Intervention Efficient Algorithm for Two-Stage Causal MDPs

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Abstract

We study Markov Decision Processes (MDP) wherein states correspond to causal graphs that stochastically generate rewards. In this setup, the learner’s goal is to identify atomic interventions that lead to high rewards by intervening on variables at each state. Generalizing the recent causal-bandit framework, the current work develops (simple) regret minimization guarantees for two-stage causal MDPs, with parallel causal graph at each state. We propose an algorithm that achieves an instance dependent regret bound. A key feature of our algorithm is that it utilizes convex optimization to address the exploration problem. We identify classes of instances wherein our regret guarantee is essentially tight, and experimentally validate our theoretical results.

1 Introduction

Recent years have seen an active interest in causal reinforcement learning. In this thread of work, a fundamental model is that of causal bandits [BFP15, LLR16, SSDS17, LB18, YHS+18, LB19, NPS21]. In the causal bandits setting, one assumes an environment comprising of causal variables that influence an outcome of interest; specifically, a reward. The goal of a learner then is to maximize her reward by intervening on certain variables (i.e., by fixing the values of certain variables). Note that the reward is assumed to be dependent on the values that the causal variables take, and the causal variables themselves may influence each other. The relationship between these causal variables is typically expressed via a directed acyclic graph (DAG), which is referred to as the causal graph [Pea09].

Of particular interest are causal settings wherein the learner is allowed to perform atomic interventions. Here, at most one causal variable can be set to a particular value, while other variables take values in accordance with their underlying distributions. Prominent results in the context of atomic interventions include [CB20] and [BGK+20].

It is relevant to note that when a learner performs an intervention in a causal graph, she gets to see

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the values that all the causal variables took. Hence, the collective dependence of the reward on the variables is observed through each intervention. That is, from such an observation, the learner may be able to make inferences about the (expected) reward under other values for the causal variables [PJS17]. In essence, with a single intervention, the learner is allowed to intervene on a variable (in the causal graph), allowed to observe all other variables, and further, is privy to the effects of such an intervention. Indeed, such an observation in a causal graph is richer than a usual sample from a stochastic process. Hence, a standard goal in causal bandits (and causal reinforcement learning, in general) is to understand the power and limitations of interventions. This goal manifests in the form of developing algorithms that identify intervention(s) that lead to high rewards, while using as few observations/interventions as possible. We use the term intervention complexity (rather than sample complexity) for our algorithm, to emphasize the point that in causal reinforcement learning one deals with a richer class of observations.

Addressing causal bandits, the notable work of Lattimore et al. [LLR16] obtains an intervention-complexity bound with a focus on atomic interventions and parallel causal graphs. While the causal bandit framework provides a meaningful (causal) extension of the classic multi-armed bandit setting, it is still not general enough to directly capture settings wherein one requires multiple states to model the environment. Specifically, causal bandits, as is, do not carry the same modelling prowess as Markov decision processes (MDP). Motivated, in part, by this consideration, recent works in causal reinforcement learning have generalized causal bandits to causal MDPs, see, e.g., [LMTY20].

The current work contributes to this thread of work and extends the causal bandit framework of Lattimore et al. [LLR16]. In particular, we develop results for two-stage causal MDPs (see Figure 1a). Such a setup is general enough to address the fact that underlying environment states can evolve, as in an MDP, while simultaneously utilizing (causal) aspects from the causal bandit setup.

We now provide a stylized example that highlights the applicability of the two-stage model. Consider a patient who visits a doctor with certain medical issues. The patient may arrive with a combination of symptoms and lifestyle factors. Some of these may include immediate symptoms, such as fever, but may also include more complex lifestyle factors, e.g., a sedentary routine or smoking. On observing the patient and before prescribing an invasive procedure, the doctor may consider prescribing certain lifestyle changes or milder medicines. This initial intervention can then lead to the patient evolving to a new set of symptoms. At this point, with fresh symptoms and lifestyle factors (i.e., in the second stage of the MDP), the doctor can finalize a course of medication. Such an interaction can be modelled as a two-stage causal MDP, and is not directly captured by the causal bandit framework. Also, the outcome of whether the patient is cured, or not, corresponds to a 0-1 reward for the interventions chosen by the doctor.

1.1 Additional Related Work

An extension to the earlier literature on causal bandits—towards causal MDPs—was proposed by Lu et al. [LMTY20]. This work considers a causal graph at each state of the MDP. Furthermore, in this model, along with the rewards, the state transitions are also (stochastically) dependent on the causal variables. We address a similar model in our two-stage causal MDP, wherein the state transitions
as well as the rewards are functions of the causal variables. It is, however, relevant to note that in [LMTY20] it is assumed that the MDP can be initialized to any state. The work of Azar et al. [AOM17] also conforms to this assumption. Hence, while these two results address a more general MDP setup (than the two-stage one), their results are not directly applicable in the current context wherein the MDP always starts at a specific state and transitions based on the chosen interventions. Indeed, the assumption that the MDP can be initialized arbitrarily might not hold in real-world domains, such as the medical-intervention example mentioned above.

Sachidananda and Brunskill [SB17] propose a Thompson-Sampling based model in a causal bandit setting to minimize cumulative regret. Nair et al. [NPS21] study the problem of online causal learning to minimize expected cumulative regret under the setting of no-backdoor graphs. They also supply an algorithm for expected simple regret minimization in the causal bandit setting with non-uniform costs associated with the interventions.

Much of the literature in causal learning assumes the causal graph structure is known. In more general settings, learning the causal graph structure is an important sub-problem; for relevant contributions to the problem of causal graph learning see [SKDV15, KSB17, KDV17], and references therein. Lu et al. [LMT21] and Maiti et al. [MNS21] extend this to the causal bandit problem. Further, under many circumstances, the structure of the causal graph can be learnt externally, or via some form of hypothesis testing [ABDK18].

The current work contributes to the growing body of work on causal reinforcement learning by developing intervention-efficient algorithms for finding near-optimal policies. We focus on simple regret minimization (i.e., near optimal policy identification) in causal MDPs.

1.2 Our Contributions

Our main contributions are summarized next.

We formulate and study two-stage causal MDPs, which encompass many of the issues that arise when considering extensions from bandits to general MDPs. At the same time, the current setup is structured enough to be amenable to a thorough analysis. A notable feature of our setting is that we do not assume that the learner has ready access to all the states, and has to rely on the transitions to reach certain states.

Here, we develop and analyze an algorithm for finding (near) optimal intervention policies. The algorithm’s objective is to minimize simple regret in an intervention efficient manner. We focus on causal MDPs wherein the nonzero transition probabilities are sufficiently high and show that, interestingly, the intervention complexity of our algorithm depends on an instance dependent structural parameter—referred to as $\lambda$ (see equation (1))—rather than directly on the number of interventions or states (Theorem 1).

Notably, our algorithm uses a convex program to identify optimal interventions. Using convex optimization to design efficient explorations is a distinguishing feature of the current work. The algorithm spends some time of the given budget learning the MDP parameters (e.g., the transition probabilities).
After this, it solves an optimization problem to design efficient exploration of the causal graphs at various states. Such an optimization problem gives rise to the structural parameter, $\lambda$, of the causal MDP instance. We note that the parameter $\lambda$ can be significantly smaller than, say, the total number of interventions in the causal MDP, as demonstrated by our experiments (see Section 5).

In fact, we provide a lower bound showing that our algorithm’s regret guarantee is tight (up to a log factor) for certain classes of two-stage causal MDPs (see Section 4).

2 Notation and Preliminaries

We consider a Markov decision process (MDP) that starts at state 0, transitions to one of $k$ states $[k] = \{1, \ldots, k\}$, receives a reward, and then finally terminates at state $S_t$; see Figure 1a. At each state $\{0, 1, \ldots, k\}$, there is a causal graph along the lines of the ones studied in [LLR16]; see Figure 1b. In particular, at state $i \in \{0, 1, \ldots, k\}$, the causal graph is composed of $n$ independent Bernoulli variables $\{X^i_1, \ldots, X^i_n\}$. For each $X^i_j \in \{0, 1\}$, the associated probability $q^i_j := P\{X^i_j = 1\}$.

In the MDP, for each state $i \in \{0, \ldots, k\}$, all the variables $X^i_1, \ldots, X^i_n$, are observable. Furthermore, we are allowed atomic interventions, i.e., we can select at most one variable and set it to either 0 or 1. We will use $I_i$ to denote the set of atomic interventions available at state $i \in \{0, \ldots, k\}$; in particular, $I_i = \{do()\} \cup \{do(X^i_j = 0), do(X^i_j = 1) : j \in [n]\}$. We note that $do()$ is an empty intervention that allows all the variables to take values from their underlying (Bernoulli) distributions. Also, $do(X^i_j = 0)$ and $do(X^i_j = 1)$ set the value of variable $X^i_j$ to 0 and 1, respectively, while leaving all the other variables to independently draw values from their respective distributions. Note that for all $i \in [k]$, we have $|I_i| = 2n + 1$. Write $N := 2n + 1$.

The model provides us with a $\{0, 1\}$ reward as we transition to the terminal state $S_t$ from an intermediate state. Depending on the state $i \in [k]$, from where we transition to $S_t$, we label the reward as $R_i$. Note that the reward $R_i$ stochastically depends on the variables $X^i_1, \ldots, X^i_n$; in particular, for all $j \in [n]$ and
each realization \( X_j^i = x_j \in \{0, 1\} \), the reward \( R_i \) is distributed as \( \mathbb{P} \{ R_i = 1 \mid X_j^i = x_1, \ldots, X_h^i = x_n \} \).

Extending this, we will write \( \mathbb{E}[R_i \mid a] \) to denote the expected value of reward \( R_i \) when intervention \( a \in \mathcal{I}_i \) is performed in state \( i \in [k] \). For instance, \( \mathbb{E}[R_i \mid do(X_j^i = 1)] \) is the expected reward when variable \( X_j^i \) is set to 1, and all the other variables independently draw values from their respective distributions.

Note that, across the states, the probabilities \( q_j^i \)s and the reward distributions are fixed but unknown. Indeed, the high-level goal of the current work is to develop an algorithm that—in a sample efficient manner—identifies interventions that maximize the expected rewards.

We denote by \( m_i \), the causal parameter from [LLR16] at state \( i \). This parameter is a crucial factor in the regret bound obtained by [LLR16]. Formally, at state \( i \), we consider the Bernoulli probabilities of the variables in increasing order, \( q_j^i \leq q_{j+1}^i \leq \cdots \leq q_{(m)}^i \), and write \( m_i := \max \{ j \mid q_j^i < 1/j \} \). In addition, let \( M \in \mathbb{N}^{k \times k} \) denote the diagonal matrix of \( m_1, \ldots, m_k \).

**Remark 1.** The probabilities \( q_j^i \)s are a priori unknown. It is, however, instructive to consider the computation of \( m_i \) from \( q_j^i \)s: (1) Without loss of generality, assume that \( \mathbb{P} \{ X_j^i = 1 \} \leq \mathbb{P} \{ X_j^i = 0 \} \) (otherwise consider the lesser of the two quantities as \( q_j^i \)) (2) Sort the \( q_j^i \)s in increasing order (3) Compute \( m_i = \max \{ j \mid q_j^i < 1/j \} \) and write \( \mathcal{I}_{m_i} := \{ do(X_j^i = 1) : q_j^i < 1/j \} \)

**MDP Notations:** At state 0, the transition to the intermediate states \( [k] \) stochastically depends on the independent Bernoulli random variables \( \{X_j^0, \ldots, X_h^0\} \). Here, \( \mathbb{P} \{ i \mid a \} \) denotes the probability of transitioning into state \( i \in [k] \) with atomic intervention atomic intervention \( a \in \mathcal{I}_0 \); recall that \( \mathcal{I}_0 \) includes the do-nothing intervention. We will collectively denote these transition probabilities as matrix \( P := [P_{a,i}] = \mathbb{P} \{ i \mid a \} \}_{a \in \mathcal{I}_0, i \in [k]} \). Furthermore, write \( p_+ \) to denote the minimum non-zero value in \( P \). Note that matrix \( P \in \mathbb{R}^{[\mathcal{I}_0] \times k} \) is fixed, but unknown.

