mid \widehat{q}_j^{k_j} < \frac{1}{2m}\}| \leq 2m$. This implies $\widehat{m} \leq 2m$.

□

The next lemma provides the confidence bound on the estimate of $\mu_{i,x}$ computed by Algorithm 3 for each i, x .

Lemma D.3
For an action $a_{i,x} \in \mathcal{A}$, at the end of $T/2$ rounds $\mathbb{P}(|\widehat{\mu}_{i,x} - \mu_{i,x}| > \epsilon) \leq \exp\big(-\epsilon^2 \frac{q_i^{k_i} T}{K_{\mathcal{G}}}\big)$, where $K_{\mathcal{G}} \geq 1$ is a constant dependent on the structure of $\mathcal{G}$ but independent of $\mathbb{P}$.

Proof. Using **Theorem 2.5** and **Theorem A.1** in Bhattacharyya et al. [2020], it can be inferred that the learner can estimate $\widehat{\mu}_{i,x}$, such that $|\widehat{\mu}_{i,x} - \mu_{i,x}| \leq \epsilon$, with probability $1-\delta_i$, using $O\big(2^{2u_i^2} \log 2^{2u_i^2} \log \frac{1}{\delta_i}/(q_i^{k_i}\epsilon^2)\big)$ samples, where $u_i = 1 + k_i(d+1)$. Hence using samples $T = K' \frac{2^{2.2u_i^2}}{q_i^{k_i}\epsilon^2} \log \frac{1}{\delta_i}$, where K' is a constant independent of the problem instance, we get, $P(|\widehat{\mu}_{i,x} - \mu_{i,x}| \leq \epsilon) \geq 1 - \delta_i$. Writing δ_i in terms of T and ϵ, and using $K_{\mathcal{G}} = \max\{1, K' 2^{2.2u_i^2}\}$,

$$\mathbb{P}(|\widehat{\mu}_{i,x} - \mu_{i,x}| > \epsilon) \leq \exp\left(-\frac{T}{K'}\frac{q_i^{k_i}\epsilon^2}{2^{2.2u_i^2}}\right) \leq \exp\left(-\epsilon^2 \frac{q_i^{k_i} T}{K_{\mathcal{G}}}\right)$$

Also by A.3, for a_0, by,

$$\mathbb{P}(|\widehat{\mu}_0 - \mu_0| \geq \epsilon) \leq \exp\left(-2\epsilon^2 \frac{T}{2}\right).$$

□

Now we are ready to prove the theorem using the above Lemmas, and let $K = 2^{k-1}K_{\mathcal{G}}$. Let $L_1 = \min_{t\in\mathbb{N}}(4NZe^{-\frac{1}{16}(1-2^{-1/k})^2 q^2 t} \leq \sqrt{\frac{144Km}{t}\log\frac{Nt}{m}})$ and $L_2 = \min_{t\in\mathbb{N}} \frac{6}{N^3}(\frac{m}{t})^4 \leq \sqrt{\frac{16Km}{t}\log\frac{Nt}{m}}$ and we assume throughout the proof that $T \geq \max\{L_1, L_2\}$. Consider $a_{i,x} \in \mathcal{Q}$. By Lemma A.3, and Lemma D.2,

$$\mathbb{P}\big(|\widehat{\mu}_{i,x} - \mu_{i,x}| \geq \epsilon \mid F = 0\big) \leq 2\exp\left(-\epsilon^2 \frac{2T}{4\widehat{m}}\right) \leq 2\exp\left(-\epsilon^2 \frac{T}{4m}\right) \leq 2\exp\left(-\epsilon^2 \frac{T}{4Km}\right)$$

If $a_{i,x} \notin \mathcal{Q}$, and $q_i^{k_i} \geq \frac{1}{m}$, then given $F = 0$ we get,

$$\mathbb{P}\big(|\widehat{\mu}_{i,x} - \mu_{i,x}| > \epsilon \mid F = 0\big) \leq \exp\left(-\epsilon^2 \frac{q_i^{k_i} T}{K_{\mathcal{G}}}\right) \leq \exp\left(-\epsilon^2 \frac{T}{4Km}\right)$$

If $a_{i,x} \notin \mathcal{Q}$, and $q_i^{k_i} < \frac{1}{m}$, then given $F = 0$ from Lemma D.1, $q_i^{k_i} \geq (\widehat{q}_i - \frac{1}{4}(1-2^{-1/k})q)^{k_i} \geq ((\frac{1}{\widehat{m}})^{1/k_i} - \frac{1}{4}(\frac{1}{m})^{1/k_i}))^{k_i} \geq ((\frac{1}{2m})^{1/k_i} - \frac{1}{4}(\frac{1}{m})^{1/k_i}))^{k_i} \geq \frac{1}{2^{k+1}m}$ we get,

$$\mathbb{P}\big(|\widehat{\mu}_{i,x} - \mu_{i,x}| > \epsilon \mid F = 0\big) \leq \exp\left(-\epsilon^2 \frac{q_i^{k_i} T}{K_{\mathcal{G}}}\right) \leq \exp\left(-\epsilon^2 \frac{T}{2^{k+1}K_{\mathcal{G}} m}\right) \leq \exp\left(-\epsilon^2 \frac{T}{4Km}\right)$$

$$\begin{aligned}\mathbb{P}\{\textit{There exists an action } a \textit{ such that } |\widehat{\mu}_a - \mu_a| > \epsilon \mid F = 0\} &\leq (4N+2)\exp\left(-\epsilon^2 \frac{T}{4Km}\right) \\ &\leq 6N\exp\left(-\epsilon^2 \frac{T}{4Km}\right)\end{aligned}$$

Substituting $\epsilon = \sqrt{\frac{16Km}{T}\log\frac{NT}{m}}$, we get,

$$E[r_T \mid F = 0] \leq 2\sqrt{\frac{16Km}{T}\log\frac{NT}{m}} + \frac{6}{N^3}\left(\frac{m}{T}\right)^4 \leq \sqrt{\frac{144Km}{T}\log\frac{NT}{m}}$$

Finally, the expected simple regret of Algorithm 1 is as follows:

$$\begin{aligned}E[r_T] &= E[r_T|F=0]\mathbb{P}(F=0) + E[r_T|F=1]\mathbb{P}(F=1) \\ &\leq E[r_T|F=0] + \mathbb{P}(F=1) \\ &\leq \sqrt{\frac{144Km}{T}\log\frac{NT}{m}} + 4NZe^{-\frac{1}{16}(1-2^{-1/k})^2 q^2 T}\end{aligned}$$

Since $T \geq \max(L_1, L_2)$ the simple regret is $\mathcal{O}\left(\sqrt{\frac{m}{T}\log\frac{NT}{m}}\right)$.

E PROOF OF THEOREM 4.1

Throughout this proof we assume the following terminology: a) a node is a root node if it has not parents, b) a node is a leaf node if it has no children. Consider an n-ary tree $\mathcal{T} \in \mathsf{T}$ on N intervenable nodes. Note that since $\mathcal{T}$ is a tree, each node X_i for $i \in [N]$ has at most one parent. In addition $\mathcal{T}$ has one special node Y, called the outcome. There is a directed from every leaf node in $\mathcal{T}$ to Y, and let $L_{\mathcal{T}}$ be the set of all leaf nodes. We use $\mathbf{V}$ to denote the set of nodes in $\mathcal{T}$, that is, $\mathbf{V} = \{X_1, \ldots, X_N, Y\}$. Without loss of generality, we assume that $X_1, \ldots, X_N$ is in the reverse topological order, that is, X_1 is a leaf node, X_N is a root node, X_{N-1} is either a root node or a child of X_N, and so on. Let $\mathcal{T}_M$ be the sub-graph of $\mathcal{T}$ defined by the nodes $X_1, \ldots, X_M$. An edge belongs to $\mathcal{T}_M$ if both its endpoints belong to $\{X_1, \ldots, X_M\}$. Further, let h be the maximum number of nodes in a (directed) path from a root node to Y. Now we define distributions $\mathbb{P}_0, \ldots, \mathbb{P}_M$ all compatible with $\mathcal{T}$ such that the optimal arm in the CBN $\mathcal{C}_i = (\mathcal{T}, \mathbb{P}_i)$ is $a_{i,1}$ for $i \in [M]$, and for $\mathcal{C}_0 = (\mathcal{T}, \mathbb{P}_0)$ every arm is an optimal arm.

Defining $\mathbb{P}_0$: For X_i not belonging to $\mathcal{T}_M$ let $\mathbb{P}_0(X_i = 1|.) = 0.5$, and for X_i belonging to $\mathcal{T}_M$ and for an appropriately chosen α let

$$
\begin{aligned}
&\mathbb{P}_0(X_i = 1) = \alpha && \text{If } X_i \text{ is a root node,}\\
&\mathbb{P}_0(X_i = 1 \mid \mathbf{Pa}(X_i) = 0) = \alpha && \text{If } X_i \text{ is not a root node,}\\
&\mathbb{P}_0(X_i = 1 \mid \mathbf{Pa}(X_i) = 1) = 1 - \alpha && \text{If } X_i \text{ is not a root node,}\\
&\mathbb{P}_0(Y = 1 \mid .) = 0.5 \quad \mathbb{P}_0(Y = 0 \mid .) = 0.5
\end{aligned}
$$

The value of α is appropriately chosen later to achieve the desired lower bound. Note that in the above equations if X_i is not a root node then $\mathbf{Pa}(X_i)$ is a singleton set. Also, $\mathbb{P}_0(Y = 1|.)$ denotes the probability of $Y = 1$ conditioned on any value of its parents. Next, we define $\mathbb{P}_i$ for $i \in [N]$.

Defining $\mathbb{P}_i$: Let L_i be the set of leaf nodes that are reachable from X_i, that is there is a directed path from X_i to every leaf node in L_i. Note that if X_i is a leaf then $L_i = \{X_i\}$. We use $L_i = \mathbf{1}$ and $L_i = \mathbf{0}$ to denote all nodes in L_i evaluated to 1 and 0 respectively. Also, let $L_{\mathcal{T}}^M$ be the set of all leaves in $\mathcal{T}_M$ and $L_i' = L_{\mathcal{T}}^M \setminus L_i$. Then

$$\mathbb{P}_i(Y|L_i = \mathbf{1}, L_i' = \mathbf{0}) = 0.5 + \epsilon\ .$$

The value of ϵ is appropriately chosen later to achieve the desired lower bound. The distributions of X_i given its parents corresponding to $\mathbb{P}_i$ is the same as those defined for $\mathbb{P}_0$.

