# Gaussian Randomized Exploration for Semi-bandits with Sleeping Arms

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## Abstract

This paper provides theoretical analyses of problem-independent upper and lower 1 regret bounds for Gaussian randomized algorithms in semi-bandits with sleeping 2 arms, where arms may be unavailable in certain rounds, and available arms satis-3 fying combinatorial constraints can be played simultaneously. We first introduce 4 the CTS-G algorithm, an adaptation of Thompson sampling with Gaussian priors, 5 achieving an upper bound of  $O(m\sqrt{NT})$  over T rounds with N arms and up to m 6 arms played per round, where O hides the logarithmic factors. Next, we present 7 CL-SG, which improves upon CTS-G by using a single Gaussian sample per round, 8 achieving a near-optimal upper regret bound of  $O(\sqrt{mNT})$ . We also establish that 9 both algorithms have lower regret bounds of  $\Omega(\sqrt{mNT \ln \frac{N}{m}})$  and  $\Omega(\sqrt{mNT})$ , 10 respectively. 11

# 12 **1** Introduction

We consider a sleeping semi-bandit problem with a fixed set  $[N] = \{1, 2, \ldots, N\}$  of N base arms 13 and each base arm  $a \in [N]$  is associated with an unknown probability distribution  $p_a$  supported on 14 [0, 1] and mean  $r_a$ . Unlike standard combinatorial bandits (Kveton et al., 2015), where a learning 15 agent, in each round  $t = 1, \ldots, T$ , plays a super arm (combinations of base arms)  $A_t \in \Theta$ , 16 where  $\Theta \subseteq 2^{[N]}$  is a *feasible set* that satisfy certain constraints, sleeping semi-bandits involve a 17 time-varying feasible set  $\Theta_t \subseteq \Theta$ , revealed at each round t. After observing the feasible set  $\Theta_t$  in 18 round t, the learning agent selects a super arm  $A_t \in \Theta_t$ , observes rewards  $r_{a,t} \sim p_a$  for each base 19 arm  $a \in A_t$ , and aims to minimize the T-round (pseudo)-regret defined as follows. 20

$$\mathcal{R}(T) := \sum_{t=1}^{T} \mathbf{E} \left[ \sum_{a \in A_t^*} r_a - \sum_{a \in A_t} r_a \right], \tag{1}$$

where  $A_t^* := \arg \max_{A \in \Theta_t} \sum_{a \in A} r_a$  denotes the optimal super arm in round t and the expectation is taken over  $\Theta_t$ ,  $A_t$ , and  $A_t^*$ . Note that  $A_t^*$  is determined by  $\Theta_t$ . We further denote by  $m := \max_{A \in \Theta} |A|$  the maximum number of base arms in any super arm.

The upper confidence bound (UCB) (Agrawal, 1995; Auer et al., 2002) and Thompson sam-24 pling (TS) (Thompson, 1933; Kaufmann et al., 2012; Agrawal & Goyal, 2012, 2017a) are two 25 leading algorithmic families for addressing stochastic bandit problems. For semi-bandit settings, the 26 minimax lower bound is established as  $\Omega(\sqrt{mNT})$  (Kveton et al., 2015; Merlis & Mannor, 2020), and 27 UCB-based algorithms achieve an upper bound of  $O(\sqrt{mNT} \ln T)$  (Kveton et al., 2015). Although 28 TS-based algorithms have been analyzed for problem-dependent bounds in semi-bandits (Wang & 29 Chen, 2018; Perrault et al., 2020), their results cannot be simply extended to reasonable problem-30 independent bounds because their bounds contain constant terms that grow exponentially with m. 31

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- <sup>32</sup> While a substantial body of literature has explored the setting of sleeping semi-bandits (Hu et al.,
- <sup>33</sup> 2019; Li et al., 2019; Wu & Li, 2024) using *upper confidence bound (UCB)*-based algorithms with an
- <sup>34</sup> upper bound of  $O(\sqrt{mNT \ln T})$ , the upper and lower bounds for *Thompson sampling (TS)*-based
- algorithms for (sleeping) semi-bandits still remain an open problem. Since TS is highly competitive
   with advanced UCB-based algorithms and widely used in large-scale applications (Chapelle & Li,
- 2011) investigating the theoretical performance of TS based algorithms is erucial
- 2011), investigating the theoretical performance of TS-based algorithms is crucial.