A map \( \pi : \{0, \ldots, k\} \to \mathcal{I}_i \), between states and interventions (performed by the algorithm), will be referred to as a policy. Specifically, \( \pi(i) \in \mathcal{I}_i \) is the intervention at state \( i \in \{0, 1, \ldots, k\} \). Note that, for any policy \( \pi \), the expected reward is equal to \( \sum_{i=1}^{k} \mathbb{E}[R_i \mid \pi(i)] \cdot \mathbb{P} \{ i \mid \pi(0) \} \).

Maximizing expected reward, at each intermediate state \( i \in [k] \), we obtain the overall optimal policy \( \pi^* \) as follows: \( \pi^*(i) = \arg \max_{a \in \mathcal{I}_i} \mathbb{E}[R_i \mid a] \), for \( i \in [k] \), and \( \pi^*(0) = \arg \max_{b \in \mathcal{I}_0} \left( \sum_{i=1}^{k} \mathbb{E}[R_i \mid \pi^*(i)] \cdot \mathbb{P} \{ i \mid b \} \right) \).

Our goal is to find a policy \( \pi \) with (expected) reward as close to that of \( \pi^* \) as possible. We will use \( \varepsilon(\pi) \) to denote the sub-optimality of a policy \( \pi \); in particular, \( \varepsilon(\pi) \) is defined as the difference between the expected rewards of \( \pi^* \) and \( \pi \).

Conforming to the standard *simple-regret* framework, the algorithm is given a time budget \( T \), i.e., the algorithm can go through the two-stages of the MDP \( T \) times. In each of these \( T \) rounds, the algorithm can perform the atomic interventions of its choice (both at state 0 and then at the resulting intermediate state). The overall goal of the algorithm is to compute a policy with high expected reward and the algorithm’s sub-optimality is defined as its regret, \( \text{Regret}_T := \mathbb{E}[\varepsilon(\hat{\pi})] \). Here, the expectation is with respect to the policy \( \hat{\pi} \) computed by the algorithm; indeed, given any two-stage causal MDP instance and time budget \( T \) to an algorithm, different policies \( \hat{\pi}_s \)s will have potentially different probabilities of being returned.
Table 1: MDP Notations

| Notation | Explanation |
|----------|-------------|
| $P \in \mathbb{R}^{N \times k}$ | Transition probabilities matrix: $P := [P_{(a,i)} = \mathbb{P}(i \mid a)]_{a \in \mathcal{I}_0, i \in [k]}$ |
| $p_+$ | $p_+ = \min\{P_{(a,i)} \mid P_{(a,i)} > 0\}$ |
| $\pi : \mathcal{S} \rightarrow \mathcal{I}$ | Policy, a map from states to interventions. $\pi(i) \in \mathcal{I}_i$ for $i \in \{0\} \cup [k]$ |
| $\mathbb{E}[R_i \mid \pi(i)]$ | Expectation of the reward at state $i$ given intervention $\pi(i)$ |
| $\pi^*$ | Optimal Policy |
| $\hat{\pi}$ | Computed policy |
| $\varepsilon(\pi)$ | Sub-optimality of $\pi$ |
| Regret$_T$ | $\mathbb{E}[\varepsilon(\hat{\pi})]$ |

**Algorithm 1** ALG-CE: Convex Exploration

Algorithm

1: **Input:** Total rounds $T$
2: $\hat{P} \leftarrow$ Estimate Transition Probabilities($\frac{T}{3}$)
3: $\hat{f} \leftarrow \arg \max_{f} \min_{\text{fq. vector } f} \hat{P}^\top f$
4: $\hat{M} \leftarrow$ Estimate Causal Parameters($\hat{f}, \frac{T}{3}$)
5: $\hat{f}^* \leftarrow \arg \min_{\text{fq. vector } f} \max_{\text{interventions } I_0} \hat{P}\hat{M}^{1/2}\left(\hat{P}\hat{f}\right)^{\frac{a-\frac{1}{2}}{2}}$
6: $\hat{R} \leftarrow$ Estimate Rewards($\hat{f}^*, \hat{f}, \frac{T}{3}$)
7: Estimate optimal policy $\hat{\pi}(i)$ for all $i \in [k]$ based on $\hat{R}$
8: Estimate $\hat{\pi}(0)$ from $\hat{P}$ and $\hat{\pi}(i)$ for all $i \in [k]$
9: **return** $\hat{\pi} = \{\pi(0), \pi(1), \ldots, \pi(k)\}$

**Algorithm 2** Estimate Transition Probabilities

Algorithm

1: **Input:** Time budget $T'$
2: for time $t \leftarrow \{1, \ldots, \frac{T'}{3}\}$ do
3: Perform do() at state 0. Transition to $i \in [k]$.
4: Count number of times state $i \in [k]$ is observed.
5: Update $\hat{q}_0^\ell = \mathbb{P}\{X_0^\ell = 1\}$
6: Using $\hat{q}_0^\ell$s, estimate $m_0$ and the set $\mathcal{I}_{m_0}$.
7: Note that $\mathcal{I}_0 = \mathcal{I}_{m_0} \cup \mathcal{I}_{m_o}$
8: for intervention $a \in \mathcal{I}_{m_o}$ at state 0 do
9: for time $t \leftarrow \{1, \ldots, \frac{T'}{3}\}$ do
10: Perform $a \in \mathcal{I}_{m_o}$. Transition to some $i \in [k]$ for each $a \in \mathcal{I}_{m_o}$.
11: Count number of times state $i$ is observed.
12: Estimate $\hat{P}_{(a,i)} = \mathbb{P}[i \mid a]$ for each $a \in \mathcal{I}_{m_o}$, $i \in [k]$
13: **return** Estimated matrix $\hat{P} = [\hat{P}_{(a,i)}]_{i \in [k], a \in \mathcal{I}_0}$

### 3 Main Algorithm and its Analysis

Our algorithm (ALG-CE) uses subroutines to estimate the transition probabilities, the causal parameters, and the rewards. From these, it outputs the best available interventions as its policy $\hat{\pi}$. Given time budget $T$, the algorithm uses the first $T/3$ rounds to estimate the transition probabilities (i.e., the matrix $P$) in **Algorithm 2**. The subsequent $T/3$ rounds are utilized in **Algorithm 3** to estimate causal parameters $m_1$s. Finally, the remaining budget is used in **Algorithm 4** to estimate the intervention-dependent reward $R_i$s, for all intermediate states $i \in [k]$.

To judiciously explore the interventions at state 0, ALG-CE computes frequency vectors $f \in \mathbb{R}^{\left|\mathcal{I}_0\right|}$. In such vectors, the $a$th component $f_a \geq 0$ denotes the fraction of time that each intervention $a \in \mathcal{I}_0$ is
We next define a key parameter $\lambda$ that specifies the regret bound in Theorem 1 (below).

$$\lambda := \min_{f, \text{vector } f} \left\| P M^{1/2} \left( P^T f \right)^{0 - \frac{1}{2}} \right\|_\infty$$

(1)

Furthermore, we will write $f^*$ to denote the optimal frequency vector in equation (1). Hence, with vector $\nu := PM^{1/2} \left( P^T f^* \right)^{0 - \frac{1}{2}}$, we have $\lambda = \max_a \nu_a^2$. Note that Step 5 in ALG-CE addresses an analogous optimization problem, albeit with the estimates $\hat{P}$ and $\hat{M}$. Also, we show in Lemma 11 (see Section B) that this optimization problem is convex and, hence, Step 5 admits an efficient implementation.

The following theorem is the main result of the current work. It upper bounds the regret of ALG-CE.

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Algorithm 3 Estimate Causal Parameters

1: **Input:** Frequency vector $\hat{f}$ and time budget $T'$
2: Update $f(a) \leftarrow \frac{1}{2} \left( \hat{f}(a) + \frac{1}{\lambda_a} \right) \forall a \in I_0$
3: **for** intervention $a \in I_0$ **do**
4:  **for** time $t \leftarrow \{1, \ldots, T' \cdot f(a)\}$ **do**
5:  Perform $a \in I_0$. Transition to some $i \in [k]$
6:  At state $i$, perform $\text{do}(\cdot)$ and observe $X_j$'s
7:  Update $\hat{q}_j = \mathbb{P} \{ X_j = 1 \}$
8:  Using $\hat{q}_j$'s, estimate $\hat{m}_i$ values\(^1\) for each state $i \in [k]$
9:  **return** $\hat{M}$, the diagonal matrix of the $\hat{m}_i$ values

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Algorithm 4 Estimate Rewards

1: **Input:** Optimal frequency $f^*$, min-max frequency $\hat{f}$, and time budget $T'$
2: Set $f(a) \leftarrow \frac{1}{2} \left( f^*(a) + \hat{f}(a) + \frac{1}{\lambda_a} \right) \forall a \in I_0$
3: **for** intervention $a \in I_0$ at state 0 **do**
4:  **for** time $t \leftarrow \{1, \ldots, f(a) \cdot T'/2\}$ **do**
5:  Perform $a \in I_0$. Transition to some $i \in [k]$
6:  Perform $\text{do}(\cdot)$ at $i \in [k]$. Observe $X_j$'s and $R_i$
7:  Find the set $I_{m_i} \forall i \in [k]$ using $\hat{q}_j$ estimates\(^3\).
8:  For all $b \in I_{m_i}$, estimate reward $\hat{R}_{(b,i)} = \mathbb{E}[R_i \mid b]$
9: **for** intervention $a \in I_0$ at state 0 **do**
10:  **for** time $t \leftarrow \{1, \ldots, f(a) \cdot T'/2\}$ **do**
11:  Perform $a \in I_0$. Transition to some $i \in [k]$
12:  Iteratively perform $b \in I_{m_i}$ and observe $R_i$
13:  Estimate mean reward $\hat{R}_{(b,i)} = \mathbb{E}[R_i \mid b] \forall b \in I_{m_i}$
14: **return** $\hat{R} = \left[ \hat{R}_{(b,i)} \right]_{i \in [k], b \in I_i}$

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\(^1\)See Remark 1

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performed by the algorithm, i.e., given time budget $T'$, the intervention $a$ will be performed $T_a T'$ times. Note that, by definition, $\sum_a f_a = 1$ and the frequency vectors are computed by solving convex programs over the estimates. The algorithm and its subroutines throughout consider empirical estimates, i.e., find the estimates by direct counting. Here, let $\hat{P}$ denote the computed estimate of the matrix $P$ and $\hat{M}$ be the estimate of the diagonal matrix $M$. We obtain a regret upper bound via an optimal frequency vector $\hat{f}^*$ (see Step 5 in ALG-CE).

Recall that for any vector $x$ (with non-negative components), the Hadamard exponentiation $\circ - \frac{1}{2}$ leads to the vector $y = x^{0 - \frac{1}{2}}$ wherein $y_i = \frac{1}{\sqrt{x_i}}$ for each component $i$.