We set $\alpha = \min\{(2h|L_{\mathcal{T}}| + 2^{h+1})^{-1}, (2^h|L_{\mathcal{T}}|M)^{-1}\}$ and hence $\alpha < \frac{1}{M}$. Using this it is easy to see that $m(\mathcal{C}_i) = M$ for $i \in [0, M]$ and $M > 4$. Additionally, in $\mathcal{C}_i$ arm $a_{i,1}$ is the optimal arm for $i \in [1, M]$ and the reward for every arm in $\mathcal{C}_0$ is 0.5. We will denote a^* as the optimal arm for every $\mathcal{C}_i$, and note that $a^* = a_{i,1}$ for $\mathcal{C}_i$, where $i \in [M]$. First, in Lemma E.1, we lower bound the regret of returning a sub-optimal arm in $\mathcal{C}_i$ at the end of T rounds. Further, in Lemma E.2, we show that any algorithm would have a non-trivial probability of returning a sub-optimal arm in at least one of the constructed CBNs. Finally, we would use Lemmas E.1 and E.2 to lower bound the expected regret of any algorithm. Let $\text{rew}_i(a_{j,x})$ denote the expected reward of action $do(X_j = x)$ under the distribution $\mathbb{P}_i$. We deviate from the usual notation of μ in this case, because the reward now depends on the arm and the corresponding distribution. We require the following sets in Lemmas E.1 and E.2: $V_1 = L_i \setminus L_j$, $V_2 = L_i \cap L_j$, $V_3 = L_j \setminus L_i$, $V_4 = L_{\mathcal{T}}^M \setminus (L_i \cup L_j)$, and $V_5 = V \setminus L_{\mathcal{T}}^M$.

Lemma E.1
For every $i \in [1, M]$, $j \in [1, N]$, $x \in \{0, 1\}$, and $(j, x) \neq (i, 1)$ the following holds: $\text{rew}_i(a_{i,1}) - \text{rew}_i(a_{j,x}) \geq 0.5\epsilon$.

Proof. For any $i, j \in [M]$, we have

$$\text{rew}_i(a_{i,1}) = 0.5 + \mathbb{P}_i(V_4 = \mathbf{0}, V_1 = \mathbf{1}, V_2 = \mathbf{1}, V_3 = \mathbf{0} \mid do(X_i = 1))(\epsilon) \tag{8}$$
$$\text{rew}_i(a_{j,1}) = 0.5 + \mathbb{P}_i(V_4 = \mathbf{0}, V_1 = \mathbf{1}, V_2 = \mathbf{1}, V_3 = \mathbf{0} \mid do(X_j = 1))(\epsilon) \tag{9}$$

Subtracting Equation 9 from Equation 8 we have

$$
\begin{aligned}
&\text{rew}_i(a_{i,1}) - \text{rew}_i(a_{j,1}) \\
&= \mathbb{P}_i(V_4 = \mathbf{0})\big[\mathbb{P}_i(V_1 = \mathbf{1}, V_2 = \mathbf{1}, V_3 = \mathbf{0} \mid do(X_i = 1)) - \mathbb{P}_i(V_1 = \mathbf{1}, V_2 = \mathbf{1}, V_3 = \mathbf{0} \mid do(X_j = 1))\big]\epsilon \\
&= \mathbb{P}_i(V_4 = \mathbf{0})\big[\mathbb{P}_i(V_3 = \mathbf{0})\mathbb{P}_i(V_1 = \mathbf{1}, V_2 = \mathbf{1} \mid do(X_i = 1)) - \mathbb{P}_i(V_1 = \mathbf{1})P(V_2 = \mathbf{1}, V_3 = \mathbf{0} \mid do(X_j = 1))\big]\epsilon \\
&\underset{(i)}{\geq} (1-\alpha)^{h|V_4|}\big[(1-\alpha)^{h(|L_i|+|V_3|)} - (2^h\alpha)\big]\epsilon \\
&\geq ((1-\alpha)^{h|L_{\mathcal{T}}|} - 2^h\alpha)\epsilon \\
&\geq ((1-h|L_{\mathcal{T}}|\alpha) - 2^h\alpha)\epsilon \\
&\geq 0.5\epsilon
\end{aligned}
$$

(i) in the above equations follows from the definitions of h and $\mathbb{P}_i$. Similarly, it can be shown that $\text{rew}_i(a_{i,1}) - \text{rew}_i(a_{j,0}) \geq 0.5\epsilon$ for $j \in [N]$, and $\text{rew}_i(a_{i,1}) - \text{rew}_i(a_{j,1}) \geq 0.5\epsilon$ for $j \in [M+1, N]$. Also $\text{rew}_i(a_{i,1}) - \text{rew}_i(a_0) \geq 0.5\epsilon$. □

Let ALG be an algorithm that outputs arm a_T at the end of T rounds. We choose $\epsilon = \min\{\frac{1}{4}, \sqrt{\frac{M}{18T}}\}$. Note that corresponding to every $\mathcal{C}_i$ for $i \in [0, M]$, ALG and $\mathbb{P}_i$ together define a probability measure on all the sampled values of the nodes of $\mathcal{T}$ over T rounds. Denote $\mathbb{D}_i$ as this measure and $\mathbb{E}_i$ as the expectation over $\mathbb{D}_i$ for $i \in [0, M]$. Let $\mathcal{G}_t$ be the sampled values of the nodes of $\mathcal{T}$ at time t and let $\mathbf{G}_t = \{\mathcal{G}_1, \ldots, \mathcal{G}_t\}$. Also, for $i \in [0, M]$ let $\mathbb{D}_i(.|\mathbf{G}_{t-1}) = \mathbb{P}_i^t(.)$; here $\mathbb{D}_i(.|\mathbf{G}_{t-1})$ denotes the probability of the sampled values of the nodes of $\mathcal{G}$ conditioned on its history till time $t-1$. Observe that conditioned on history $\mathbf{G}_{t-1}$, ALG determines an arm, say a_t, to pull at time t (either deterministically or in a randomized way), and for $j, j' \in [1, N]$ if $a_t = a_{j,x}$ then $\mathbb{P}_i^t(X_{j'} = x|do(X_j = x)) = \mathbb{P}_i(X_{j'} = x|do(X_j = x))$.

Lemma E.2
For any algorithm ALG *there exists an* $i \in [M]$ *such that* $\mathbb{D}_i\{a_T \neq a_{i,1}\} \geq \frac{\frac{M}{4e}-1}{M}$.

Proof. We use $KL(\mathbb{D}_0, \mathbb{D}_i)$ to denote the KL divergence between $\mathbb{D}_0$ and $\mathbb{D}_i$ for any $i \in [M]$. Let $N_T^{(i,1)}$ be the number of times ALG plays the arm $a_{i,1}$ at the end of T rounds. Also, let $\mathcal{B} = \{a_{i,1} \mid i \leq M \textit{ and } \mathbb{E}_0[N_T^{(i,1)}] \leq 2T/M\}$. Observe that $|\mathcal{B}| \geq M/2$, as otherwise the sum of the expected number of arm pulls of arms not in $\mathcal{B}$ would be greater than T. First, using Lemma 2.6 from Tsybakov [2008], we have,

$$\mathbb{D}_0(a_T = a_{i,1}) + \mathbb{D}_i(a_T \neq a_{i,1}) \geq \frac{1}{2} \cdot \exp\left(-KL(\mathbb{D}_0, \mathbb{D}_i)\right)$$

Rearranging and summing the above equation over arms in $\mathcal{B}$, and observing that $\sum_{a_{i,1} \in \mathcal{B}} \mathbb{D}_0(a_T = a_{i,1}) \leq 1$ we have

$$\sum_{a_{i,1} \in \mathcal{B}} \mathbb{D}_i\{a_T \neq a_{i,1}\} \geq \frac{1}{2} \cdot \sum_{a_{i,1} \in \mathcal{B}} \exp(-KL(\mathbb{D}_0, \mathbb{D}_i)) - 1 \tag{10}$$

Now we bound $\exp(-KL(\mathbb{D}_0, \mathbb{D}_i))$ for every i such that $a_{i,1} \in \mathcal{B}$. Using the chain rule for product distributions (see Auer et al. [1995] and Chapter 2 in Slivkins [2019]) the KL divergence of $\mathbb{D}_0$ and $\mathbb{D}_i$ for any $i \in [M]$ can be written as

$$KL(\mathbb{D}_0, \mathbb{D}_i) = \sum_{t=1}^{T} KL(\mathbb{D}_0(\mathcal{G}_t|\mathbf{G}_{t-1}), \mathbb{D}_i(\mathcal{G}_t|\mathbf{G}_{t-1}) = \sum_{t=1}^{T} KL(\mathbb{P}_0^t(\mathcal{G}_t), \mathbb{P}_i^t(\mathcal{G}_t)) \tag{11}$$