This work addresses long-standing gaps in the literature by introducing two algorithms with provable theoretical guarantees. The first algorithm, CTS-G, is an adaptation of TS with Gaussian priors specifically designed for sleeping semi-bandits, achieving an upper bound of  $\tilde{O}(m\sqrt{NT})$ , where  $\tilde{O}$  hides the logarithmic factors, and a lower bound of  $\Omega(\sqrt{mNT} \ln \frac{N}{m})$ . We further introduce

- 42 CL-SG, which improves upon CTS-G both theoretically and practically by employing only a single
- 43 Gaussian sample, resulting in tighter bounds: an upper bound of  $\tilde{O}(\sqrt{mNT})$  and a lower bound of
- 44  $\Omega(\sqrt{mNT})$ . CL-SG is minimax-optimal up to logarithmic factors compared to the known lower

bound for combinatorial bandits (Kveton et al., 2015; Merlis & Mannor, 2020).

# 46 **2** Gaussian Randomized Algorithms

We first present some notations specific to this section. Let  $n_{a,t} := \sum_{\tau=1}^{t-1} \mathbf{1}[a \in A_{\tau}]$  denote the total number of times that base arm  $a \in [N]$  has been pulled at the beginning of round t. Let  $\hat{r}_{a,n_{a,t}} := \frac{\sum_{\tau=1}^{t-1} \mathbf{1}[a \in A_{\tau}] \cdot r_{a,\tau}}{n_{a,t}}$  denote the empirical mean of base arm a at the beginning of round t, which is the average of  $n_{a,t}$  i.i.d. random variables according to reward distribution  $p_a$ . Let  $\mathcal{F}_t$ collect all the actions and observed rewards up to the end of round t

In Sec. 2.1, we present CTS-G, an algorithm enjoying  $\tilde{O}(m\sqrt{NT})$  and  $\Omega(\sqrt{mNT \ln \frac{N}{m}})$  upper and lower regret bounds. In Sec. 2.2, we present CL-SG, an algorithm enjoying  $\tilde{O}(\sqrt{mNT})$  and  $\Omega(\sqrt{mNT})$  upper and lower regret bounds. The practical performance of both algorithms is discussed in Appendix A, and all the detailed proofs can be found in Appendix C to D.

## 56 2.1 Combinatorial Thompson Sampling with Gaussian Priors (CTS-G)

CTS-G presented in Alg. 1 is a direct adaptation of TS with Gaussian priors (Agrawal & Goyal, 2017b) 57 to the sleeping semi-bandit problems. The core idea is to use posterior distributions to model the mean 58 reward  $r_a$  of each base arm  $a \in [N]$ . In each round t, CTS-G draws a Gaussian posterior sample  $w_{a,t} \sim \mathcal{N}(\hat{r}_{a,n_{a,t}}, \frac{\gamma m \ln t}{n_{a,t}+1})$  for each  $a \in [N]$ , where  $\gamma > 0$  is a constant parameter to control the 59 60 exploration level.<sup>1</sup> We can view the collection  $w_t = \{w_{a,t}, \forall a \in [N]\}$  of all posterior samples as 61 the "sampled problem instance" based on which the learning agent conducts learning in round t. Then, 62 based on the revealed feasible set  $\Theta_t$ , CTS-G plays the super arm  $A_t \in \arg \max_{A \in \Theta_t} \sum_{a \in A} w_{a,t}$ with the highest aggregated value of posterior samples and observes each individual base arm's 63 64 random reward. 65

**Theorem 1.** (1) The regret of CTS-G is  $O\left(m \ln(T)\sqrt{NT}\right)$ . (2) There exists a problem instance such that CTS-G suffers  $\Omega\left(\sqrt{mNT \ln\left(\frac{N}{m}\right)}\right)$  regret.