We next define a key parameter $\lambda$ that specifies the regret bound in Theorem 1 (below).

\[ \lambda := \min_{f, \text{vector } f} \left\| P M^{1/2} \left( P^T f \right)^{0 - \frac{1}{2}} \right\|_\infty \]

(1)
The result requires the algorithm’s time budget to be at least

\[ T_0 := \tilde{O} \left( \frac{N \max(m_i)}{p^+} \right) \]  

(2)

**Theorem 1.** Let parameter \( \lambda \) be as defined in equation (1). Then, given number of rounds \( T \geq T_0 \), \( \text{ALG-CE} \) achieves regret

\[ \text{Regret}_T \in \mathcal{O} \left( \sqrt{\frac{1}{T} \max \left\{ \lambda, \frac{m_0}{p^+} \right\} \log (NT)} \right) \]

### 3.1 Proof of Theorem 1

We prove the theorem, we analyze the algorithm’s execution as falling under either **good event** or **bad event**, and tackling the regret under each.

**Definition 1.** We define five events, \( E_1 \) to \( E_5 \), the intersection of which we call as **good event**, \( E \), i.e.,

\[ \text{good event } E \equiv \bigcap_{i \in [5]} E_i. \]

\( E_1 \): \( \sum_{i=1}^{k} \left| \hat{P}(a,i) - P(a,i) \right| \leq \frac{p^+}{2} \quad \forall a \in \mathcal{I}_0. \) That is, for every intervention \( a \in \mathcal{I}_0 \), the empirical estimate of transition probability in each of Algorithms 2, 3 and 4 is good, up to an absolute factor of \( p^+/3 \).

\( E_2 \): Estimate \( \hat{m}_0 \in \left[ \frac{2}{3} m_0, 2m_0 \right] \) in Algorithm 2. In other words, our estimate for causal parameter \( m_0 \) for state 0 in Algorithm 2 is relatively good.

\( E_3 \): \( \hat{m}_i \in \left[ \frac{2}{3} m_i, 2m_i \right] \), for all states \( i \in [k] \). That is, our estimate of \( m_i \) parameter is relatively good for every state \( i \in [k] \), in Algorithms 3 and 4.

\( E_4 \): \( \sum_{i \in [k]} \left| \hat{P}(a,i) - P(a,i) \right| \leq \eta' \), for all interventions \( a \in \mathcal{I}_0 \). Here, random variable \( \eta' := \sqrt{\frac{150 m_0}{T p^+}} \log \left( \frac{3T}{k} \right) \) and \( \hat{P}(a,i) \) is the estimated transition probability computed in Algorithm 2.

\( E_5 \): \( \left| \mathbb{E} [R_i | a] - \hat{R}(a,i) \right| \leq \hat{\eta}_i \) for all \( i \in [k] \) and all \( a \in \mathcal{I}_i \); here \( \hat{\eta}_i = \sqrt{\frac{2T m_i}{T (p^+ f^*)_i}} \log (2TN) \).

**Definition 2.** We define **bad event** \( F \), as the complement of the intersection of events \( E_1 \) - \( E_5 \), as defined above, i.e., **bad event** \( F \equiv E^c \).

Before we proceed with the proof, we state below a corollary which provides a multiplicative bound on \( \hat{P} \) with respect to \( P \), complementing the additive form of \( E_1 \).

**Corollary 1.** Under event \( E_1 \), for all interventions \( a \in \mathcal{I}_0 \) and states \( i \in [k] \), we have:

\[ \frac{2}{3} P(a,i) \leq \hat{P}(a,i) \leq \frac{4}{3} P(a,i) \]

**Proof.** Event \( E_1 \) ensures that \( \sum_{i=1}^{k} \left| \hat{P}(a,i) - P(a,i) \right| \leq \frac{p^+}{3} \), for each interventions \( a \in \mathcal{I}_0 \) and states \( i \in [k] \). This, in particular, implies that for each intervention \( a \in \mathcal{I}_0 \) and state \( i \in [k] \) the following inequality holds.

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\[ \text{Recall that } \hat{f}^* \text{ denotes the optimal frequency vector computed in Step 5 of ALG-CE. Also, } (\hat{P}^T \hat{f}^*), \text{ denotes the } i \text{th component of the vector } P^T f^*. \]
holds: $|\hat{P}_{(a,i)} - P_{(a,i)}| \leq \frac{p_+^2}{3}$. Note that if $P_{(a,i)} = 0$, then the algorithm will never observe state $i$ with intervention $a$, i.e., in such a case $\hat{P}_{(a,i)} = P_{(a,i)} = 0$. For the nonzero $P_{(a,i)}$s, recall that (by definition), $p_+ = \min\{P_{(a,i)} \mid P_{(a,i)} > 0\}$. Therefore, for any nonzero $P_{(a,i)}$, the above-mentioned inequality gives us $|\hat{P}_{(a,i)} - P_{(a,i)}| \leq \frac{1}{3} P_{(a,i)}$. Equivalently, $\hat{P}_{(a,i)} \leq \frac{4}{3} P_{(a,i)}$ and $\hat{P}_{(a,i)} \geq \frac{2}{3} P_{(a,i)}$. Therefore, for all $P_{(a,i)}$s the corollary holds.

Considering the estimates $\hat{P}$ and $\hat{M}$, along with frequency vector $\hat{f}^*$ (computed in Step 5), we define random variable $\hat{\lambda} := \left\| \hat{P} \hat{M}^{1/2} \left( \hat{P}^\top \hat{f}^* \right)^{\frac{\alpha - 2}{2}} \right\|_\infty^2$. Note that $\hat{\lambda}$ is a surrogate for $\lambda$. We will, in fact, show that, under the good event, $\hat{\lambda}$ is close to $\lambda$ (Lemma 3).

Recall that $\text{Regret}_T := \mathbb{E}[\varepsilon(\pi)]$ and here the expectation is with respect to the policy $\pi$ computed by the algorithm. We can further consider the expected sub-optimality of the algorithm and the quality of the estimates (in particular, $\hat{P}$, $\hat{M}$ and $\hat{\lambda}$) under good event (E).

Based on the estimates returned at Step 5 of ALG-CE, either the good event holds, or we have the bad event (though this is unknown to our algorithm). We obtain the regret guarantee by first bounding sub-optimality of policies computed under the good event, and then bound the probability of the bad event.

**Lemma 1.** For the optimal policy $\pi^*$, under the good event (E), we have

$$\sum_{i \in [k]} P_{(\pi^*(0),i)} \mathbb{E} [R_i \mid \pi^*(i)] \leq \sum_{i \in [k]} \hat{P}_{(\pi^*(0),i)} \hat{R}_{(\pi^*(i),i)} + O \left( \sqrt{\max \{\hat{\lambda}, \frac{m_0}{\mathbb{P}^*_+} \} \log (NT) } \right)$$

**Proof.** Consider the expression

$$\sum_{i \in [k]} P_{(\pi^*(0),i)} \mathbb{E} [R_i \mid \pi^*(i)] - \sum_{i \in [k]} \hat{P}_{(\pi^*(0),i)} \hat{R}_{(\pi^*(i),i)}.$$

We can add and subtract $\sum_{i \in [k]} P_{(\pi^*(0),i)} \hat{R}_{(\pi^*(i),i)}$ and take common terms out to reduce the expression:

$$\sum_{i \in [k]} P_{(\pi^*(0),i)} \left( \mathbb{E} [R_i \mid \pi^*(i)] - \hat{R}_{(\pi^*(i),i)} \right) + \sum_{i \in [k]} \hat{R}_{(\pi^*(i),i)} \left( P_{(\pi^*(0),i)} - \hat{P}_{(\pi^*(0),i)} \right)$$

Note that:

(a) $\hat{R}_{(\pi^*(i),i)} \leq 1$

(b) $\sum_{i \in [k]} |\hat{P}_{(\pi^*(0),i)} - P_{(\pi^*(0),i)}| \leq \eta'$ (from E4)

(c) $|\mathbb{E} [R_i \mid \pi^*(i)] - \hat{R}_{(\pi^*(i),i)}| \leq \hat{\eta}_i$ (from E5)

Furthermore, it follows from Corollary 1 that (component-wise) $P \leq \frac{3}{2} \hat{P}$. Hence, the above-mentioned expression is bounded above by

$$\sum_{i \in [k]} \frac{3}{2} \hat{P}_{(\pi^*(0),i)} \hat{\eta}_i + \eta'$$
Note that the definition of \( \hat{\lambda} \) ensures \( \sum_{i \in [k]} \hat{P}_{(\pi^*(0),i)} \hat{\eta}_i = O\left( \sqrt{\frac{\hat{\lambda}}{T} \log(NT)} \right) \). Further, \( \eta' = O\left( \sqrt{\frac{m_0}{T p_+} \log(\frac{T}{K})} \right) \).

Therefore,

\[
\sum_{i \in [k]} P_{(\pi^*(0),i)} \eta_i + \eta' = O\left( \sqrt{\max\{\hat{\lambda}, \frac{m_0}{p_+}\} \log(NT)} \right) T
\]

This establishes the lemma.

We now state another similar lemma for any policy \( \hat{\pi} \) computed under good event.

**Lemma 2.** Let \( \hat{\pi} \) be a policy computed by ALG-CE under the good event \( E \). Then,

\[
\sum_{i \in [k]} P_{(\hat{\pi}(0),i)} \mathbb{E}[R_i \mid \hat{\pi}(i)] \geq \sum_{i \in [k]} \hat{P}_{(\hat{\pi}(0),i)} \hat{R}_{(\hat{\pi}(i),i)} - O\left( \sqrt{\max\{\hat{\lambda}, \frac{m_0}{p_+}\} \log(NT)} \right) T
\]

**Proof.** Consider the expression:

\[
\sum_{i \in [k]} P_{(\hat{\pi}(0),i)} \hat{R}_{(\hat{\pi}(i),i)} - \sum_{i \in [k]} P_{(\hat{\pi}(0),i)} \mathbb{E}[R_i \mid \hat{\pi}(i)]
\]

We can add and subtract \( \sum_{i \in [k]} P_{(\hat{\pi}(0),i)} \hat{R}_{(\hat{\pi}(i),i)} \) to get:

\[
\sum_{i \in [k]} \hat{R}_{(\hat{\pi}(i),i)} \left( \hat{P}_{(\hat{\pi}(0),i)} - P_{(\hat{\pi}(0),i)} \right) + \sum_{i \in [k]} P_{(\hat{\pi}(0),i)} \left( \hat{R}_{(\hat{\pi}(i),i)} - \mathbb{E}[R_i \mid \hat{\pi}(i)] \right)
\]

Analogous to Lemma 1, one can show that this expression is bounded above by

\[
\eta' + \sum_{i \in [k]} \frac{3}{2} \hat{P}_{(\hat{\pi}(0),i)} \hat{\eta}_i = O\left( \sqrt{\max\{\hat{\lambda}, \frac{m_0}{p_+}\} \log(NT)} \right) T
\]

We can also bound \( \hat{\lambda} \) to within a constant factor of \( \lambda \).

**Lemma 3.** Under the good event, we have \( \hat{\lambda} \leq 8\lambda \).

**Proof.** Corollary 1 ensures that given event \( E_1 \) (and, hence, the good event), \( \frac{2}{3} P \leq \hat{P} \leq \frac{4}{3} P \). In addition, note that event \( E_3 \) gives us \( \hat{M} \leq 2M \). From these observations we obtain the desired bound:

\[
\hat{\lambda} = \hat{P} \hat{M}^{\frac{1}{2}} \left( \hat{P}^{\top} \hat{f}^* \right)^{\frac{1}{2}} \leq \hat{P} \hat{M}^{\frac{1}{2}} \left( \hat{P}^{\top} f^* \right)^{\frac{1}{2}} \leq 8PM^{\frac{1}{2}} \left( P^{\top} f^* \right)^{\frac{1}{2}} = 8\lambda
\]

Here, the first inequality follows from the fact that \( \hat{f}^* \) is the minimizer of the \( \hat{\lambda} \) expression, and for the second inequality, we substitute the appropriate bounds of \( \hat{P} \) and \( \hat{M} \).