Each term on the right hand side of the above summation can be computed as follows:

$$
\begin{aligned}
KL(\mathbb{P}_0^t, \mathbb{P}_i^t) &= \sum_{\mathbf{v}} \mathbb{P}_0^t(V = \mathbf{v}) \log \frac{\mathbb{P}_0^t(\mathbf{V} = \mathbf{v})}{\mathbb{P}_i^t(\mathbf{V} = \mathbf{v})} \\
&\underset{(i)}{=} \sum_{x, \mathbf{v_5}} \mathbb{P}_0^t(Y = x, L_i = \mathbf{1}, L_i' = \mathbf{0}, V_5 = \mathbf{v_5}) \log \frac{\mathbb{P}_0^t(Y = x | L_i = \mathbf{1}, L_i' = \mathbf{0}, V_5 = \mathbf{v_5})}{\mathbb{P}_i^t(Y = x | L_i = \mathbf{1}, L_i' = \mathbf{0}, V_5 = \mathbf{v_5})} \\
&\underset{(ii)}{=} 0.5 \cdot \mathbb{P}_0^t(L_i = \mathbf{1}, L_i' = \mathbf{0}) \Big[\log \frac{0.5}{0.5 + \epsilon} + \log \frac{0.5}{0.5 - \epsilon} \Big] \\
&\underset{(iii)}{\leq} 0.5 \Big(\mathbb{P}_0^t\{do(X_i = 1)\} + 2^h |L_{\mathcal{T}}| \alpha \Big) \log \frac{0.25}{0.25 - \epsilon^2} \\
&= -0.5 \Big(\mathbb{P}_0^t\{do(X_i = 1)\} + 2^h |L_{\mathcal{T}}| \alpha \Big) \log(1 - 4\epsilon^2) \\
&= 0.5 \Big(\mathbb{P}_0^t\{do(X_i = 1)\} + 2^h |L_{\mathcal{T}}| \alpha \Big) \Big(4\epsilon^2 + \frac{(4\epsilon^2)^2}{2} + \frac{(4\epsilon^2)^3}{3} + \dots \Big) \\
&\leq 6 \Big(\mathbb{P}_0^t\{do(X_i = 1)\} + 2^h |L_{\mathcal{T}}| \alpha \Big) \epsilon^2 \, . \qquad (12)
\end{aligned}
$$

In the above equations: (i) follows by observing that for every other evaluation of $\mathbf{V}$ the distributions $\mathbb{P}_0^t$ and $\mathbb{P}_i^t$ are same hence the corresponding terms in KL divergence amount to zero, (ii) follows from the definitions of $\mathbb{P}_0^t$ and $\mathbb{P}_i^t$, and (iii) follows by observing that

$$
\mathbb{P}_0^t(L_i = \mathbf{1}, L_i' = \mathbf{0}) \leq \mathbb{P}_0^t\{do(X_i = 1)\} + 2^h |L_{\mathcal{T}}| \alpha \, .
$$

Using Equations 11 and 12, we have for every $a_{i,1} \in \mathcal{B}$,

$$
KL(\mathbb{D}_0, \mathbb{D}_i) \leq \sum_{t=1}^{T} 6 \big(\mathbb{E}_0[N_T^{(i,1)}] + 2^h |L_{\mathcal{T}}| \alpha T \big) \epsilon^2 \underset{(i)}{\leq} \frac{18T}{M} \epsilon^2 \leq 1 \, , \qquad (13)
$$

where (i) follows from the definition of $\mathcal{B}$. Finally, using Equations 10 and 13, and $|\mathcal{B}| \geq M/2$, we have

$$
\begin{aligned}
\sum_{a_{i,1} \in \mathcal{B}} \mathbb{D}_i\{a_T \neq a_{i,1}\} &\geq \frac{1}{2} \sum_{a_{i,1} \in \mathcal{B}} \exp(-KL(\mathbb{D}_0, \mathbb{D}_i)) - 1 \\
&\geq \frac{|\mathcal{B}|}{2e} - 1 \\
&\geq \frac{M}{4e} - 1 \, .
\end{aligned}
$$

Therefore as $|\mathcal{B}| \leq M$, by averaging argument there exists an $i \in [M]$ such that

$$
\mathbb{D}_i\{a_T^* \neq a_{i,1}\} \geq \frac{\frac{M}{4e} - 1}{M} \, .
$$

□

From Lemmas E.1 and E.2 for any algorithm ALG, if $\epsilon < \frac{1}{4}$ then the expected simple regret of ALG can be upper bounded as follows

$$
r_{\texttt{ALG}}(T) \geq \mathbb{D}_i\{a_T^* \neq a_{i,1}\} \frac{1}{2} \epsilon \geq \frac{\frac{M}{4e} - 1}{M} \cdot (\frac{1}{2} \epsilon) \geq \frac{\frac{M}{4e} - 1}{2M} \sqrt{\frac{M}{18T}} \, . \qquad (14)
$$

On the contrary, if $\epsilon \geq \frac{1}{4}$ then $M \geq T$, so $\sqrt{M/T} = \Omega(1)$ and regret $r_{\texttt{ALG}}(T) \geq \Omega(1)$. Hence, for any algorithm there exists an $i \in [0, M]$ such that the expected simple regret of the algorithm on $\mathcal{C}_i$ is $\Omega\Big(\sqrt{\frac{m(\mathcal{C}_i)}{T}} \Big)$.

F PROOF OF THEOREM 4.2

We begin by constructing the causal graph $\mathcal{G}$ on $N+1$ nodes $\{X_1, \ldots, X_N, Y\}$, where $N \geq 3$. In $\mathcal{G}$, X_N is the parent of $X_1, \ldots, X_{N-1}$ and there is a directed edge form each node to the outcome node Y. The strategy remains the same as in the proof of Theorem 4.1; Now given $q_1, q_2, \ldots, q_N$, compatible with the graph $\mathcal{G}$, we will construct $\mathbb{P}_0, \ldots, \mathbb{P}_N$ such that on at least one CBN $\mathcal{C}_i = (\mathcal{G}, \mathbb{P}_i)$ the expected simple regret of any algorithm is tight. Also, without loss of generality, assume that $q_1 \leq q_2 \leq \cdots \leq q_N$.

Defining $\mathbb{P}_0$: For all the nodes in the graph $\mathcal{G}$, we define the distribution $\mathbb{P}_0$ as follows:

$$\begin{aligned}
&\mathbb{P}_0(X_N = 1) = q_N \\
&\mathbb{P}_0(X_i = 1 | X_N = 0) = \frac{q_i}{1 - q_N} \\
&\mathbb{P}_0(X_i = 1 | X_N = 1) = \frac{1}{2} \\
&\mathbb{P}_0(Y = 1 | .) = 0.5
\end{aligned}$$

$\mathbb{P}_0(Y = 1|.)$ denotes the probability of $Y = 1$ conditioned on any value of the parents. Also, note that since $q_1, \ldots, q_N$ are compatible with the given graph $\mathcal{G}$, we have, for any $i \neq N$, $q_i = \min_{x_i, x_N} \mathbb{P}_0(X_i = x_i, X_N = x_N) \leq \mathbb{P}_0(X_i = 1, X_N = 1) = q_N/2$. In addition, $\mathbb{P}_0(X_i = 1|X_N = 0) = q_i/(1 - q_N) \leq 2q_i$. Let $M = m(\mathcal{C}_i)$ for all $i \in [N]$ and $M' = M - 1$.

Case a: $M \geq 12$.

Defining $\mathbb{P}_i$: For $i = N$, define $\mathbb{P}_N(Y = 1|X_N = 1) = 0.5 + \epsilon$, and for $i \neq N$, $\mathbb{P}_i(Y = 1|X_i = 1, X_N = 0) = 0.5 + \epsilon$. The remaining conditional distributions are same as those of $\mathbb{P}_0$.

Now, it is easy to see that the optimal action for $\mathbb{P}_i$ is $a_{i,1}$. As in proof of Theorem 4.1, let $\text{rew}_i(a_{j,x})$ denote the expected reward of action $do(X_j = x)$ under the distribution $\mathbb{P}_i$.

Lemma F.1
For every $i \in [M']$, $j \in [N]$, $x \in \{0, 1\}$, and $(j, x) \neq (i, 1)$ the following holds: $\text{rew}_i(a_{i,1}) - \text{rew}_i(a_{j,x}) \geq 0.1\epsilon$.

Proof. For $i = N$, the regret for choosing a sub-optimal arm a is $\text{rew}_N(a_{N,1}) - \text{rew}_N(a) \geq (1 - q_N)\epsilon \geq 0.5\epsilon$. For $i \neq N$, the regret for choosing a sub-optimal arm $a_{j,x}$, where $j \neq N$ is as follows:

$$\begin{aligned}
\text{rew}_i(a_{i,1}) - \text{rew}_i(a_{j,x}) &\geq (1 - q_N)\epsilon - q_i\epsilon \\
&\geq \left(1 - \frac{3q_N}{2}\right)\epsilon \\
&\geq 0.25\epsilon
\end{aligned}$$

For $j = N$, the regret is as follows:

$$\begin{aligned}
&\text{rew}_i(a_{i,1}) - \text{rew}_i(a_{N,0}) = (1 - q_1)\epsilon - \mathbb{P}_i(X_i = 1|X_N = 0)\epsilon \geq (0.5 - 2q_i)\epsilon \\
&\text{rew}_i(a_{i,1}) - \text{rew}_i(a_{N,1}) = (1 - q_1)\epsilon \geq 0.5\epsilon
\end{aligned}$$

Hence, if $q_i \leq 1/M' \leq \frac{1}{5}$, the regret of pulling a sub-optimal arm is 0.1ϵ.

□

Let ALG be an algorithm that outputs arm a_T at the end of T rounds. We choose $\epsilon = \min\{\frac{1}{4}, \sqrt{\frac{M'}{24T}}\}$. For $i \in [N]$, denote $\mathbb{D}_i$ as the measure on all the sampled values of the nodes of $\mathcal{G}$ over T rounds and $\mathbb{E}_i$ as the expectation over $\mathbb{D}_i$. Let $\mathcal{G}_t$ be the sampled values of the nodes of $\mathcal{G}$ at time t and let $\mathbf{G}_t = \{\mathcal{G}_1, \ldots, \mathcal{G}_t\}$. Also, for $i \in [0, M']$ let $\mathbb{D}_i(.|\mathbf{G}_{t-1}) = \mathbb{P}_i^t(.)$. Note that ALG determines the arm a_t conditioned on $\mathbf{G}_{t-1}$ (either in a deterministic or randomized way). Also for $j, j' \in [1, N]$, if $a_t = a_{j,x}$ and $j' \neq j$, then $\mathbb{P}_i^t(X_{j'} = x|do(X_j) = x) = \mathbb{P}_i(X_{j'} = x|do(X_j = x))$.

Lemma F.2
For any algorithm ALG, there exists an $i \in [M']$, such that $\mathbb{D}_i\{a_T \neq a_{i,1}\} \geq \frac{\frac{M'}{4e} - 1}{M'}$.