**Discussion.** Theorem 1 states that CTS-G is worst-case optimal up to an extra  $\ln(T)\sqrt{m}$  factor. 68 Compared with UCB-based algorithms for sleeping semi-bandits, our upper bound has an extra 69 factor of  $\sqrt{m \ln T}$  with the ones by Hu et al. (2019); Li et al. (2019), which are  $O(\sqrt{mNT \ln T})$ . 70 However, it is important to note a significant aspect of our model: unlike the assumptions in Hu et al. 71 (2019); Li et al. (2019), our bound is derived without relying on stochastic assumptions regarding 72 the availability of arms. Furthermore, the upper bound is minimax optimal up to an extra  $\ln(T)\sqrt{m}$ 73 factor as compared to the  $\Omega\left(\sqrt{mNT}\right)$  minimax lower bound for combinatorial bandits shown in 74 Merlis & Mannor (2020). 75

<sup>&</sup>lt;sup>1</sup>In practice, we only need to draw posterior samples for available arms to improve efficiency.

<sup>76</sup> **Upper bound proof sketch.** The theoretical analysis is non-trivial due to overlapping base arms <sup>77</sup> among super arms, the dynamic nature of the optimal super arm  $A_t^*$ , and its unobservability, as only the <sup>78</sup> played super arm  $A_t$  is observed in each round t To decompose the regret, we define a high probability

<sup>79</sup> event for the empirical estimates. Let  $\mathcal{E}_t := \left\{ |r_a - \hat{r}_{a,n_{a,t}}| \le \sqrt{\frac{3 \ln(Nt)}{n_{a,t}+1}}, \forall a \in [N] \right\}$  be the <sup>80</sup> event that the empirical means are close to their true means by the beginning of round t. Let <sup>81</sup>  $t' = \max\{\sqrt{m}, 4\}$  and  $\mathbf{E}_{\Theta_t}[\cdot] := \mathbf{E}[\cdot | \Theta_t]$ . Then, we decompose the regret defined in (1) as

$$\mathcal{R}(T) \leq \underbrace{\sum_{t=t'}^{T} \mathbf{E}\left[\sum_{a \in A_t^*} r_a - \mathbf{E}_{\Theta_t}\left[\sum_{a \in A_t} w_{a,t}\right]\right]}_{=:I_1, \text{ optimism term}} + \underbrace{\sum_{a \in A_t}^{T} \mathbf{E}\left[\mathbf{E}_{\Theta_t}\left[\sum_{a \in A_t} (w_{a,t} - r_a) \mathbf{1}[\mathcal{E}_t]\right]\right]}_{=:I_2, \text{ deviation term}} + mt' + O(1)$$

The deviation term  $I_2$  is easy to analyze as we can observe  $A_t$ , and is upper bounded by  $\tilde{O}(m\sqrt{NT})$ via using concentration bounds. The center question is how to upper bound the optimism term, which measures the gap between the maximum amount of true reward  $\sum_{a \in A_t^*} r_a$  the learning agent could achieve and the expected maximum amount of reward  $\sum_{a \in A_t^*} w_{a,t}$  the learning agent can observe in round t. Intuitively, if the learning agent is lucky, i.e., the history  $\mathcal{F}_{t-1}$  gives  $\sum_{a \in A_t^*} r_a \leq$  $\mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} w_{a,t} \right]$ , there is no regret in round t for this term. Let  $(\cdot)^+ := \max \{\cdot, 0\}$  be an activation function. Then, we have

$$\sum_{a \in A_t^*} r_a - \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} w_{a,t} \right] \leq \left( \sum_{a \in A_t^*} r_a - \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} w_{a,t} \right] \right)^+ .$$
(2)

Let  $c(\gamma)$  be a constant only depending on  $\gamma$ . In our novel technical Lemma 1, inspired by Russo (2019), we show

$$\left(\sum_{a\in A_t^*} r_a - \mathbf{E}_{\Theta_t} \left[\sum_{a\in A_t} w_{a,t}\right]\right)^+ \leq c(\gamma) \cdot \mathbf{E}_{\Theta_t} \left[ \left(\sum_{a\in A_t} w_{a,t} - \mathbf{E}_{\Theta_t} \left[\sum_{a\in A_t} w_{a,t}\right]\right)^+ \right]$$
(3)

which tackles the challenge brought by the unobservability of  $A_t^*$ .