**Corollary 2.** Let \( \hat{\pi} \) be a policy computed by ALG-CE under good event \( E \), then

\[
\varepsilon(\hat{\pi}) = O\left( \sqrt{\max\{\lambda, \frac{m_0}{p_+}\} \log(NT)} \right) T
\]
Proof. Since \textsc{Alg-CE} selects the optimal policy (with respect to the estimates),
\[
\sum \hat{P}_{(\pi^*(0),i)} \hat{R}_{(\pi^*(i),i)} \leq \sum \hat{P}_{(\hat{\pi}(0),i)} \hat{R}_{(\hat{\pi}(i),i)}
\]
Combining this with Lemmas 1 and 2, we get under good event:
\[
\sum_{i \in [k]} P_{(\pi^*(0),i)} E[R_i | \pi^*(i)] - \sum_{i \in [k]} P_{(\hat{\pi}(0),i)} E[R_i | \hat{\pi}(i)] = O \left( \sqrt{\max \left\{ \lambda, \frac{m_0}{p_+} \right\} \frac{\log NT}{T} } \right)
\]
Note the left-hand-side of this expression is equal to $\varepsilon(\hat{\pi})$. Finally, using Lemma 3, we get that
\[
\varepsilon(\hat{\pi}) = O \left( \sqrt{\max \left\{ \lambda, \frac{m_0}{p_+} \right\} \frac{\log NT}{T} } \right)
\]
The corollary stands proved. □

Corollary 2 shows that under the good event, the (true) expected reward of $\pi^*$ and $\hat{\pi}$ are within $O \left( \sqrt{\max \left\{ \lambda, \frac{m_0}{p_+} \right\} \frac{\log NT}{T} } \right)$ of each other.

In Lemma 4 (stated below and proved in Appendix A.6) we will show that\footnote{Recall that, by definition, $F = E_c$.} \( \mathbb{P} \left\{ \bigcup_{i \in [5]} \neg E_i \right\} = \mathbb{P} \{ F \} \leq \frac{5k}{T} \),
for appropriately large $T$.

**Lemma 4** (Bound on Bad Event). Write $T_0 := O \left( \frac{N \max(m_0)}{p_+} \log (2NT) \right) = \tilde{O} \left( \frac{N \max(m_0)}{p_+} \right)$. Then for any $T > T_0$:
\[
\mathbb{P} \{ F \} \leq \frac{5k}{T}
\]
The above-mentioned bounds together establish Theorem 1 (i.e., bound the regret of \textsc{Alg-CE}):
\[
\text{Regret}_T = \mathbb{E}[\varepsilon(\pi)] = \mathbb{E}[\varepsilon(\hat{\pi}) | E] \mathbb{P} \{ E \} + \mathbb{E}[\varepsilon(\pi') | F] \mathbb{P} \{ F \}
\]
Since the rewards are bounded between 0 and 1, we have $\varepsilon(\pi') \leq 1$, for all policies $\pi'$. In addition, the fact that $\mathbb{P} \{ E \} \leq 1$ gives us $\text{Regret}_T \leq \mathbb{E}[\varepsilon(\pi) | E] + \mathbb{P} \{ F \}$. Therefore, Corollary 2 along with Lemma 4, lead to the stated regret guarantee
\[
\text{Regret}_T = O \left( \sqrt{\max \left\{ \lambda, \frac{m_0}{p_+} \right\} \frac{\log NT}{T} } \right) + \frac{5k}{T} = \tilde{O} \left( \sqrt{\max \left\{ \lambda, \frac{m_0}{p_+} \right\} \frac{\log NT}{T} } \right)
\]

4 Lower Bound

This section provides a lower bound on regret for a family of instances. For any number of states $k$, we show that there exist transition matrices $P$ and reward distributions $(\mathbb{E}[R_i | a])$ such that regret achieved by \textsc{Alg-CE} (Theorem 1) is tight, up to log factors.
There exists a transition matrix $P$, reward distributions, and probabilities $q_j^0$ corresponding to causal variables $\{X_j^0\}_{j \in [n]}$, such that for any $q_j^i$, corresponding to causal variables at states $i \in [k]$, the simple regret achieved by any algorithm is

$$\text{Regret}_T \in \Omega \left( \sqrt{\frac{\lambda}{T}} \right)$$

### 4.1 Theorem 2: Proof Setup

This section establishes Theorem 2. We will identify a collection of two-stage causal MDP instances and show that, for any given algorithm $A$, there exists an instance in this collection for which $A$’s regret is $\Omega \left( \sqrt{\frac{\lambda}{T}} \right)$.

First we describe the collection of instances and then provide the proof.

For any integer $k > 1$, consider $n = (k-1)$ causal variables at each state $i \in \{0, 1, \ldots, k\}$. The transition matrix $P$ is set to be deterministic. Specifically, for each $i \in [n]$, we have $\mathbb{P}\{i \mid do(X_0^i = 1)\} = 1$. For all other interventions at state 0, we transition to state $k$ with probability 1. Such a transition matrix can be achieved by setting $q_0^0 = 0$ for all $i \in [k-1]$. As before, the total number of interventions $N := 2n + 1 = 2k - 1$.

Now consider a family of $Nk + 1$ instances $\{\mathcal{F}_0\} \cup \{\mathcal{F}_{(a,i)}\}_{i \in [k], a \in \mathcal{I}_i}$. Here, $\mathcal{F}_0$ and each $\mathcal{F}_{(a,i)}$ is a two-stage causal MDP with the above-mentioned transition probabilities. The instances differ in the rewards at the intermediate states. In particular, in instance $\mathcal{F}_0$, we set the reward distributions such that $\mathbb{E}[R_i \mid a] = \frac{1}{2}$ for all states $i \in [k]$ and interventions $a \in \mathcal{I}_i$. For each $i \in [k]$ and $a \in \mathcal{I}_i$, instance $\mathcal{F}_{(a,i)}$ differs from $\mathcal{F}_0$ only at state $i$ and for intervention $a$. Specifically, by construction, we will have $\mathbb{E}[R_i \mid a] = \frac{1}{2} + \beta$, for a parameter $\beta > 0$. The expected rewards under all other interventions will be 1/2, the same as in $\mathcal{F}_0$.

Given any algorithm $A$, we will consider the execution of $A$ over all the instances in the family. The execution of algorithm $A$ over each instance induces a trace, which may include the realized transition probabilities $\hat{P}$, the realized variable probabilities $\hat{q}_j^i$ for $i \in [k]$ and $j \in [n]$ and the corresponding $\hat{m}_i$s, and the realized rewards $\hat{R}$. Each of such realizations (random variables) has a corresponding distribution (over many possible runs of the algorithm). We call the measures corresponding to these random variables under the instances $\mathcal{F}_0$ and $\mathcal{F}_{(a,i)}$ as $\mathcal{P}_0$ and $\mathcal{P}_{(a,i)}$, respectively.

### 4.2 Proof of Theorem 2

For any algorithm $A$ and given time budget $T$, we first consider the $A$’s execution over instance $\mathcal{F}_0$. As mentioned previously, $\mathcal{P}_0$ denotes the trace distribution induced by the algorithm for $\mathcal{F}_0$. In particular, write $r_i$ to denote the expected number of times state $i$ is visited, $r_i := \mathbb{E}_{\mathcal{P}_0}[\text{state } i \text{ is visited}] / T$.

Recall the construction of the set $\mathcal{I}_{m_i}$ (for each intermediate state $i \in [k]$) from Remark 1 in Section 2. In particular, $m_i := \max\{j \mid q_j^i < \frac{1}{2}\}$ and $\mathcal{I}_{m_i} := \{do(X_j^i = 1) \mid q_j^i < \frac{1}{2}\}$, where the Bernoulli probabilities of the variables at state $i$ are sorted to satisfy $q_1^i \leq q_2^i \leq \cdots \leq q_{m_i}^i$. Note that these
definitions do not depend on the algorithm at hand. The algorithm, however, may choose to perform
different interventions different number of times. Write \( N_{(a,i)} \) to denote the expected (under \( \mathcal{P}_0 \)) number
of times intervention \( a \) is performed by the algorithm at state \( i \). Furthermore, let random variable \( T_{(a,i)} \)
denote the number of times intervention \( a \) is observed at state \( i \). Hence, \( \mathbb{E}_{\mathcal{P}_0}[T_{(a,i)}] \) is the expected
number of times intervention \( a \) is observed.\(^4\)

Using the expected values for algorithm \( A \) and instance \( \mathcal{F}_0 \), we define a subset of \( \mathcal{I}_{m_i} \) as follows:
\[ J_i := \left\{ a \in \mathcal{I}_{m_i} : N_{(a,i)} \leq 2 \frac{Tr_i}{m_i} \right\}. \]

**Proposition 4.1.** The set \( J_i \) is non-empty. In particular,
\[ m_i/2 \leq |J_i| \leq m_i. \]

**Proof.** The upper bound on the size of subset \( J_i \) follows directly from its definition: since \( J_i \subseteq \mathcal{I}_{m_i} \) we have \( |J_i| \leq |\mathcal{I}_{m_i}| = m_i \).

For the lower bound on the size of \( J_i \), note that \( Tr_i \) is the expected number of times state \( i \) is visited
by the algorithm. Therefore,
\[ \sum_{a \in \mathcal{I}_{m_i}} N_{(a,i)} \leq Tr_i \quad (3) \]

Furthermore, by definition, for each intervention \( b \in \mathcal{I}_{m_i} \setminus J_i \) we have \( N_{(b,i)} \geq 2 \frac{Tr_i}{m_i} \). Hence, assuming
\( |\mathcal{I}_{m_i} \setminus J_i| > \frac{m_i}{2} \) would contradict inequality 3. This observation implies that \( |\mathcal{I}_{m_i} \setminus J_i| \leq \frac{m_i}{2} \) and, hence,
\( |J_i| \geq \frac{m_i}{2} \). This completes the proof. \( \square \)

Recall that \( T_{(a,i)} \) denotes the number of times intervention \( a \) is observed at state \( i \). The following
proposition bounds \( \mathbb{E}[T_{(a,i)}] \) for each intervention \( a \in J_i \).

**Proposition 4.2.** For every intervention \( a \in J_i \)
\[ \mathbb{E}_{\mathcal{P}_0}[T_{(a,i)}] \leq 3 \frac{Tr_i}{m_i}. \]

**Proof.** Any intervention \( a \in J_i \subseteq \mathcal{I}_{m_i} \) may be observed either when it is explicitly performed by the
algorithm or as a random realization (under some other intervention, including do-nothing). Since \( a \in \mathcal{I}_{m_i} \), the probability that \( a \) is observed as part of some other intervention is at most \( \frac{1}{m_i} \). Therefore, the expected number of times that \( a \) is observed by the algorithm—without explicitly performing it—is at most \( \frac{Tr_i}{m_i} \).\(^5\) Recall that the expected number of times state \( i \) is visited is equal to \( Tr_i \).

For any intervention \( a \in J_i \), by definition, the expected number of times \( a \) is performed \( N_{(a,i)} \leq 2 \frac{Tr_i}{m_i} \). Therefore, the proposition follows:
\[ \mathbb{E}[T_{(a,i)}] \leq \frac{Tr_i}{m_i} + N_{(a,i)} \leq 3 \frac{Tr_i}{m_i}. \]

\(^4\)Note that \( a \) can be observed while performing the do-nothing intervention. Also, the expected value \( N_{(a,i)} \) accounts
for the number of times \( a \) is explicitly performed and not just observed.

\(^5\)Here, we use the fact that the realization of \( a \) is independent of the visitation of state \( i \).
We now state two known results for KL divergence.