Proof. We use $KL(\mathbb{D}_0, \mathbb{D}_i)$ to denote the KL divergence between $\mathbb{D}_0$ and $\mathbb{D}_i$ for any $i \in [N]$. Let $N_T^{(i,1)}$ be the number of times ALG plays the arm $a_{i,1}$ at the end of T rounds. Also, let $\mathcal{B} = \{a_{i,1} \mid i \leq M' \textit{ and } \mathbb{E}_0[N_T^{(i,1)}] \leq 2T/M'\}$. Observe that $|\mathcal{B}| \geq M'/2$, as otherwise the sum of the expected number of arm pulls of arms not in $\mathcal{B}$ would be greater than T. First, using Lemma 2.6 from Tsybakov [2008], we have,

$$\mathbb{D}_0(a_T = a_{i,1}) + \mathbb{D}_i(a_T \neq a_{i,1}) \geq \frac{1}{2} \cdot \exp\left(-KL(\mathbb{D}_0, \mathbb{D}_i)\right)$$

Rearranging and summing the above equation over arms in $\mathcal{B}$, and observing that $\sum_{a_{i,1} \in \mathcal{B}} \mathbb{D}_0(a_T = a_{i,1}) \leq 1$ we have

$$\sum_{a_{i,1} \in \mathcal{B}} \mathbb{D}_i\{a_T \neq a_{i,1}\} \geq \frac{1}{2} \cdot \sum_{a_{i,1} \in \mathcal{B}} \exp(-KL(\mathbb{D}_0, \mathbb{D}_i)) - 1 \tag{15}$$

Now we bound $\exp(-KL(\mathbb{D}_0, \mathbb{D}_i))$ for every i such that $a_{i,1} \in \mathcal{B}$. Using the chain rule for product distributions (see Auer et al. [1995] and Chapter 2 in Slivkins [2019]) the KL divergence of $\mathbb{D}_0$ and $\mathbb{D}_i$ for any $i \in [M]$ can be written as

$$KL(\mathbb{D}_0, \mathbb{D}_i) = \sum_{t=1}^{T} KL(\mathbb{D}_0(\mathcal{G}_t|\mathbf{G}_{t-1}), \mathbb{D}_i(\mathcal{G}_t|\mathbf{G}_{t-1}) = \sum_{t=1}^{T} KL(\mathbb{P}_0^t(\mathcal{G}_t), \mathbb{P}_i^t(\mathcal{G}_t)) \tag{16}$$

Now each term in the summation can be written as, for $i \neq N$,

$$\begin{aligned}
&KL(\mathbb{P}_0^t, \mathbb{P}_i^t) \\
&= \sum_{\mathbf{v}} \mathbb{P}_0^t(\mathbf{v}) \log \frac{\mathbb{P}_0^t(\mathbf{v})}{\mathbb{P}_i^t(\mathbf{v})} \\
&= \sum_{y} \mathbb{P}_0^t(Y = y|X_N = 0, X_i = 1)\mathbb{P}_0^t(X_N = 0, X_i = 1) \log \frac{\mathbb{P}_0^t(Y = y|X_N = 0, X_i = 1)}{\mathbb{P}_i^t(Y = y|X_N = 0, X_i = 1)} \\
&= 0.5\mathbb{P}_0^t(X_N = 0, X_i = 1)\left[\log \frac{0.5}{0.5 + \epsilon} + \log \frac{0.5}{0.5 - \epsilon}\right] \\
&\leq 6\mathbb{P}_0^t(X_N = 0, X_i = 1)\epsilon^2
\end{aligned} \tag{17}$$

For $i = N$,

$$\begin{aligned}
KL(\mathbb{P}_0^t, \mathbb{P}_i^t) &= \sum_{\mathbf{v}} \mathbb{P}_0^t(\mathbf{v}) \log \frac{\mathbb{P}_0^t(\mathbf{v})}{\mathbb{P}_i^t(\mathbf{v})} \\
&= \sum_{y} \mathbb{P}_0^t(Y = y|X_N = 1)\mathbb{P}_0^t(X_N = 1) \log \frac{\mathbb{P}_0^t(Y = y|X_1 = 1)}{\mathbb{P}_i^t(Y = y|X_N = 1)} \\
&= 0.5\mathbb{P}_0^t(X_N = 1)\left[\log \frac{0.5}{0.5 + \epsilon} + \log \frac{0.5}{0.5 - \epsilon}\right] \\
&\leq 6\mathbb{P}_0^t(X_N = 1)\epsilon^2
\end{aligned} \tag{18}$$

Using Equation 17 and 18 in equation 16, we get when $q_i \leq \frac{1}{M'}$

$$\begin{aligned}
KL(\mathbb{D}_0, \mathbb{D}_i) &\leq 6\left[\mathbb{E}_0[N_T^{(i,1)}] + \frac{2}{M'}T\right]\epsilon^2 \\
&\leq \frac{24T}{M'}\epsilon^2 \\
&\leq 1
\end{aligned}$$

Now putting the value of $KL(\mathbb{D}_0, \mathbb{D}_i)$ in Equation 15 we get the following,

$$\begin{aligned}\sum_{a_{i,1}\in\mathcal{B}} \mathbb{D}_i\{a_T \neq a_{i,1}\} &\geq \frac{1}{2}\sum_{a_{i,1}\in\mathcal{B}} \exp(-KL(\mathbb{D}_0, \mathbb{D}_i)) - 1 \\ &\geq \frac{|\mathcal{B}|}{2e} - 1 \\ &\geq \frac{M'}{4e} - 1\,.\end{aligned}$$

Therefore as $|\mathcal{B}| \leq M'$, by averaging argument there exists an $i \in [M']$ such that

$$\mathbb{D}_i\{a_T^* \neq a_{i,1}\} \geq \frac{\frac{M'}{4e} - 1}{M'}\,.$$

From Lemmas F.1 and F.2 for any algorithm ALG, if $\epsilon < \frac{1}{4}$ then the expected simple regret of ALG can be upper bounded as follows

$$r_{\texttt{ALG}}(T) \geq \mathbb{D}_i\{a_T^* \neq a_{i,1}\} \cdot (0.1\epsilon) \geq \frac{\frac{M'}{4e} - 1}{M'} \cdot (0.1\epsilon) \geq \frac{\frac{M'}{4e} - 1}{10M'}\sqrt{\frac{M'}{24T}}\,. \tag{19}$$

Otherwise, if $\epsilon \geq \frac{1}{4}$, $M' \geq T$, so $\sqrt{M'/T} = \Omega(1)$ and regret $r_{\texttt{ALG}}(T) \geq \Omega(1)$.

Hence, it is proved that regret is lower bounded by $\Omega\big(\sqrt{\frac{M}{T}}\big)$.

□

Case b: $M < 12$. Define N distributions $\mathbb{P}_1, \ldots, \mathbb{P}_N$ as follows. We choose $\epsilon = \sqrt{\frac{1}{45T}}$. The rest of conditional distributions remain same as $\mathbb{P}_0$. For all $i \in [N]$,

$$\mathbb{P}_i(Y = 1|X_i = 1) = 0.5 + \epsilon$$

Now, the optimal arm for action $\mathbb{P}_i$ is $a_{i,1}$, and the regret of pulling a sub-optimal arm in place of the optimal arm $a_{i,1}$ is $(1 - q_i)\epsilon \geq 0.5 \cdot \epsilon$. Each term in the summation of Equation 16 can be written as

$$\begin{aligned}KL(\mathbb{P}_0^t, \mathbb{P}_i^t) &= \sum_{\mathbf{v}} \mathbb{P}_0(\mathbf{v}) \log \frac{\mathbb{P}_0^t(\mathbf{v})}{\mathbb{P}_i^t(\mathbf{v})} \\ &= \sum_{y} \mathbb{P}_0^t(Y = y|X_i = 1)\mathbb{P}_0^t(X_i = 1) \log \frac{\mathbb{P}_0^t(Y = y|X_i = 1)}{\mathbb{P}_i^t(Y = y|X_i = 1)} \\ &= 0.5\mathbb{P}_0^t(X_i = 1)\left[\log \frac{0.5}{0.5 + \epsilon} + \log \frac{0.5}{0.5 - \epsilon}\right] \\ &\leq 6\mathbb{P}_0^t(X_i = 1)\epsilon^2\end{aligned}$$

Since $\mathbb{P}_0(X_i = 1|.) \leq 0.5$.

$$KL(\mathbb{D}_0, \mathbb{D}_i) \leq 6\left[\mathbb{E}_0[N_T^{(i,1)}] + \frac{T}{2}\right]\epsilon^2 \tag{20}$$

Note that $\mathbb{E}_0[N_T^{(i,1)}] \leq T$

$$KL(\mathbb{D}_0, \mathbb{D}_i) \leq 9T\epsilon^2 \leq 0.2 \tag{21}$$

Now putting the value of $KL(\mathbb{D}_0, \mathbb{D}_i)$ in Equation 15 we get the following,

$$\begin{aligned}\sum_{i\in[N]} \mathbb{D}_i\{a_T \neq a_{i,1}\} &\geq \frac{1}{2}\sum_{i\in[N]} \exp(-KL(\mathbb{D}_0, \mathbb{D}_i)) - 1 \\ &\geq \frac{N}{2e^{0.2}} - 1\,.\end{aligned}$$

Hence any algorithm ALG there exists an i such that the regret incurred by it is

$$r_{\texttt{ALG}}(T) \geq 0.5\mathbb{D}_i(a_T \neq a_{i,1})\epsilon \geq \frac{\frac{N}{2e^{0.2}} - 1}{N}\sqrt{\frac{1}{45T}} \tag{22}$$

Finally, from Equations 19 and 22 it follows that the expected simple regret of any algorithm is $\Omega(\sqrt{\frac{M}{T}})$, where M depends on $\mathbf{q}$ and k_i for $i \in [N]$.

G PROOF OF THEOREM 5.1

Throughout the proof we use a^* to denote the optimal arm. First, we prove a few lemmas, and then use it to bound the expected cumulative regret of CRM−ALG. Recall the definitions of E_t, O_t and C_t^x from Section G. In this section we need to keep the context of which X_i the C_t^x corresponds to, therefore, we refer to it as $C_t^{i,x}$ instead. The following lemma shows that the expectation of $\widehat{\mu}_{i,x}$ as defined in Equation 5 is equal to $\mu_{i,x}$ for every i, x.