Next, via introducing an independent "ghost" copy  $\tilde{w}_{a,t} \sim \mathcal{N}(\hat{r}_{a,n_{a,t}}, \frac{\gamma m \ln t}{n_{a,t}+1})$  of  $w_{a,t}$ , we show

$$\mathbf{E}_{\Theta_t} \left[ \left( \sum_{a \in A_t} w_{a,t} - \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} w_{a,t} \right] \right)^+ \right] \leq \mathbf{E}_{\Theta_t} \left[ \left| \sum_{a \in A_t} (w_{a,t} - \tilde{w}_{a,t}) \right| \right], \quad (4)$$

<sup>93</sup> which gets rid of the introduced activation function.

Since  $w_{a,t} - \tilde{w}_{a,t} \sim \mathcal{N}\left(0, \frac{2\gamma m \ln t}{n_{a,t}+1}\right)$ , we only need to deal with Gaussian random variables and have

$$\sum_{t=t'}^{T} \mathbf{E} \left[ \left| \sum_{a \in A_t} \left( w_{a,t} - \tilde{w}_{a,t} \right) \right| \right] \leq O \left( m \ln T \sqrt{\gamma NT} \right).$$
(5)

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**Lower bound proof sketch.** Inspired by Theorem 1.4 in Agrawal & Goyal (2017b), the lower bound is refined by constructing a path selection problem with N links (base arms) and K paths (super arms) of m links. This reduces the semi-bandits to K independent path selections, and the result follows using the anti-concentration inequality for Gaussian variables (Appendix C.7)

#### 101 2.2 Combinatorial Learning with Single Gaussian Seed (CL-SG)

Since the upper bound of CTS-G still has an extra  $\ln(T)\sqrt{m}$  factor from the minimax lower bound Merlis & Mannor (2020) for combinatorial bandits, we are motivated to improve the upper bound by controlling the amount of randomness injected within the learning algorithm.

Inspired by Xiong et al. (2022), we devise CL-SG which enjoys a  $O(\sqrt{mNT})$  regret bound. The key idea behind the removal of the extra  $\sqrt{m}$  factor as compared to the regret of CTS-G (Alg. 1) is CL-SG uses a single random seed  $w_t \sim \mathcal{N}(0, 1)$  to perturb the empirical estimates of all the base arms, as shown in Alg. 2. After drawing  $w_t$ , we construct  $\bar{r}_{a,t} = \hat{r}_{a,n_{a,t}} + w_t \cdot \sqrt{\frac{\gamma \ln t}{n_{a,t}+1}}$ for all the base arms  $a \in [N]$ , where constant  $\gamma > 0$  controls the exploration level. Then, we play  $A_t = \arg \max_{A \in \Theta_t} \sum_{a \in A} \bar{r}_{a,t}$  from the feasible set  $\Theta_t$  in round t.

**Theorem 2.** (1) The regret of CL-SG is  $O\left(\ln T\sqrt{mNT}\right)$ . (2) There exists a problem instance such that CL-SG suffers  $\Omega\left(\sqrt{mNT}\right)$  regret.

**Discussion.** The extra  $\sqrt{m}$  in CTS-G comes from the *m* factor in the variance of the Gaussian posterior sample  $w_{a,t}$ , necessary to keep  $c(\gamma)$  bounded by a constant. To bound  $c(\gamma)$ , we must lower bound  $\Pr_{\Theta_t} \left( \sum_{a \in A_t^*} w_{a,t} - \hat{r}_{a,n_{a,t}} \ge \sum_{a \in A_t^*} \sqrt{\frac{4 \ln t}{n_{a,t}+1}} \right)$ , requiring the Cauchy-Schwarz inequality to bring the summation inside the square root for the RHS term in the probability, which scales with  $\sqrt{m}$ , i.e.,  $\sum_{a \in A_t^*} \sqrt{\frac{4 \ln t}{n_{a,t}+1}} \le \sqrt{m \sum_{a \in A_t^*} \frac{4 \ln t}{n_{a,t}+1}}$ . This fact further results in an extra *m* in the variance of CTS-G Gaussian samples for the probability to be lower bounded by a constant. On the other hand, with CL-SG, using a single  $w_t$ , we lower bound a similar probability,  $\Pr\left(\sum_{a \in A_t^*} w_t \sqrt{\frac{\gamma \ln t}{n_{a,t}+1}} \ge \sum_{a \in A_t^*} \sqrt{\frac{4 \ln t}{n_{a,t}+1}}\right)$ , allowing us to divide both sides by  $\sum_{a \in A_t^*} \sqrt{\frac{4 \ln t}{n_{a,t}+1}}$  and avoid the extra *m* in the variance.