**Bretagnolle-Huber Inequality (Theorem 14.2 in [LS20])**: Let \( P \) and \( P' \) be any two measures on the same measurable space. Let \( E \) be any event in the sample space with complement \( E^c \). Then,
\[
P_P\{E\} + P_{P'}\{E^c\} \geq \frac{1}{2} \exp \left( -\text{KL}(P, P') \right).
\] (4)

**Bound on KL-Divergence with number of observations (Adaptation of Equation 17 in Lemma B1 from [ACBFS95])**: Let \( P_0 \) and \( P_{(a,i)} \) be any two measures with differing expected rewards (for exactly the intervention \( a \) at state \( i \)) by an amount \( \beta \). Then,
\[
\text{KL}(P_0, P_{(a,i)}) \leq 6\beta^2 \mathbb{E}_{P_0}[T_{(a,i)}]
\] (5)

We prove the above inequality in Appendix C.

Using this bound on KL divergence and Proposition 4.2, we have, for all states \( i \in [k] \) and interventions \( a \in J_i \):
\[
\text{KL}(P_0, P_{(a,i)}) \leq 6\beta^2 \cdot 3 \frac{\text{Tr}_i}{m_i} = 18 \frac{\text{Tr}_i \beta^2}{m_i}.
\] (6)

Substituting this in the Bretagnolle-Huber Inequality, we obtain, for any event \( E \) in the sample space along with all states \( i \in [k] \) and all interventions \( a \in J_i \):
\[
P_{P_{(a,i)}}\{E\} + P_{P_0}\{E^c\} \geq \frac{1}{2} \exp \left( -18 \frac{\text{Tr}_i \beta^2}{m_i} \right).
\] (7)

We now define events to lower bound the probability that Algorithm \( \mathcal{A} \) returns a sub-optimal policy. In particular, write \( \hat{\pi} \) to denote the policy returned by algorithm \( \mathcal{A} \). Note that \( \hat{\pi} \) is a random variable.

For any \( \ell \in [k] \) and any intervention \( b \), write \( G_1(b, \ell) \) to denote the event that—under the returned policy \( \hat{\pi} \)—intervention \( b \) is not chosen at state \( \ell \), i.e., \( G_1(b, \ell) := \{\hat{\pi}(\ell) \neq b\} \). Also, let \( G_2(\ell) \) denote the event that policy \( \hat{\pi} \) does not induce a transition to \( \ell \) from state 0, i.e., \( G_2(\ell) := \{\hat{\pi}(0) \neq \ell\} \). Furthermore, write \( G(b, \ell) := G_1(b, \ell) \cup G_2(\ell) \). Note that the complement \( G^c(b, \ell) = G_1^c(b, \ell) \cap G_2^c(\ell) = \{\hat{\pi}(\ell) = b\} \cap \{\hat{\pi}(0) = \ell\} \).

Considering measure \( P_0 \), we note that for each state \( \ell \in [k] \) there exists an intervention \( \alpha_\ell \in J_\ell \) with the property that \( \mathbb{P}_{P_0}\{G_1^c(\alpha_\ell, \ell)\} = \mathbb{P}_{P_0}\{\hat{\pi}(\ell) = \alpha_\ell\} \leq \frac{1}{|J_\ell|} \). This follows from the fact that \( \sum_{a \in J_\ell} \mathbb{P}_{P_0}\{\hat{\pi}(\ell) = a\} \leq 1 \). Therefore, for each state \( \ell \in [k] \) there exists an intervention \( \alpha_\ell \) such that \( \mathbb{P}_{P_0}\{G^c(\alpha_\ell, \ell)\} \leq \frac{1}{|J_\ell|} \).

This bound and inequality 7 imply that for all states \( \ell \in [k] \) there exists an intervention \( \alpha_\ell \) that satisfies
\[
\mathbb{P}_{P_{(\alpha_\ell, \ell)}}\{G(\alpha_\ell, \ell)\} \geq \frac{1}{2} \exp \left( -18 \frac{\text{Tr}_\ell \beta^2}{m_\ell} \right) - \frac{1}{|J_\ell|}.
\] (8)
We will set
\[
\beta = \min \left\{ \frac{1}{3}, \sqrt{\frac{\sum_{\ell \in [k]} m_\ell}{18T}} \right\}
\]  \(\text{ (9)}\)

Therefore \(\beta\) takes value either \(\sqrt{\frac{\sum_{\ell \in [k]} m_\ell}{18T}}\) or \(\frac{1}{3}\). We will address these over two separate cases.

Case 1: \(\beta = \sqrt{\frac{\sum_{\ell \in [k]} m_\ell}{18T}}\).

We wish to substitute this \(\beta\) value in Equation 8. Towards this, we will state a proposition.

**Proposition 4.3.** There exists a state \(s \in [k]\) such that
\[
\sqrt{\frac{m_s}{18T r_s}} \geq \sqrt{\frac{\sum_{\ell \in [k]} m_\ell}{18T}}
\]

**Proof.** First, we note the following claim considering all vectors \(\rho = \{\rho_1, \ldots, \rho_k\}\) in the probability simplex \(\Delta\).

**Claim 4.1.** For any given set of integers \(m_1, m_2, \ldots, m_k\), we have
\[
\min_{(\rho_1, \rho_2, \ldots, \rho_k) \in \Delta} \left( \max_{\ell \in [k]} \frac{m_\ell}{\rho_\ell} \right) \geq \sum_{\ell \in [k]} m_\ell
\]

**Proof.** Assume, towards a contradiction, that for all \(\ell \in [k]\), we have \(\frac{m_\ell}{\rho_\ell} < \sum_{\ell \in [k]} m_\ell\). Then, \(\rho_\ell > \frac{m_\ell}{\sum_{\ell \in [k]} m_\ell}\), for all \(\ell \in [k]\). Therefore, \(\sum_{\ell \in [k]} \rho_\ell > \sum_{\ell \in [k]} \frac{m_\ell}{\sum_{\ell \in [k]} m_\ell} = 1\). However, this is a contradiction as \(\sum_{\ell \in [k]} \rho_\ell = 1\).

An immediate consequence of Claim 4.1 is that
\[
\min_{(r_1, r_2, \ldots, r_k) \in \Delta} \left( \max_{\ell \in [k]} \sqrt{\frac{m_\ell}{18T r_\ell}} \right) \geq \sqrt{\frac{\sum_{\ell \in [k]} m_\ell}{18T}}
\]

Therefore, irrespective of how \(r_i\)s are chosen, there always exists a state \(s \in [k]\) such that \(\sqrt{\frac{m_s}{18T r_s}} \geq \sqrt{\frac{\sum_{\ell \in [k]} m_\ell}{18T}}\).

For such a state \(s \in [k]\) that satisfies Proposition 4.3, we note that, \(\frac{m_s}{18T r_s} \geq \beta^2\) or \(\frac{18T r_s \beta^2}{m_s} \leq 1\).

Let us now restate Equation 8 for such a state \(s\). There exists a state \(s \in [k]\) and an intervention \(\alpha_s\) that satisfies
\[
\Pr_{\mathcal{P}(\alpha_s, s)} \{G(\alpha_s, s)\} \geq \frac{1}{2} \exp \left( -18 \frac{T r_s \beta^2}{m_s} \right) - \frac{1}{|\mathcal{J}_s|} \geq \frac{1}{2e} - \frac{1}{|\mathcal{J}_s|} \tag{10}
\]

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Note that the last inequality lower bounds the to probability of selecting a non-optimal policy when the
classification \( \mathcal{A} \) is executed on instance \( \mathcal{F}_{\alpha, s} \). Furthermore, in instance \( \mathcal{F}_{\alpha, s} \), for any non-optimal policy \( \hat{\pi} \) we have \( \epsilon(\hat{\pi}) = (1/2 + \beta) - \frac{1}{2} = \beta \). Therefore, we can lower bound \( \mathcal{A} \)'s regret over instance \( \mathcal{F}_{\alpha, s} \) as follows:

\[
\text{Regret}_T = \mathbb{E}[\epsilon(\hat{\pi})] = \mathbb{P}_{\mathcal{P}_{\alpha, s}}(G(\alpha, s)) \cdot \mathbb{E}[	ext{Regret} | G(\alpha, s)] + \mathbb{P}_{\mathcal{P}_{\alpha, s}}(G'(\alpha, s)) \cdot \mathbb{E}[	ext{Regret} | G'(\alpha, s)] \\
\geq \left[ \frac{1}{2e} - \frac{1}{|\mathcal{J}_s|} \right] \beta + \mathbb{P}_{\mathcal{P}_{\alpha, s}}(G'(\alpha, s)) \cdot 0 \\
= \left[ \frac{1}{2e} - \frac{1}{|\mathcal{J}_s|} \right] \beta
\]

(12)

Note that we can construct the instances to ensure that \( m_\ell \geq 8 \), for all states \( \ell \), and, hence, \( \left( \frac{1}{2e} - \frac{1}{|\mathcal{J}_s|} \right) = \Omega(1) \) (see Proposition 4.1). Therefore Equation 12 gives us:

\[
\text{Regret}_T = \Omega(\beta) = \Omega \left( \sqrt{\sum_{\ell \in [k]} m_\ell} \right)
\]

(13)

**Case 2** We now consider the case when \( \beta = \frac{1}{3} \). In such a case, \( \sqrt{\frac{\sum_{\ell \in [k]} m_\ell}{18T}} > \frac{1}{3} \).

We showed in Proposition 4.3 that there exists a state \( s \in [k] \) such that \( \sqrt{\frac{m_s}{18T_s}} \geq \sqrt{\frac{\sum_{\ell \in [k]} m_\ell}{18T}} \). Combining the two statements, there exists a state \( s \) such that \( \sqrt{\frac{m_s}{18T_s}} \geq \frac{1}{3} \). We now restate Inequality 8 for such a state \( s \in [k] \):

\[
\mathbb{P}_{\mathcal{P}_{\alpha, s}}(G(\alpha, s)) \geq \frac{1}{2} \exp \left( -9\beta^2 \right) - \frac{1}{|\mathcal{J}_s|} = \frac{1}{2e} - \frac{1}{|\mathcal{J}_s|}
\]

Following the exact same procedure as in Case 1, we can derive that \( \text{Regret}_T \geq \left[ \frac{1}{2e} - \frac{1}{|\mathcal{J}_s|} \right] \beta \). We saw in Case 1 that it is possible to construct instances such that \( \left[ \frac{1}{2e} - \frac{1}{|\mathcal{J}_s|} \right] = \Omega(1) \). Therefore the following holds for Case 2 also:

\[
\text{Regret}_T = \Omega(\beta) = \Omega \left( \sqrt{\sum_{\ell \in [k]} m_\ell} \right)
\]

(14)

Inequalities 13 and 14 imply that there exists a state \( s \) and an intervention \( \alpha_s \) such that, under instance \( \mathcal{F}_{(\alpha_s, s)} \), algorithm \( \mathcal{A} \)'s regret satisfies

\[
\text{Regret}_T = \Omega \left( \sqrt{\sum_{\ell \in [k]} m_\ell} \right)
\]

(15)

We complete the proof of Theorem 2 by showing that in the current context \( \lambda = \sum_{\ell \in [k]} m_\ell \).
Proposition 4.4. For the chosen transition matrix

\[ \lambda := \min_{\text{fq. vector } f} \left\| PM^{1/2} \left( P^\top f \right)^{\circ - \frac{1}{2}} \right\|_\infty^2 = \sum_{\ell \in [k]} m_\ell \]

Proof. Recall that all the instances, \( \mathcal{F}_0 \) and \( \mathcal{F}_{(a,i)} \), have the same (deterministic) transition matrix \( P \). Also, parameter \( \lambda \) is computed via Equation 1.