Lemma G.1
$\widehat{\mu}_{i,x}(t)$ is an unbiased estimator of $\mu_{i,x}$, that is $\mathbb{E}[\widehat{\mu}_{i,x}(t)] = \mu_{i,x}$. Moreover $\mathbb{P}(|\widehat{\mu}_{i,x}(t) - \mu_{i,x}| \geq \epsilon) \leq 2\exp(-2(N_t^{i,x} + C_t^{i,x})\epsilon^2)$.

Proof. We begin by restating the the definition of $\widehat{\mu}_{i,x}$ from Equation 5.

$$\widehat{\mu}_{i,x}(t) = \frac{\sum_{j \in S_t^{i,x}} \mathbb{1}\{Y_j = 1\} + \sum_{c \in [C_t^{i,x}]} Y_c^{i,x}}{N_t^{i,x} + C_t^{i,x}}$$

We note that in Equation 5, $Y_c^{i,x}$ is a random variable such that $\mathbb{E}[Y_c^{i,x}] = \mu_{i,x}$. Note that this holds because we partition the time steps where arm a_0 was pulled into odd and even instances O_t and E_t.Taking expectation on both sides of the above equation we have

$$\begin{aligned}
&\mathbb{E}[\widehat{\mu}_{i,x}(t)] \\
&= \mathbb{E}\left[\frac{\sum_{j \in S_t^{i,x}} \mathbb{1}\{Y_j = 1\} + \sum_{c \in [C_t^{i,x}]} Y_c^{i,x}}{N_t^{i,x} + C_t^{i,x}}\right] \\
&= \sum_{a=1}^{\infty}\sum_{b=0}^{\infty} \mathbb{E}\left[\frac{\sum_{j \in S_t^{i,x}} \mathbb{1}\{Y_j = 1\} + \sum_{c \in [C_t^{i,x}]} Y_c^{i,x}}{N_t^{i,x} + C_t^{i,x}} \;\middle|\; N_t^{i,x} = a, C_t^{i,x} = b\right]\mathbb{P}(N_t^{i,x} = a, C_t^{i,x} = b) \\
&= \sum_{a=1}^{\infty}\sum_{b=0}^{\infty} \left(\frac{a\mu_{i,x} + b\mu_{i,x}}{a+b}\right)\mathbb{P}(N_t^{i,x} = a, C_t^{i,x} = b) \\
&= \mu_{i,x}\sum_{a=1}^{\infty}\sum_{b=0}^{\infty} \mathbb{P}(N_t^{i,x} = a, C_t^{i,x} = b) \\
&= \mu_{i,x}
\end{aligned}$$

Next we prove the concentration inequality part of the lemma, which is similar to Chernoff-Hoeffding inequality (Lemma A.3) for our estimator.

$$
\begin{aligned}
&\mathbb{P}\Bigg(\frac{\sum_{j\in S_t^{i,x}} \mathbb{1}\{Y_j=1\}+\sum_{c\in[C_t^{i,x}]} Y_c^{i,x}}{N_t^{i,x}+C_t^{i,x}} \geq \mu_{i,x}+\epsilon\Bigg)\\
&=\mathbb{P}\Bigg(\sum_{j\in S_t^{i,x}} \mathbb{1}\{Y_j=1\}+\sum_{c\in[C_t^{i,x}]} Y_c^{i,x} \geq (N_t^{i,x}+C_t^{i,x})\mu_{i,x}+(N_t^{i,x}+C_t^{i,x})\epsilon\Bigg)\\
&\overset{(i)}{\leq} \min_{\lambda>0} E\Bigg[\exp\Big(\lambda(\sum_{j\in S_t^{i,x}}(\mathbb{1}\{Y_j=1\}-\mu_{i,x})+\sum_{c\in[C_t^{i,x}]}(Y_c^{i,x}-\mu_{i,x}))\Big)\Bigg]e^{-\lambda(N_t^{i,x}+C_t^{i,x})\epsilon}\\
&=\min_{\lambda>0} E\Bigg[\prod_{j\in S_t^{i,x}}\exp\big(\lambda(\mathbb{1}\{Y_j=1\}-\mu_{i,x})\big)\prod_{c\in[C_t^{i,x}]}\exp\big(\lambda(Y_c^{i,x}-\mu_{i,x})\big)\Bigg]e^{-\lambda(N_t^{i,x}+C_t^{i,x})\epsilon}\\
&\overset{(ii)}{=} \min_{\lambda>0}\prod_{j\in S_t^{i,x}} E\Bigg[\exp\big(\lambda(\mathbb{1}\{Y_j=1\}-\mu_{i,x})\big)\Bigg]\prod_{c\in[C_t^{i,x}]} E\Bigg[\exp\big(\lambda(Y_c^{i,x}-\mu_{i,x})\big)\Bigg]e^{-\lambda(N_t^{i,x}+C_t^{i,x})\epsilon}\\
&\overset{(iii)}{\leq} \min_{\lambda>0}\exp\Bigg(\frac{N_t^{i,x}\lambda^2}{8}+\frac{C_t^{i,x}\lambda^2}{8}-\lambda(N_t^{i,x}+C_t^{i,x})\epsilon\Bigg)\\
&\leq \exp\left(-2(N_t^{i,x}+C_t^{i,x})\epsilon^2\right)
\end{aligned}
\tag{23}
$$

In the above equations, the inequality in (i) follows from Lemma A.1, the equality in (ii) follows from the fact that each term in the product are independent, and (iii) follows from Lemma A.2. Following the same steps as above we get the following two sided bound

$$
\mathbb{P}(|\widehat{\mu}_{i,x}(t)-\mu_{i,x}|\geq\epsilon)\leq 2\exp\left(-2(N_t^{i,x}+C_t^{i,x})\epsilon^2\right). \tag{24}
$$

□

Next we show that the estimates of μ_a at the end of T rounds is good with high probability.

Lemma G.2
Let $p=\min_{i,x,\mathbf{z}}\mathbb{P}(X_i=x,\mathbf{Pa}(X_i)=\mathbf{z})$. Then for sufficiently large $T\in\mathbb{N}$, at the end of T rounds the following hold:

1. $\mathbb{P}\Big(|\widehat{\mu}_0(T)-\mu_0|\geq\frac{\Delta_0}{4}\Big)\leq 2T^{-\frac{\Delta_0^2}{8}}$.
2. *Let $\widehat{p}_{\mathbf{z},T}^{i,x}=\frac{1}{|O_T|}\sum_{t\in O_T}\mathbb{1}\{X_i(t)=x,\mathbf{Pa}(X_i)(t)=\mathbf{z}\}$, and $\widehat{p}_T^{i,x}=\min_{\mathbf{z}}\widehat{p}_{\mathbf{z},T}^{i,x}$. Then $\mathbb{P}\big(\widehat{p}_T^{i,x}\geq\frac{p}{2}\big)\geq 1-Z_iT^{-\frac{p^2}{4}}$, where Z_i is the size of the domain from which $\mathbf{Pa}(X_i)$ takes values.*
3. $\mathbb{P}\Big(|\widehat{\mu}_{i,x}(T)-\mu_{i,x}|\geq\frac{\Delta_0}{4}\Big)\leq 2T^{-\frac{p\Delta_0^2}{32}}+Z_iT^{-\frac{p^2}{4}}$.

Proof. a) Since $\beta\geq 1$, at the end of T rounds arm a_0 is pulled by Algorithm 2 at least $(\ln T)$ times. Hence, $N_T^0\geq(\ln T)$, and by A.3,

$$
\mathbb{P}\Big(|\widehat{\mu}_0(T)-\mu_0|\geq\frac{\Delta_0}{4}\Big)\leq 2e^{-\frac{\Delta_0^2}{8}\ln T}=2T^{-\frac{\Delta_0^2}{8}}
$$

b) In this part we show, using union bound, that the estimation of $\widehat{p}_T^{i,x}$ being less that $p/2$ have low probability. Since, $|O_T|\geq N_T^0/2$, by Lemma A.3, we have,

$$
\mathbb{P}\Bigg(\widehat{p}_{\mathbf{z},T}^{i,x}>p_{\mathbf{z}}^{i,x}-\frac{p}{2}\geq\frac{p}{2}\Bigg)\geq 1-e^{-2\frac{p^2}{4}\frac{\ln T}{2}}=1-T^{-\frac{p^2}{4}}
$$

Now using this we get,

$$
\mathbb{P}\Bigg(\widehat{p}_T^{i,x}\leq\frac{p}{2}\Bigg)=\mathbb{P}\Bigg(\min_{\mathbf{z}}\widehat{p}_{\mathbf{z},T}^{i,x}\leq\frac{p}{2}\Bigg)\leq\sum_{\mathbf{z}}\mathbb{P}\Bigg(\widehat{p}_{\mathbf{z},T}^{i,x}\leq\frac{p}{2}\Bigg)\leq Z_iT^{-\frac{p^2}{4}} \tag{25}
$$

c) Let the conditional probability distribution $\mathbb{P}(. \mid \widehat{p}_T^{i,x} > \frac{p}{2})$ be denoted by $\mathbb{P}_p$. Since $\beta \geq 1$, $N_T^0 \geq \ln T$. Further if $\widehat{p}_T^{i,x} > \frac{p}{2}$ then $C_T^{i,x} > \frac{p}{2}\frac{N_T^0}{2} \geq \frac{p}{4}\ln T$ (from the definition of $C_T^{i,x}$). Hence, from Lemma G.1 we have

$$\mathbb{P}_p\left(|\widehat{\mu}_{i,x}(T) - \mu_{i,x}| \geq \frac{\Delta_0}{4}\right) \leq 2\exp\left(-\frac{\Delta_0^2}{32}p\ln T\right) = 2T^{-\frac{p\Delta_0^2}{32}} \tag{26}$$

Finally by the law of total probability and using Equations 25 and 26

$$\begin{aligned}\mathbb{P}\left(|\widehat{\mu}_{i,x}(T) - \mu_{i,x}| \geq \frac{\Delta_0}{4}\right) &\leq \mathbb{P}_p\left(|\widehat{\mu}_{i,x}(T) - \mu_{i,x}| \geq \frac{\Delta_0}{4}\right) + \mathbb{P}\left(\widehat{p}_T^{i,x} \leq \frac{p}{2}\right)\\ &\leq 2T^{-\frac{p\Delta_0^2}{32}} + Z_i T^{-\frac{p^2}{4}}\end{aligned}$$

□

Next we show that β as set in `CRM-ALG` is bounded in expectation. Lemma G.3 and its proof is similar to Lemma 8.6 in Nair et al. [2021].