Consider any frequency vector \( f \) over the interventions \( \{1, \ldots, N\} \). From the chosen transition matrix, we have the following:

\[
P = \begin{bmatrix}
1 & 0 & \ldots & 0 \\
0 & 1 & \ldots & 0 \\
\vdots \\
0 & 0 & \ldots & 1 \\
0 & 0 & \ldots & 1 \\
\end{bmatrix} \quad PM^{1/2} = \begin{bmatrix}
\sqrt{m_1} & 0 & \ldots & 0 \\
0 & \sqrt{m_2} & \ldots & 0 \\
\vdots \\
0 & 0 & \ldots & \sqrt{m_k} \\
\end{bmatrix} \quad P^\top f = \left[ \begin{array}{c}
 f_1 \\
f_2 \\
\vdots \\
f_{k-1} \\
f_k + \ldots + f_N \\
\end{array} \right]
\]

From here, we can compute the following:

\[
PM^{1/2} \left( P^\top f \right)^{\circ - \frac{1}{2}} = \left[ \begin{array}{c}
\sqrt{m_1}/f_1, \ldots, \sqrt{m_{k-1}}/f_{k-1}, \sqrt{m_k}/(f_k + \ldots + f_N), \ldots, \sqrt{m_k}/(f_k + \ldots + f_N) \end{array} \right]^\top
\]

That is, for all \( \ell \in [k-1] \), the \( \ell \)th component of the vector \( PM^{1/2} \left( P^\top f \right)^{\circ - \frac{1}{2}} \) is equal to \( \sqrt{m_\ell} \). All the remaining components are \( \sqrt{m_k}/(f_k + \ldots + f_N) \).

Write \( \rho_\ell := f_\ell \) for all \( \ell \in [k-1] \) and \( \rho_k = \sum_{j=k}^N f_j \). Since \( f \) is a frequency vector, \( (\rho_1, \ldots, \rho_k) \in \Delta \). In addition,

\[
PM^{1/2} \left( P^\top f \right)^{\circ - \frac{1}{2}} = \left[ \begin{array}{c}
\sqrt{m_1}/\rho_1, \ldots, \sqrt{m_{k-1}}/\rho_{k-1}, \sqrt{m_k}/\rho_k, \ldots, \sqrt{m_k}/\rho_k \end{array} \right]^\top
\]

Therefore, by definition, \( \lambda = \min_{(\rho_1, \ldots, \rho_k) \in \Delta} \left( \max_{\ell \in [k]} \frac{m_\ell}{\rho_\ell} \right) \). Now, using a complementary form of Claim 4.1 we obtain \( \lambda = \sum_{\ell \in [k]} m_\ell \). The proposition stands proved.

Finally, substituting Proposition 4.4 into Equation 15, we obtain that there exists an instance \( \mathcal{F}_{(a,s)} \) for which algorithm \( \mathcal{A} \)'s regret is lower bounded as follows

\[
\text{Regret}_T = \Omega \left( \sqrt{\frac{\lambda}{T}} \right). \tag{16}
\]

This completes the proof of Theorem 2.
5 Experiments

We first describe ALG-UE (Uniform Exploration Algorithm), the baseline algorithm that we compare ALG-CE with. This is followed by a complete description of our experimental setup. Finally, we present and discuss our main results.

Uniform Exploration (ALG-UE): This algorithm uniformly explores all the interventions in the instance. It first performs all the interventions \( a \in I_0 \) at the start state 0 in a round robin manner. On transitioning to any state \( i \in [k] \), it performs interventions \( b \in I_i \) in a round robin manner.

Setup: We consider an MDP with a start state 0, \( k = 25 \) intermediate states and a terminal state. At each state we have a causal graph with \( n = 25 \) variables. The number of interventions is therefore \( N = 2n + 1 = 51 \). Our reward is a Bernoulli random variable, with probability \( 0.5 + \epsilon \), if \( X_1^1 = 1 \) and 0.5 for every other intervention (we use \( \epsilon = 0.3 \) in our experiments). Note that the reward function is unknown to the algorithm. Like in Lattimore et al. [LLR16], we set \( q_{ij} = 0 \) for \( j \leq m_i \) and 0.5 otherwise. In our setup, we set all \( m_i \) values for all intermediate states \( i \in [k] \) to be the same. On taking action \( a = do() \) at state 0, we transition uniformly to one of the intermediate states. On taking action \( do(X_i^0 = 1) \) (at state 0), where \( i \in [n] \), we transition with probability \( \frac{1}{k} \) to state \( i \) (we take \( k = n \) for these experiments) and probability \( \frac{1}{k} - \frac{1}{k(k-1)} \) to any other state. Recall that \( q_i^0 = P(X_i^0 = 1) \). Then, for all interventions \( do(X_i^0 = 1) \), we have a transition probability vector given by \( p(X_i^0 = 1) \) which is computed from \( (1 - q_i^0)p(X_i^0 = 0) + q_i^0 p(X_i^0 = 1) = p_{do()} \).

We perform two experiments on the above model. In the first one, we run ALG-CE and ALG-UE for time horizon \( T = \{1000, \ldots, 25000\} \). In the second experiment, we run ALG-CE and ALG-UE for a fixed time horizon \( T = 25000 \) with \( \lambda \) varying in the set \( \{50, 75, \ldots, 625\} \). To vary \( \lambda \), we vary \( m_i \) for the intermediate states in the set \( \{2, 3, \ldots, 25\} \). In both the experiments we average the regret over 10000 independent runs for each setting. We use CVXPY [DB16] to solve the optimization problem at Step 5 in ALG-CE.
Results: In Figure 2a, we compare the expected simple regret of ALG-CE and ALG-UE obtained in the first experiment. Our plots indicate that ALG-CE outperforms ALG-UE and its regret falls rapidly as $T$ increases. In Figure 2b, we plot the expected simple regret against $\lambda$ for ALG-CE and ALG-UE that was obtained in Experiment 2, and empirically validate their relationship that was proved in Theorem 1.

Figure 2b shows that ALG-CE outperforms ALG-UE for a wide range of $\lambda$s. This highlights the applicability of ALG-CE, specifically in instances wherein $\lambda$ is dominated by the other instance parameters. This also substantiates the relevance of using causal information; note that, by construction, ALG-UE uses such information, whereas ALG-UE does not.

6 Conclusion and Future Work

We studied extensions of the causal bandits framework into causal MDPs by considering a two-stage setup. This accounted for non-trivial extensions from [LLR16] by considering multiple states as well as transitions between states. We developed the Convex Exploration algorithm for minimizing simple regret in this model. We also identified an instance dependent parameter $\lambda$, and proved that the regret of this algorithm is $\tilde{O}\left(\sqrt{\frac{1}{T} \max\{\lambda, \frac{m_0}{p}\}}\right)$. The current work also established that, for certain families of instances, this upper bound is essentially tight. Finally, we showed through experiments that our algorithm performs better than uniform (naive) exploration in a range of settings.

Instead of addressing MDPs, in their unruly generality, this work considers a stepped extension of causal bandits. Building upon this, a natural way forward would be to consider multi-stage MDPs. This would likely entail the development of an exploration algorithm that solves optimization problems at various stages of the MDP. Furthermore, while our work relies on the parallel causal graph model of Lattimore et al. [LLR16], an active area of research is to address general causal graphs for causal bandits. Extending causal MDPs to such contexts is an interesting direction of future work.

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Appendices

A Bounding the Probability of Bad Event

Recall that the good event corresponds to $\bigcap_{i \in [5]} E_i$ (see Definition 1). Write $F := \neg \bigcap_{i \in [5]} E_i$ and note that, for the regret analysis, we require an upper bound on $P\{F\} = P\{\neg \bigcap_{i \in [5]} E_i\} = P\{\bigcup_{i \in [5]} \neg E_i\}$.

Towards this, in this section we address $P\{\neg E_i\}$, for each of the events $E_1$-$E_5$, and then apply the union bound.

A.1 $E_1$: Probability Bound

The next lemma upper bounds the probability of $\neg E_1$.

**Lemma 5.** In each of Algorithms 2, 3 and 4 and for all interventions $a \in I_0$, we have

$$P\{\neg E_1\} = P\left\{\sum_{i=1}^{k} |\hat{P}_{(a,i)} - P_{(a,i)}| > \frac{p_+}{3}\right\} < \frac{k}{T}$$

whenever $T \geq \max\left\{\frac{1620N}{p_+}, \frac{2025N}{p_+} \log\left(\frac{9NT}{k}\right)\right\}$.

**Proof.** On performing any intervention $a \in I_0$ at state 0, the intermediate state that we visit follows a multinomial distribution. Hence, we can apply Devroye’s inequality (for multinomial distributions) to obtain a concentration guarantee; we state the inequality next in our notation.

**Lemma 6** (Restatement of Lemma 3 in [Dev83]). Let $T_a$ be the number of times intervention $a \in I_0$ is performed in state 0. Then, for any $\eta > 0$ and any $T_a \geq \frac{20s}{\eta^2}$, we have

$$P\left\{\sum_{i=1}^{k} |\hat{P}_{(a,i)} - P_{(a,i)}| > \eta\right\} \leq 3 \exp\left(-\frac{T_a \eta^2}{25}\right)$$

Here, $s$ is the support of the distribution (i.e., the number of states that can be reached from $a$ with a nonzero probability).

Note that each intervention $a \in I_0$ is performed at least $T_a = \frac{T}{9N}$ times across Algorithms 2, 3 and 4. Setting $\eta = \frac{p_+}{3}$ and $T_a = \frac{T}{9N}$ above, we get that for each intervention $a \in I_0$, in each subroutine:

$$P\left\{\sum_{i=1}^{k} |P_{(a,i)} - \hat{P}_{(a,i)}| > \frac{p_+}{3}\right\} \leq 3 \exp\left(-\frac{Tp_+^2}{9N \cdot 9 \cdot 25}\right) = 3 \exp\left(-\frac{Tp_+^2}{2025N}\right)$$

Note that to apply the inequality, we require $\frac{T}{9N} \geq \frac{180s}{p_+^2}$, i.e., $T \geq \frac{1620sN}{p_+^2}$. In the current context, the support size $s$ is at most $\frac{1}{p_+}$; this follows from the fact that on performing any intervention $a \in I_0$, at most $\frac{1}{p_+}$ states can have $P_{(a,i)} \geq p_+$. Hence, the requirement reduces to $T \geq \frac{1620sN}{p_+^2}$.
Next, we union bound the probability over the \( N \) interventions (at state 0) and the three subroutines, to obtain that, for any intervention \( a \in \mathcal{I}_0 \) and in any subroutine,
\[
P \left\{ \sum_{i=1}^{k} \left| P_{(a,i)} - \hat{P}_{(a,i)} \right| > \frac{p_+}{3} \right\} \leq 3N \cdot 3 \exp \left( -\frac{Tp_+^2}{2025N} \right) = 9N \exp \left( -\frac{Tp_+^2}{2025N} \right)
\]

Note that \( 9N \exp \left( -\frac{Tp_+^2}{2025N} \right) \leq \frac{k}{T} \), for any \( T \geq \frac{2025N}{p_+^2} \log \left( \frac{9NT}{k} \right) \). Hence, for any \( T \geq \max \left\{ \frac{1620N}{p_+^3} \frac{2025N}{p_+^2} \log \left( \frac{9NT}{k} \right) \right\} \), we have:
\[
P[\neg E_1] \leq 9N \exp \left( -\frac{Tp_+^2}{2025N} \right) \leq \frac{k}{T}
\]

This completes the proof of the lemma.

### A.2 \( E_2 \): Probability Bound

In this section, we bound the probabilities that our estimated \( \hat{m}_i \)'s are far away from the true causal parameters \( m_i \)'s.

**Lemma 7.** For any \( T \geq 144m_0 \log \left( \frac{TN}{k} \right) \), in Algorithm 2,
\[
P[\neg E_2] = P \left\{ \hat{m}_0 \notin \left[ \frac{2}{3}m_0, 2m_0 \right] \right\} \leq \frac{k}{T}
\]

*Proof.* We allocate time \( \frac{T}{3} \) to Algorithm 2. Lemma 8 in [LLR16] ensures that, for any \( \delta \in (0, 1) \) and \( T \geq 48m_0 \log \left( \frac{N}{\delta} \right) \), we have \( \hat{m}_0 \in \left[ \frac{2}{3}m_0, 2m_0 \right] \), with probability at least \((1 - \delta)\). Setting \( \delta = \frac{k}{T} \), we get the required probability bound.

### A.3 \( E_3 \): Probability Bound

Next, we address \( P\{\neg E_3 \mid E_1\} \).

**Lemma 8.** For any \( T \geq \frac{648 \max(m_i)N}{p_+} \log \left( 2NT \right) \), in each of Algorithms 3 and 4, we have
\[
P \left\{ \exists i \in [k], \quad \hat{m}_i \notin \left[ \frac{2}{3}m_i, 2m_i \right] \mid E_1 \right\} \leq \frac{k}{T}
\]

*Proof.* Fix any reachable state \( i \in [k] \). Corresponding to such a state, there exists an intervention \( \alpha \in \mathcal{I}_0 \) such that \( P_{(a,i)} \geq p_+ \). Event \( E_1 \) (Corollary 1) implies that \( \hat{P}_{(a,i)} \geq \frac{2}{3} \hat{P}_{(a,i)} \geq \frac{2}{3}p_+ \).

Now, write \( T_i \) to denote the number of times state \( i \in [k] \) is visited by the Algorithms 3 and 4. Recall that in the subroutines we estimate \( \hat{P}_{(a,i)} \) by counting the number of times state \( i \) was reached and simultaneously intervention \( \alpha \) observed. Furthermore, note that we allocate to every intervention at least \( \frac{T}{9N} \) time (See Steps 2 in both the subroutines). In particular, intervention \( \alpha \) was necessarily observed \( \frac{T}{9N} \) times. Therefore, \( \hat{P}_{(a,i)} \leq \frac{T_i}{\left( \frac{9N}{T} \right)} \). This inequality leads to a useful lower bound: \( T_i \geq \frac{T}{9N} P_{(a,i)} \geq \frac{2p_+}{9N} \).
We now restate Lemma 8 from [LLR16]: Let $T_i$ be the number of times state $i \in [k]$ is observed. Then,
\[
\Pr\left\{ \hat{m}_i \notin \left[ \frac{2}{3} m_i, 2m_i \right] \right\} \leq 2N \exp\left( -\frac{T_i}{48m_i} \right)
\]
Since $T_i \geq \frac{2 T p_+}{4 N}$, this guarantee from [LLR16] corresponds to
\[
\Pr\left\{ \hat{m}_i \notin \left[ \frac{2}{3} m_i, 2m_i \right] \mid E_1 \right\} \leq 2N \exp\left( -\frac{T p_+}{648N m_i} \right) \leq 2N \exp\left( -\frac{T p_+}{648N \max(m_i)} \right)
\]
Union bounding over all states $i \in [k]$ and the two Algorithms 3 and 4, we obtain:
\[
\Pr\left\{ \exists i \in [k] \text{ in Algorithms 3, 4 with } \hat{m}_i \notin \left[ \frac{2}{3} m_i, 2m_i \right] \mid E_1 \right\} \leq 2Nk \exp\left( -\frac{T p_+}{648N \max(m_i)} \right)
\]
Finally, substituting the value of $T \geq \frac{648 \max(m_i)N}{p_+} \log (2NT)$, gives us:
\[
\Pr\{ \exists i \in [k] \text{ in Algorithms 3, 4 with } \hat{m}_i \notin \left[ \frac{2}{3} m_i, 2m_i \right] \mid E_1 \} 
\leq 2Nk \exp\left( -\frac{T p_+}{648N \max(m_i)} \cdot \left[ \frac{648 \max(m_i)N}{p_+} \log (2NT) \right] \right)
\]
\[= \frac{k}{T} \]
This completes the proof. \(\Box\)

A.4 \(E_4\): Probability Bound

The following lemma provides an upper bound for $\Pr\{\neg E_4 \mid E_2\}$.

Lemma 9. Let $\eta' := \sqrt{\frac{150m_0}{p_+} \log \left( \frac{3T}{k} \right)}$. Then,
\[
\Pr\{\neg E_4 \mid E_2\} = \Pr\left\{ \sum_{i \in [k]} |P_{(a,i)} - \hat{P}_{(a,i)}| > \eta' \mid E_2 \right\} \leq \frac{k}{T}
\]

Proof. As in the proof of Lemma 5, we will use Devroye’s inequality. Write $T_a$ to denote the number of times intervention $a \in I_0$ is observed (in state 0) in Algorithm 2.

For any $\eta \in (0,1)$ and with $T_a \geq \frac{20s}{\eta^2}$, Devroye’s inequality gives us
\[
\Pr\left\{ \sum_{i=1}^{k} |\hat{P}_{(a,i)} - P_{(a,i)}| > \eta \right\} \leq 3 \exp\left( -\frac{T_a \eta^2}{25} \right)
\]
Here, $s$ is the size of the support of the multinomial distribution.

We first show that $T_a$ is sufficiently large, for each intervention $a \in I_0$. Recall that we allocate time $\frac{T}{3}$ to Algorithm 2. Furthermore, we observe each intervention in state 0, at least $\frac{T}{3m_0}$ times, either as
part of the do-nothing intervention or explicitly in Step 10 of Algorithm 2. Now, event $E_2$ ensures that $\hat{m}_0 \in [3m_0, 2m_0]$. Hence, each intervention $a \in \mathcal{I}_0$ is observed $T_a \geq \frac{T}{3m_0} \geq \frac{T}{32m_0} = \frac{T}{6m_0}$ times.

Substituting this inequality for $T_a$ in the above-mentioned probability bound, when $T \geq \frac{120m_0}{\eta^2}$, we obtain:

$$\mathbb{P} \left\{ \sum_{i=1}^{k} \hat{P}_{(a,i)} - P_{(a,i)} > \eta \right\} \leq 3 \exp \left( - \frac{T\eta^2}{150m_0} \right)$$

As observed in Lemma 5, the support size $s$ is at most $\frac{1}{p_+}$. Therefore, the requirement on $T$ reduces to $T \geq \frac{120m_0}{\eta^2p_+}$.

Setting $\eta = \sqrt{\frac{150m_0}{Tp_+} \log \left( \frac{3T}{k} \right)}$ gives us

$$\mathbb{P} \left\{ \sum_{i=1}^{k} \hat{P}_{(a,i)} - P_{(a,i)} > \sqrt{\frac{150m_0}{Tp_+} \log \left( \frac{3T}{k} \right)} \right\} \leq 3 \exp \left( - \frac{T}{150m_0} \left[ \sqrt{\frac{150m_0}{Tp_+} \log \left( \frac{3T}{k} \right)} \right]^2 \right) \leq \frac{k}{T}.$$ 

Therefore

$$\mathbb{P} \left\{ \sum_{i=1}^{k} \hat{P}_{(a,i)} - P_{(a,i)} > \eta \right\} \leq \frac{k}{T}$$

This probability bound requires $T \geq \frac{120m_0}{\eta^2p_+}$. That is, $\eta \geq \sqrt{\frac{120m_0}{Tp_+}}$. This inequality is satisfied by our choice of $\eta$. Hence, the lemma stands proved. \hfill $\Box$

### A.5 $E_5$: Probability Bound

The next lemma bounds $\mathbb{P}\{\neg E_5 \mid E_1, E_3\}$.

**Lemma 10.** Let $\hat{\eta}_i = \sqrt{\frac{2m_i}{T(p_+ + f_i)}} \log (2TN)$. Then,

$$\mathbb{P} \left\{ \exists i \in [k] \text{ and } a \in \mathcal{I}_i \text{ such that } \left| \mathbb{E} [R_i \mid a] - \hat{R}_{(a,i)} \right| > \hat{\eta}_i \mid E_3, E_1 \right\} \leq \frac{k}{T}$$

Equivalently,

$$\mathbb{P}\{\neg E_5 \mid E_3, E_1\} \leq \frac{k}{T}$$

**Proof.** For intermediate states $i \in [k]$, we denote the realization of the causal parameters $m_i$ and the transition probabilities $P$ in Algorithm 4, as $\hat{m}_i$ and $\hat{P}$, respectively. The estimates in the previous subroutines are denoted by $\hat{m}_i$ and $\hat{P}$.

Event $E_1$ gives us $P_{(a,i)} \in \left[ \frac{3}{4} \hat{P}_{(a,i)}, \frac{3}{2} \hat{P}_{(a,i)} \right]$ and $\hat{P}_{(a,i)} \in \left[ \frac{3}{4} P_{(a,i)}, \frac{3}{2} P_{(a,i)} \right]$. Hence, the estimates across the subroutines are close enough: $\hat{P}_{(a,i)} \in \left[ \frac{3}{4} P_{(a,i)}, 2 \hat{P}_{(a,i)} \right]$. Similarly, event $E_3$ gives us $\hat{m}_i \in \left[ \frac{1}{3} \hat{m}_i, 3 \hat{m}_i \right]$.

Write $\hat{T}_i$ to denote the number of times state $i \in [k]$ was visited in Algorithm 4. For all states $i \in [k]$, we first establish a useful lower bound on $\hat{T}_i$, under events $E_1$ and $E_3$. The relevant observation here is that
the estimate $\tilde{P}_{(\alpha, i)}$ was computed in Algorithm 4 by counting the number of times state $i$ was visited with intervention $\alpha \in \mathcal{I}_0$ (at state 0). By construction, in Algorithm 4 each intervention $\alpha \in \mathcal{I}_0$ was performed at least $\frac{T \hat{f} \alpha}{3}$ times. Furthermore, given that $\tilde{P}_{(\alpha, i)}$ was computed via the visitation count, we get that state $i$ is visited with intervention $\alpha \in \mathcal{I}_0$ at least $\tilde{P}_{(\alpha, i)} T \hat{f} \alpha$ times. Therefore,

$$\tilde{T}_i \geq \sum_{\alpha \in \mathcal{I}_0} \tilde{P}_{(\alpha, i)} \frac{T \hat{f} \alpha}{9} = \frac{T}{9} (\tilde{P} \hat{f}^*)_i \geq \frac{T}{18} (\tilde{P} \hat{f}^*_*)_i$$

Here, the last inequality follows from the above-mentioned proximity between $\hat{P}$ and $\tilde{P}$.

Now, note that, at each state $i \in [k]$, Algorithm 4 (by construction) observes every intervention $a \in \mathcal{I}_i$ at least $\tilde{T}_{(a, i)}$ times. Write $\tilde{T}_{(a, i)}$ to denote the number of times intervention $a \in \mathcal{I}_i$ is observed in this subroutine. Hence,

$$\tilde{T}_{(a, i)} \geq \frac{\tilde{T}_i}{m_i} \geq \frac{1}{m_i} \frac{T}{18} (\tilde{P} \hat{f}^*)_i \geq \frac{1}{3m_i} \frac{T}{18} (\tilde{P} \hat{f}^*_*)_i$$

(17)

For each state $i \in [k]$ and intervention $a \in \mathcal{I}_i$, define the event $\neg E_5(a, i)$ as $|E_{[R_i | a]} - \tilde{R}_{(a, i)}| > \hat{\eta}_i$. Hoeffding’s inequality gives us:

$$\mathbb{P}\{\neg E_5(a, i) | E_1, E_3\} \leq 2 \exp \left(-\frac{T (\tilde{P} \hat{f}^*_*)_i \hat{\eta}^2_i}{27 m_i} \right) \leq 2 \exp \left(-\frac{T \log (2TN)}{27m_i} \right)$$

The last inequality is obtained by substituting Equation 17.