Lemma G.3
Let $L = \arg\min_{t\in\mathbb{N}}\left\{\frac{t^{\frac{p^2\Delta_0^2}{32}}}{\ln t} \geq 3N(Z+3)\right\}$*, where* $Z = \max_i Z_i$*, and suppose* `CRM-ALG` *pulls arms for T rounds, where* $T \geq \max(L, e^{\frac{50}{\Delta_0^2}})$*, and let* $a^* \neq a_0$*. Then at the end of T rounds,* $\frac{8}{9\Delta_0^2} \leq \mathbb{E}[\beta^2] \leq \frac{50}{\Delta_0^2}$.

Proof. Before proceeding to the proof of the lemma we make the following two observations.

Observation G.4
1. If $a^* \neq a_0$ *then* $\Delta_0 = \mu_{a^*} - \mu_0$
2. Let $\widehat{\mu}^* = \max_{i,x}(\widehat{\mu}_{i,x}(T))$*. If* $|\widehat{\mu}_0(T) - \mu_0| \leq \frac{\Delta_0}{4}$ *and* $|\widehat{\mu}_{i,x}(T) - \mu_{i,x}| \leq \frac{\Delta_0}{4}$ *for all* (i,x) *then* $\frac{\Delta_0}{2} \leq \widehat{\mu}_{a^*} - \widehat{\mu}_0(T) \leq \frac{3\Delta_0}{2}$*, and* $\frac{32}{9\Delta_0^2} \leq \beta^2 \leq \frac{32}{\Delta_0^2}$*. Notice that since* $T \geq e^{\frac{50}{\Delta_0^2}}$*,* $\frac{32}{\Delta_0^2} \leq \ln T$.

Let U_0 be the event that $|\widehat{\mu}_0(T) - \mu_0| \leq \frac{\Delta_0}{4}$, and for any i, x let $U_{i,x}$ be the event $|\widehat{\mu}_{i,x}(T) - \mu_{i,x}| \leq \frac{\Delta_0}{4}$. Also let $U = (\cap_{i,x} U_{i,x}) \cap U_0$. If $\overline{U}_0$, $\overline{U}_{i,x}$, and $\overline{U}$ denote the compliment of the events $U_0, U_{i,x}$, and U respectively, then

$$\mathbb{P}(\overline{U}_0) \leq 2T^{-\frac{\Delta_0^2}{8}}\ , \text{ and}$$

$$\text{for a fixed } (i,x) \quad \mathbb{P}(\overline{U}_{i,x}) \leq 2T^{-\frac{p\Delta_0^2}{32}} + Z_i T^{-\frac{p^2}{4}}\ .$$

Hence applying union bound,

$$\begin{aligned}\mathbb{P}(\overline{U}) &\leq 2N\left(\frac{2}{T^{\frac{p\Delta_0^2}{32}}} + \frac{Z}{T^{\frac{p^2}{4}}}\right) + \frac{2}{T^{\frac{\Delta_0^2}{8}}}\\ &\leq 2N\left(\frac{2}{T^{\frac{p^2\Delta_0^2}{32}}} + \frac{Z}{T^{\frac{p^2\Delta_0^2}{32}}}\right) + \frac{2N}{T^{\frac{p^2\Delta_0^2}{32}}} \qquad \text{as } p \leq 1, \Delta_0 \leq 1\\ &\leq \frac{2N(Z+3)}{T^{\frac{p^2\Delta_0^2}{32}}} = \delta\end{aligned}$$

We will use the above arguments to first show that $\mathbb{E}[\beta^2] \geq \frac{8}{9\Delta_0^2}$. From part 2 of Observation we have that the event U implies $\beta^2 \geq \frac{32}{9\Delta_0^2}$. Since $\mathbb{P}\{U\} \geq 1 - \delta$,

$$\mathbb{E}[\beta^2] \geq \frac{32}{9\Delta_0^2}(1-\delta) = \frac{32}{9\Delta_0^2} - \frac{32\delta}{9\Delta_0^2}$$

Since T satisfies $\frac{T^{\frac{p^2\Delta_0^2}{32}}}{\ln T} \geq 3N(Z+3)$, this implies $\frac{32\delta}{9\Delta_0^2} \leq \frac{24}{9\Delta_0^2}$, and hence $\mathbb{E}[\beta^2] \geq \frac{8}{9\Delta_0^2}$. Similarly, from part 2 of Observation we have that the event U implies $\beta^2 \leq \frac{32}{\Delta_0^2}$. If U does not hold then $\beta^2 \leq \ln T$. Hence using the fact that T satisfies $\frac{T^{\frac{p^2\Delta_0^2}{32}}}{\ln T} \geq 3N(Z+3)$, and hence $\delta \ln T \leq \frac{18}{\Delta_0^2}$, we get,

$$\mathbb{E}[\beta^2] \leq \frac{32}{\Delta_0^2}(1-\delta) + \delta \ln T \leq \frac{32}{\Delta_0^2} + \delta \ln T \leq \frac{50}{\Delta_0^2} \ .$$

□

Lemma G.5
Suppose $a^* \neq a_{i,x}$. Then at the end of T rounds the following holds:

$$\mathbb{E}[N_T^{i,x}] \leq \max\left(0, \frac{8\ln T}{\Delta_{i,x}^2} + 1 - \frac{1}{4} \cdot p_{i,x} \cdot \eta_T^{i,x} \cdot \mathbb{E}[N_T^0]\right) + \frac{\pi^2}{3} \ .$$

Further if $a^* \neq a_0$ then

$$\mathbb{E}[N_T^0] \leq \left(\mathbb{E}[\beta^2]\ln T + \frac{8\ln T}{\Delta_0^2} + 1\right) + \frac{\pi^2}{3} \ .$$

Proof. Let $F_T^{i,x} = N_T^{i,x} + C_T^{i,x}$. Then,

$$N_T^{i,x} = \sum_{t \in T} \mathbb{1}\{a_t = a_{i,x}\} \ . \tag{27}$$

$$N_T^{i,x} \leq \max(0, \ell - C_T^{i,x}) + \sum_{t \in T} \mathbb{1}\{a_t = a_{i,x}, F_t^{i,x} \geq \ell\} \tag{28}$$

Here, we make an observation regarding the expected value of $C_T^{i,x}$.

Observation G.6
$\mathbb{E}[C_T^{i,x}] = \mathbb{E}[\min_{\mathbf{z}} \widehat{p}_{\mathbf{z},T}^{i,x} \lceil N_T^0/2 \rceil] \geq \frac{1}{4} \cdot p_{i,x} \cdot \mathbb{E}[N_T^0] \cdot (1 - Z_i T^{-\frac{p_{i,x}^2}{2}}) = \frac{1}{4} \cdot p_{i,x} \cdot \eta_T^{i,x} \cdot \mathbb{E}[N_T^0]$

Proof. Note that the expectation of $\min_{\mathbf{z}} \widehat{p}_{\mathbf{z},T}^{i,x}$ is over the distribution of the CBN and that of N_T^0 over the distribution in the observation across all T rounds. Recall $p_{i,x} = \min_{\mathbf{z}} p_{\mathbf{z}}^{i,x}$. By Lemma A.3, we have,

$$\mathbb{P}\left(\widehat{p}_{\mathbf{z},T}^{i,x} > p_{\mathbf{z}}^{i,x} - \frac{p_{i,x}}{2} \geq \frac{p_{i,x}}{2}\right) \geq 1 - e^{-2\frac{p_{i,x}^2}{4}\frac{\ln T}{2}} = 1 - T^{-\frac{p_{i,x}^2}{4}}$$

Now using this we get,

$$\mathbb{P}\left(\widehat{p}_T^{i,x} \leq \frac{p_{i,x}}{2}\right) \leq \mathbb{P}\left(\min_{\mathbf{z}} \widehat{p}_{\mathbf{z},T}^{i,x} \leq \frac{p_{i,x}}{2}\right) \leq \sum_{\mathbf{z}} \mathbb{P}\left(\widehat{p}_{\mathbf{z},T}^{i,x} \leq \frac{p_{i,x}}{2}\right) \leq Z_i T^{-\frac{p_{i,x}^2}{4}}$$

We can now bound the expectation of $C_T^{i,x}$ for sufficiently large T as follows:

$$\begin{aligned}
\mathbb{E}[\min_{\mathbf{z}} \widehat{p}^{i,x}_{\mathbf{z},T} \lceil N_T^0/2 \rceil] &\geq \frac{1}{2}\mathbb{E}[\min_{\mathbf{z}} \widehat{p}^{i,x}_{\mathbf{z},T} N_T^0] \\
&= \frac{1}{2}\sum_{a=1}^{\infty} a \cdot \mathbb{E}[\min_{\mathbf{z}} \widehat{p}^{i,x}_{\mathbf{z},T} \mid N_T^0 = a]\mathbb{P}(N_T^0 = a) \\
&\geq \frac{1}{2}\sum_{a=1}^{\infty} a \cdot \frac{p_{i,x}}{2} \cdot \mathbb{P}\left(\min_{\mathbf{z}} \widehat{p}^{i,x}_{\mathbf{z},T} > \frac{p_{i,x}}{2} \mid N_T^0 = a \right)\mathbb{P}(N_T^0 = a) \\
&\geq \frac{1}{2}\sum_{a=1}^{\infty} a \cdot \frac{p_{i,x}}{2} \cdot \mathbb{P}\left(\min_{\mathbf{z}} \widehat{p}^{i,x}_{\mathbf{z},T} > \frac{p_{i,x}}{2} \mid N_T^0 = a \right)\mathbb{P}(N_T^0 = a) \\
&\geq \frac{p_{i,x}}{4}\mathbb{E}[N_T^0] \cdot \max\left\{0, 1 - Z_i T^{-\frac{p_{i,x}^2}{4}}\right\} \\
&= \frac{1}{4} \cdot p_{i,x} \cdot \eta_T^{i,x} \cdot \mathbb{E}[N_T^0]
\end{aligned} \tag{29}$$

□

Taking expectation of Equation 28, we get

$$\mathbb{E}[N_T^{i,x}] \leq \max\left\{0, \ell - \frac{p_{i,x}}{4} \cdot \eta_T^{i,x} \cdot \mathbb{E}[N_T^0]\right\} + \sum_{t \in [\ell+1,T]} \mathbb{P}(a_t = a_{i,x}, F_t^{i,x} \geq \ell) \tag{30}$$

Now we bound $\sum_{t\in[l+1,T]} \mathbb{P}(a(t) = a_{i,x}, F_t^{i,x} \geq \ell)$, and assuming $a^* \neq a_0$. The proof for $a^* = a_0$ is similar. We use $F_T^{a^*}$ to denote the effective number of pulls of a^* at the end of T rounds. Also, for better clarity, we use $\widehat{\mu}_{i,x}(F_T^{i,x}, T)$ (instead of $\widehat{\mu}_{i,x}(T)$) and $\widehat{\mu}_0(N_T^0, T)$ (instead of $\widehat{\mu}_0(T)$) to denote the empirical estimates of $\mu_{i,x}$ and μ_0 computed by Algorithm 2 at the end of T rounds.

$$\begin{aligned}
&\sum_{t\in[\ell+1,T]} \mathbb{P}\left(a_t = a_{i,x}, F_t^{i,x} \geq \ell \right) \\
&= \sum_{t\in[\ell,T-1]} \mathbb{P}\left(\widehat{\mu}_{a^*}(F_t^{a^*}, t) + \sqrt{\frac{2\ln t}{F_t^{a^*}}} \leq \widehat{\mu}_{i,x}(F_t^{i,x}, t) + \sqrt{\frac{2\ln(t)}{F_t^{i,x}}},\ \ F_t^{i,x} \geq \ell \right) \\
&\leq \sum_{t\in[0,T-1]} \mathbb{P}\left(\min_{s\in[0,t]} \widehat{\mu}_{a^*}(s,t) + \sqrt{\frac{2\ln t}{s}} \leq \max_{s_j\in[\ell-1,t]} \widehat{\mu}_{i,x}(s_j,t) + \sqrt{\frac{2\ln t}{s_j}} \right) \\
&\leq \sum_{t\in[T]} \sum_{s\in[0,t-1]} \sum_{s_j\in[\ell-1,t]} \mathbb{P}\left(\widehat{\mu}_{a^*}(s,t) + \sqrt{\frac{2\ln t}{s}} \leq \widehat{\mu}_{i,x}(s_j,t) + \sqrt{\frac{2\ln t}{s_j}} \right)
\end{aligned}$$

If $\widehat{\mu}_{a^*}(s,t) + \sqrt{\frac{2\ln t}{s}} \leq \widehat{\mu}_{i,x}(s_j,t) + \sqrt{\frac{2\ln t}{s_j}}$ is true then at least one of the following events is true

$$\widehat{\mu}_{a^*}(s,t) \leq \mu_{a^*} - \sqrt{\frac{2\ln t}{s}}\ , \tag{31a}$$

$$\widehat{\mu}_{i,x}(s_j,t) \geq \mu_{i,x} + \sqrt{\frac{2\ln t}{s_j}}\ , \tag{31b}$$

$$\mu_{a^*} \leq \mu_{i,x} + 2\sqrt{\frac{2\ln t}{s_j}}\ . \tag{31c}$$

The probability of the events in Equations 31a and 31b can be bounded using Chernoff-Hoeffding inequality

$$\mathbb{P}\left\{\widehat{\mu}_{a^*}(s,t) \leq \mu_{a^*} - \sqrt{\frac{2\ln t}{s}}\right\} \leq t^{-4} \ ,$$

$$\mathbb{P}\left\{\widehat{\mu}_{i,x}(s_j,t) \geq \mu_{i,x} + \sqrt{\frac{2\ln t}{s_j}}\right\} \leq t^{-4} \ .$$

Also if $\ell \geq \lceil \frac{8\ln T}{\Delta_{i,x}^2} \rceil$ then the event in Equation 31c is false, i.e. $\mu_{a^*} > \mu_{i,x} + 2\sqrt{\frac{2\ln t}{s_j}}$. Thus for $\ell = \frac{8\ln T}{\Delta_{i,x}^2} + 1 \geq \lceil \frac{8\ln T}{\Delta_{i,x}^2} \rceil$, which implies

$$\sum_{t\in[\ell+1,T]} \mathbb{P}\{a(t) = a_{i,x}, F_t^{i,x} \geq \ell\} \leq \sum_{t\in[T]} \sum_{s\in[0,t-1]} \sum_{s_j\in[\ell-1,t]} 2t^{-4} \leq \frac{\pi^2}{3} \tag{32}$$

If $a^* = a_0$ then using the exact arguments as above we can show that Equation 32 still holds. Hence, using Equations 30 and 32 we have if $a^* \neq a_{i,x}$ then

$$\mathbb{E}[N_T^{i,x}] \leq \max\left\{0, \frac{8\ln T}{\Delta_{i,x}^2} + 1 - \frac{p_{i,x}}{4} \cdot \eta_T^{i,x} \cdot \mathbb{E}[N_T^0]\right\} + \frac{\pi^2}{3} \ .$$

The arguments used to bound $\mathbb{E}[N_T^0]$, when $a^* \neq a_0$ is similar. In this case the equation corresponding to Equation 30 is

$$\mathbb{E}[N_T^0] \leq \mathbb{E}[\beta^2]\ln T + \ell + \sum_{t\in[\ell+1,T]} \mathbb{P}\{a(t) = a_0, N_t^0 \geq \ell\} \ . \tag{33}$$

Also the same arguments as above can be used to show that for $\ell = \frac{8\ln T}{\Delta_0^2} + 1$,

$$\sum_{t\in T} \mathbb{P}\{a(t) = a_0, N_t^0 \geq \ell\} \leq \frac{\pi^2}{3} \ . \tag{34}$$

Finally using Equations 33 and 34, we have

$$\mathbb{E}[N_T^0] \leq \left(\mathbb{E}[\beta^2]\ln T + \frac{8\ln T}{\Delta_0^2} + 1\right) + \frac{\pi^2}{3} \ .$$

Lemma G.7
If $a^* = a_0$ then at the end of T rounds the following is true:

$$\mathbb{E}[N_T^0] \geq T - \left(2N(1 + \frac{\pi^2}{3}) + \sum_{i,x} \frac{8\ln T}{\Delta_{i,x}^2}\right) \ .$$

Proof. At the end of T rounds we have

$$N_T^0 + \sum_{i,x} N_T^{i,x} = T \ .$$

Taking expectation on both sides of the above equation and rearranging the terms we have,

$$\mathbb{E}[N_T^0] = T - \sum_{i,x} \mathbb{E}[N_T^{i,x}] \ .$$

Now we use Lemma G.5 to conclude that

$$\mathbb{E}[N_T^0] \geq T - \left(2N(1 + \frac{\pi^2}{3}) + \sum_{i,x} \frac{8\ln T}{\Delta_{i,x}^2}\right) \ .$$

□

Now that we have bounds on $\mathbb{E}[N_T^0]$ and $\mathbb{E}[N_T^{i,x}]$, we can bound the regret as follows.

Case a ($a^* = a_0$): In this case we bound the expected cumulative regret of Algorithm 2. From Lemma G.5 and G.7 for any T satisfying both $T^{-\frac{p_{i,x}^2}{4}} > Z_i$ and

$$T \geq \frac{4}{p_{i,x} \cdot \eta_T^{i,x}} \left(1 + \frac{8 \ln T}{\Delta_{i,x}^2}\right) + \left(2N(1 + \frac{\pi^2}{3}) + \sum_{i,x} \frac{8 \ln T}{\Delta_{i,x}^2}\right) \tag{35}$$

we have $\mathbb{E}[N_T^{i,x}] \leq \frac{\pi^2}{3}$. Notice that Equation 35 holds for sufficiently large T. Hence the cumulative regret caused by pulling sub-optimal arms $a_{i,x}$ is

$$\mathbb{E}[R(T)] \leq \sum_{\Delta_a > 0} \Delta_a \frac{\pi^2}{3} \tag{36}$$

Case b ($a^* \neq a_0$): In this case we bound the regret of pulling sub-optimal arms when $T \geq \max(L, e^{\frac{50}{\Delta_0^2}})$, where L is as defined in Lemma G.3. Note that this is satisfied for sufficiently large T. Hence from Lemma G.3 and Lemma G.5, we have for $a^* \neq a_{i,x}$ and for a_0

$$\mathbb{E}[N_T^{i,x}] \leq \max\left\{0, 1 + 8 \ln T \left(\frac{1}{\Delta_{i,x}^2} - \frac{p_{i,x} \cdot \eta_T^{i,x}}{36 \Delta_0^2}\right)\right\} + \frac{\pi^2}{3} \tag{37}$$

$$\mathbb{E}[N_T^0] \leq \frac{58 \ln T}{\Delta_0^2} + 1 + \frac{\pi^2}{3} \tag{38}$$

Hence the cumulative regret can be written as

$$\mathbb{E}[R(T)] \leq \Delta_0 \left(\frac{58 \ln T}{\Delta_0^2} + 1 + \frac{\pi^2}{3}\right) + \sum_{\Delta_{i,x} > 0} \Delta_{i,x} \left(\max\left\{0, 1 + 8 \ln T \left(\frac{1}{\Delta_{i,x}^2} - \frac{p_{i,x} \cdot \eta_T^{i,x}}{36 \Delta_0^2}\right\}\right) + \frac{\pi^2}{3}\right) \tag{39}$$

□

H ADDITIONAL EXPERIMENTS

In this section, we provide three additional experiments. In Experiment 3, we compare the simple regret of `SRM-ALG` with baselines `UE` and `SR` as m increases. In Experiment 4 we compare `SRM-ALG` with a simple regret minimization algorithm `CB` (referred to as Propagating Inference in figures), given in Algorithm 3 in Yabe et al. [2018] and in Experiment 5, we compare `CRM-ALG` with `UCB` in situations where observational arm is not the best arm.