Recall that $\hat{\eta}_i = \sqrt{\frac{27m_i}{T(\tilde{P} \hat{f}^*_*)_i} \log (2TN)}$. Hence, the previous inequality corresponds to

$$\mathbb{P}\{\neg E_5(a, i) | E_1, E_3\} \leq 2 \exp \left(-\frac{T (\tilde{P} \hat{f}^*_*)_i \hat{\eta}^2_i}{27m_i} \right) = \frac{1}{TN}$$

Note that $\neg E_5 = \bigcup_{i \in [k]} \bigcup_{a \in \mathcal{I}_i} E_5(a, i)$. Taking a union bound over all states $i \in [k]$ and interventions $a \in \mathcal{I}_i$, we obtain

$$\mathbb{P}\{\neg E_5 | E_1, E_3\} \leq \frac{kN}{TN} = \frac{k}{T}$$

This completes the proof.

A.6 Bound on bad event (F):

Here we restate and prove Lemma 4.

**Lemma 4 (Bound on Bad Event).** Write $T_0 := \mathcal{O} \left( \frac{N \max(m_i)}{p_+} \log (2NT) \right) = \widetilde{\mathcal{O}} \left( \frac{N \max(m_i)}{p_+} \right)$. Then for any $T > T_0$:

$$\mathbb{P}\{F\} \leq \frac{5k}{T}.$$
Proof. To summarize the statements of Lemmas 5, 7, 8, 9 and 10, let $T \geq T_0$ where $T_0$ is given by:

$$T_0 = \max \left\{ \frac{1620N}{p_+^3}, \frac{2025N}{p_+^2} \log \left( \frac{9NT}{k} \right), 144m_0 \log \left( \frac{Tn}{k} \right), \frac{864 \max(m_i)N}{p_+} \log (2nT) \right\}$$

$$= \mathcal{O} \left( \frac{N \max(m_i)}{p_+^3} \log (2NT) \right)$$

Then we obtain:

$$\mathbb{P}\{F\} = \mathbb{P} \left\{ \bigcup_{i \in [5]} \neg E_i \right\} \leq \mathbb{P}\{\neg E_1\} + \mathbb{P}\{\neg E_2\} + \mathbb{P}\{\neg E_3 \mid E_1\} + \mathbb{P}\{\neg E_4 \mid E_2\} + \mathbb{P}\{\neg E_5 \mid E_3, E_1\} \leq \frac{5k}{T}$$

This completes the proof.

B Convexity of the Optimization Problems

Proposition B.1. Let $\hat{f} = \arg \max_{\mathbf{f} \in \mathbb{R}^k} \min_{\pi \in \mathcal{P}_k} \hat{\mathbf{P}}^\top f$. Then, finding $\hat{f}$ is an LP.

Proof. We rewrite the above $\max_{\mathbf{f} \in \mathbb{R}^k} \min_{\pi \in \mathcal{P}_k} \hat{\mathbf{P}}^\top f$ as a simpler program:

$$\max_{\mathbf{f}} z$$

subject to

$$\hat{\mathbf{P}}^\top_1 \mathbf{f} \geq z$$

$$\ldots$$

$$\hat{\mathbf{P}}^\top_N \mathbf{f} \geq z$$

$$\mathbf{f} \cdot \mathbf{1} = 1$$

$$\mathbf{f} \succeq 0$$

Where $N = |\mathcal{I}_0|$. This is equivalent to the standard form of a linear program, and hence is an LP.

Lemma 11. $\min_{\mathbf{f} \in \mathbb{R}^k} \max_{\pi \in \mathcal{P}_k} \hat{\mathbf{P}} \hat{\mathbf{M}}^{-\frac{1}{2}} \left[ \hat{\mathbf{P}}^\top \mathbf{f} \right]^{0 - \frac{1}{2}}$ is a convex optimization problem.

Proof. First we write the min-max in terms of a single minimization. First let us use the shorthand
\[
A := \hat{P}M^{\frac{1}{2}} \text{ and } \{A_1, \ldots, A_N\} \text{ (where } N := |I_0|) \text{ denote the rows of the matrix }
\]

\[
\text{OPT}: \min_f z
\]

subject to \[
A_1 \cdot \left[\hat{P}^\top f\right]^{0-\frac{1}{2}} \leq z
\]

\[
\ldots
\]

\[
A_N \cdot \left[\hat{P}^\top f\right]^{0-\frac{1}{2}} \leq z
\]

\[
f \cdot 1 = 1
\]

\[
f \succeq 0
\]

Proposition B.2. For any \( a \in \mathbb{R}_+ \), the function \( g(x) := ax^{-\frac{1}{2}} \) is convex in \( x \).

Proof. We observe that the second derivative is positive. \( \square \)

Proposition B.3. The constraint equations of OPT are convex in \( f \)

Proof. Consider the first constraint of the problem. We can simplify this to get \[
\sum_{i \in [k]} \frac{A_{1i}}{\sqrt{P^{(i,i)}_f}}.
\]

Note that the \( i \)th term in the summand (i.e., \( \frac{A_{1i}}{\sqrt{P^{(i,i)}_f}} \)) is of the form \( f(x) = c(v^\top x)^{-\frac{1}{2}} \) for some \( c \in \mathbb{R}_+ \) and \( v \in \mathbb{R}_+^N \). Let \( x_1, x_2 \in \mathbb{R}^N \) be any two vectors, and scalar \( \lambda \in [0,1] \). We wish to show that \( f(\lambda x_1 + (1-\lambda)x_2) \leq \lambda f(x_1) + (1-\lambda)f(x_2) \).

We have \( f(\lambda x_1 + (1-\lambda)x_2) = c(v^\top(\lambda x_1 + (1-\lambda)x_2))^{-\frac{1}{2}} = c(\lambda v^\top x_1 + (1-\lambda)v^\top x_2)^{-\frac{1}{2}} \)

But \( ax^{-\frac{1}{2}} \) is convex as per Proposition B.2. Therefore \( c(\lambda v^\top x_1 + (1-\lambda)v^\top x_2)^{-\frac{1}{2}} \leq \lambda c(v^\top x_1)^{-\frac{1}{2}} + (1-\lambda)c(v^\top x_2)^{-\frac{1}{2}} = \lambda f(x_1) + (1-\lambda)f(x_2) \), as required.

Since \( \frac{A_{1i}}{\sqrt{P^{(i,i)}_f}} \) is convex, the sum \( \sum_{i \in [k]} \frac{A_{1i}}{\sqrt{P^{(i,i)}_f}} \) is convex as well. Similarly, all the other constraints are also convex. \( \square \)

Since the constraints are convex in \( f \) and the objective is linear, OPT is convex. \( \square \)

C Proof of KL-Divergence Inequality

For completeness, we provide a proof of inequality (5).

Lemma 12. \( \text{KL}(P_0, P_{(a,i)}) \leq 6\beta_1^2 \mathbb{E}_{P_0}[T_{(a,i)}] \)

Proof of Inequality (5). This proof is based on Lemma B1 in [ACBFS95]. We define a couple of notations for this proof. Let \( R_{t-1} \) indicate the filtration (of rewards and other observations) up to time \( t-1 \).
and $R_t$ indicate the reward at time $t$ for this proof.

$$\text{KL}(\mathcal{P}_0, \mathcal{P}_{(a,i)}) = \text{KL} \left[ \mathbb{P}_{\mathcal{P}_0}(R_T, R_{T-1}, \ldots, R_1) \parallel \mathbb{P}_{\mathcal{P}_{(a,i)}}(R_T, R_{T-1}, \ldots, R_1) \right]$$

We now state (without proof) a useful lemma for bounding the KL divergence between random variables over a number of observations.

**Chain Rule for entropy (Theorem 2.5.1 in [CT06]):** Let $X_1, \ldots, X_T$ be random variables drawn according to $P_1, \ldots, P_T$. Then

$$H(X_1, X_2, \ldots, X_T) = \sum_{t=1}^{T} H(X_t | X_{t-1}, X_{t-2}, \ldots, X_1)$$

where $H(\cdot)$ is the entropy associated with the random variables.

Using the chain rule for entropy

$$\text{KL}(\mathcal{P}_0, \mathcal{P}_{(a,i)}) = \sum_{t=1}^{T} \text{KL} \left[ \mathbb{P}_{\mathcal{P}_0}(R_t | R_{t-1}) \parallel \mathbb{P}_{\mathcal{P}_{(a,i)}}(R_t | R_{t-1}) \right]$$

Let $a_t$ be the intervention chosen by the Algorithm $A$ at time $t$. Then:

$$= \sum_{t=1}^{T} \mathbb{P}_{\mathcal{P}_0}\{a_t \neq a | R_{t-1}\} \left( \frac{1}{2} \parallel \frac{1}{2} \right) + \mathbb{P}_{\mathcal{P}_0}\{a_t = a | R_{t-1}\} \text{KL} \left( \frac{1}{2} \parallel \frac{1}{2} + \beta_i \right)$$

Since $\text{KL} \left( \frac{1}{2} \parallel \frac{1}{2} \right) = 0$, we get:

$$= \sum_{t=1}^{T} \mathbb{P}_{\mathcal{P}_0}\{a_t = a | R_{t-1}\} \text{KL} \left( \frac{1}{2} \parallel \frac{1}{2} + \beta_i \right)$$

$$= \text{KL} \left( \frac{1}{2} \parallel \frac{1}{2} + \beta_i \right) \sum_{t=1}^{T} \mathbb{P}_{\mathcal{P}_0}\{a_t = a | R_{t-1}\}$$

$$= \text{KL} \left( \frac{1}{2} \parallel \frac{1}{2} + \beta_i \right) \mathbb{E}_{\mathcal{P}_0}[T_{(a,i)}]$$

**Claim C.1.** $\text{KL} \left( \frac{1}{2} \parallel \frac{1}{2} + \beta_i \right) = -\frac{1}{2} \log_2(1 - 4\beta_i^2) \leq 6\beta_i^2$

**Proof.**

$$\text{KL} \left( \frac{1}{2} \parallel \frac{1}{2} + \beta_i \right) = \frac{1}{2} \log_2 \left[ \frac{\frac{1}{2} \parallel \frac{1}{2} + \beta_i}{\frac{1}{2} + \beta_i} \right] + (1 - \frac{1}{2}) \log_2 \left[ \frac{(1 - \frac{1}{2})}{(1 - \frac{1}{2} + \beta_i)} \right]$$

$$= \frac{1}{2} \log_2 \left[ \frac{\frac{1}{2} \parallel \frac{1}{2} + \beta_i}{\frac{1}{2} + \beta_i} \right] + \frac{1}{2} \log_2 \left[ \frac{1}{1 - 2\beta_i} \right] = \frac{1}{2} \log_2 \left[ \frac{1}{1 - 4\beta_i^2} \right] = -\frac{1}{2} \log_2 \left[1 - 4\beta_i^2 \right]$$

$$= -\frac{1}{2 \ln(2)} \ln \left[1 - 4\beta_i^2 \right] \leq \frac{4\beta_i^2}{2 \ln(2)} < 6\beta_i^2$$

where the last inequality is obtained from the Taylor series expansion of the log.

It follows that: $\text{KL}(\mathcal{P}_0, \mathcal{P}_1) \leq 6\beta_i^2 \mathbb{E}_{\mathcal{P}_0}[T_{(a,i)}]$. 

\[ \square \]