We mention few issues faced while implementing `CB` using the details from Yabe et al. [2018] and how we resolved them: (a) In Step (3) of Algorithm 1 in Yabe et al. [2018] (which is a subroutine for `CB`), they iterate over all possible assignments to the parents of each node. Specifically, the algorithm would be exponential time in the in-degree of the reward node Y and therefore it runs efficiently only when Y has a small number of parents. `SRM-ALG` does not face this issue. To compare both algorithms we therefore created instances where in-degree of Y was small. (b) Another issue faced while implementing their algorithm is in an inequality condition specified in Equation 4 of Yabe et al. [2018]. We observe that this inequality is trivially satisfied unless the time period becomes very large (of the order of $\geq 10^{10}$) even for their experiments given in Section 5 of Yabe et al. [2018]. Since running the algorithms for such a long time period is not feasible, we run both algorithms till we see clear convergence of `SRM-ALG`. (c) A third problem we faced was in setting the time period range for our experiments. They use $T \in \{C, 2C, \ldots, 9C\}$, but in Step 3 of Algorithm 1 and Step 4 of Algorithm 2 in Yabe et al. [2018], they estimate probabilities using $T/3C$ samples. This would leave them with at most 3 samples for such an estimation which would give noisy and unreliable estimates. Instead of using this set of values for T, we use equally spaced points in a time range where we see clear convergence of `SRM-ALG` (d) Finally, it is not discussed how the optimization problem giving $\widehat{\eta}$ in Step 12 of Algorithm 2 of Yabe et al. [2018] is solved, and in the experiments they use a fixed value for $\widehat{\eta}$. Since there is no technique proposed to solve the optimization problem, we also use the same fixed $\widehat{\eta}$ that they used.

Experiment 3 **(Regret vs. m):** This experiment compares the expected simple regret of SRM−ALG with UE and SR for CBNs with different values of function m from the set $M = \{10 + 2k : k \in [20]\}$. For this experiment, we fix the time horizon to $T = 1600$. We randomly generate 35 DAGs on $N + 1$ nodes $X_1, \ldots, X_N$ and Y. For each generated DAG $\mathcal{G}$ and $m \in M$, we use the same process as Experiment 1 to set the CPDs of $\mathcal{G}$. For each of the 35 random CBNs thus obtained, we run SRM−ALG, MAB, SR for time horizon T and average the regret over 100 independent runs. We repeat this experiment for $N = 100$ and $N = 200$. For $N = 100$, we plot the mean regret over all the 35 random CBNs vs. m in Fig. 4. The same plot for $N = 200$ is provided in Fig. 5. Our plots validate the $\sqrt{m}$ dependence of regret (for fixed T) in the case of SRM−ALG. From these plots, we can notice that as N increases, regret of SRM−ALG remains the same i.e. only depends on m (as shown in Theorem 3.1), whereas regret of MAB and SR increases as expected from their regret guarantees given above. So for larger values of N, SRM−ALG becomes strictly better in terms of regret even for a wide range of values of m.

Experiment 4 **(Comparison with Yabe et al. [2018]):** This experiment compares the expected simple regret of SRM−ALG with CB as T increases. We run the algorithms on 50 CBNs such that for every constructed CBN $\mathcal{C}$, it has 10 intervenable nodes and $m(\mathcal{C}) = 5$. The CBNs are constructed as follows: a) randomly generate 50 DAGs on 11 nodes $X_1, \ldots, X_{10}$ and Y, and let $X_1 \prec \ldots \prec X_{10} \prec Y$ be the topological order in each such DAG, b) $\mathbf{Pa}(X_i)$ contains at most 1 node chosen uniformly at random from $X_1, \ldots, X_{i-1}$, and $\mathbf{Pa}(Y) = \{X_6, \ldots, X_10\}$, c) $\mathbb{P}(X_i \mid \mathbf{Pa}(X_i)) = 0.5$ for $i \in [5]$ and $\mathbb{P}(X_i|\mathbf{Pa}(X_i)) = 1/10$ for $i \in [6, 10]$, d) uniformly at random choose a X_j from $\mathbf{Pa}(Y)$ and set the CPD of Y as $\mathbb{P}(Y|\ldots, X_j = 1, \ldots) = 0.5 + \epsilon$ and $\mathbb{P}(Y|\ldots, X_j = 0, \ldots) = 0.5 - \epsilon'$ where $\epsilon = 0.3$ and $\epsilon' = q\epsilon/(1 - q)$ for $q = 1/10$. The choice of the conditional probability distributions (CPDs) in (c) ensures $m(\mathcal{C}) = 5$ for every CBN $\mathcal{C}$ that is generated. We note that the above strategy to generate CBNs is a generalization of of the one used in Lattimore et al. [2016] to define parallel bandit instances with a fixed m. For each of the 50 random CBN, we run SRM−ALG and CB for multiple values of the time horizon T in $[500, 2500]$ and average the regret over 30 independent runs. Finally, we calculate the mean regret over all the 50 random CBNs and plot mean regret vs. T in Fig. 6. As seen in the Fig. 6, SRM−ALG has a much lower regret as compared to CB which incurs a regret of $\tilde{O}(\sqrt{N/T})$ in comparison to SRM−ALG's regret of $\tilde{O}(\sqrt{m/T})$ that was proved in Theorem 3.1.

Experiment 5 **(Cumulative Regret vs. T, General Case):** This experiment compares the cumulative regret of CRM−ALG with UCB as T increases. The algorithms are run on 12 CBNs such that for every constructed CBN $\mathcal{C}$, it has 10 intervenable nodes. The CBNs are constructed as follows: a) randomly generate 12 DAGs on 11 nodes $X_1, \ldots, X_{10}$ and Y, and let $X_1 \prec \ldots \prec X_{10} \prec Y$ be the topological order in each such DAG, b) $\mathbf{Pa}(X_i)$ contains at most 1 node chosen uniformly at random from $X_1, \ldots, X_{i-1}$, and $\mathbf{Pa}(Y)$ contains X_i for all i, c) $\mathbb{P}(X_i \mid \mathbf{Pa}(X_i)) = 0.5$ for $i \in [10]$ and, d) uniformly at random choose a X_j from $\mathbf{Pa}(Y)$ and set the CPD of Y as $\mathbb{P}(Y|\ldots, X_j = 1, \ldots) = 0.5 + \epsilon$ and $\mathbb{P}(Y|\ldots, X_j = 0, \ldots) = 0.5 - \epsilon'$ where $\epsilon = 0.1$ and $\epsilon' = q\epsilon/(1 - q)$ for $q = 1/2$, that is an interventional arm is the best arm. We run CRM−ALG and UCB for a sufficiently large T and average the cumulative regrets over 30 independent runs. Fig. 7 demonstrates that cumulative regret of CRM−ALG gets better compared to that of UCB for large enough T as expected by result in Theorem 5.1.

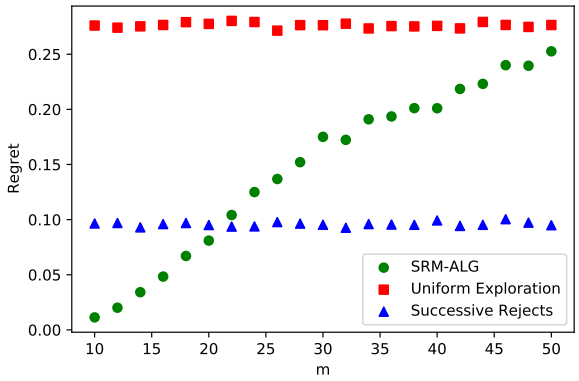

Figure 4: Regret vs m, $N = 100$

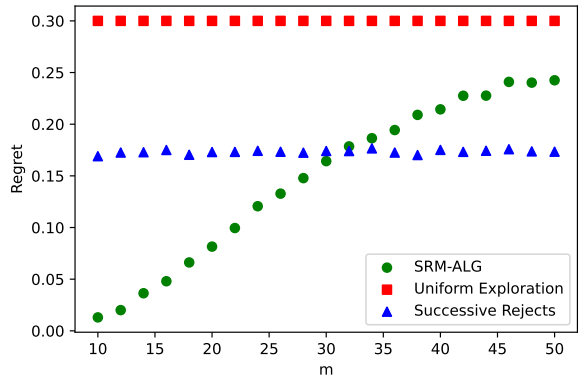

Figure 5: Regret vs m, $N = 200$

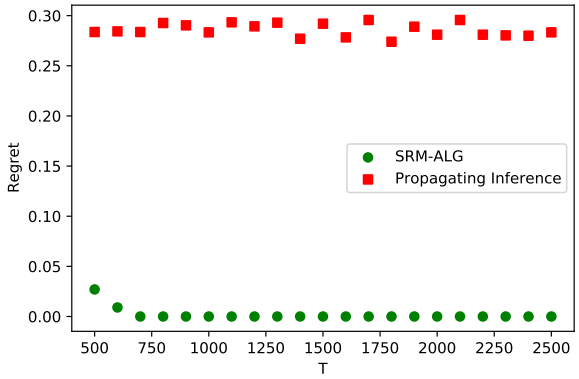

Figure 6: Simple Regret vs T

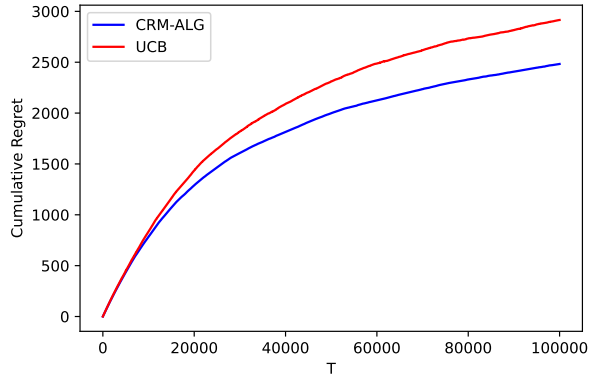

Figure 7: Cumulative Regret vs T