The lower-bound proof considers the same problem instance to Theorem 1 but differs in addressing 122 the arms' dependency in CL-SG due to the common  $w_t$ . Let  $\Delta := \sqrt{\frac{N}{mT}}$  be the reward gap between 123 each suboptimal arm and the optimal super arm, and let  $Q_A(t)$  be the number of times that super 124 arm A has been played at the beginning of round t. Then, denote by  $B_t^* := \{Q_{A_1}(t) > t - cT\}$ 125 the event that the optimal super arm  $A_1$  has been observed enough times at the beginning of 126 round t, where  $c \in (0, 1)$  is a constant. It is easy to prove that the regret is lower bounded 127 by  $cT \cdot m \cdot \Delta = \Omega(\sqrt{mNT})$  when  $B_t^*$  is false for some  $t \in [T]$ . The main challenge is 128 to demonstrate that, conditioned on the past histories  $F_{t-1}$  that lead to the happening of event 129  $B_t^*$ , the probability of playing a suboptimal super arm is at least a constant probability  $p_0$ , i.e., 130  $\Pr\left(\exists A \in \Theta \setminus A_1 : A_t = A \mid \mathcal{F}_{t-1} = F_{t-1}\right) \geq p_0$ . This leads to lower bound a probability 131 that the empirical estimates of suboptimal arms are larger than the optimal super arm, i.e., 132

$$\Pr\left(\exists A \in \Theta \setminus A_{1} : \sum_{a \in A} \hat{r}_{a,Q_{A}(t)} + w_{t} \sqrt{\frac{\gamma \ln t}{Q_{A}(t) + 1}} > \sum_{b \in A_{1}} \hat{r}_{b,Q_{A_{1}}(t)} + w_{t} \sqrt{\frac{\gamma \ln t}{Q_{A_{1}}(t) + 1}} \mid \mathcal{F}_{t-1} = F_{t-1} \right)$$

$$\geq \Pr\left(\exists A \in \Theta \setminus A_{1} : w_{t} \left(1 - \sqrt{\frac{Q_{A}(t) + 1}{Q_{A_{1}}(t) + 1}}\right) > \Delta \sqrt{Q_{A}(t) + 1} \mid \mathcal{F}_{t-1} = F_{t-1} \right).$$

This requires analyzing the play ratio between suboptimal and optimal super arms, while in the lower-bound analysis of Theorem 1, we can avoid this situation by independently considering the estimates of the optimal super arm is smaller than 0, and that of suboptimal arms is larger than 0. The trick to address this ratio is to only consider the regret from  $\alpha T$  to T, with  $\alpha \in (0, 1)$  such that  $\frac{Q_A(t)+1}{Q_{A_1}(t)+1} \leq \frac{cT+1}{(\alpha-c)T+1}$  is a constant by tuning c and  $\alpha$ . Then, by applying the anti-concentration bound for Gaussian variables and solving a non-trivial optimization problem, we can prove such a  $p_0$ exists, and regret is lower bounded by  $(1 - \alpha)T \cdot p_0 \cdot m\Delta = \Omega(\sqrt{mNT})$ .

## 140 3 Conclusion

In this paper, we have studied the problem of sleeping semi-bandits and presented CTS-G and CL-SG with theoretical guarantees. Our results bridge the existing gap in the literature by providing upper and lower bounds for TS-based algorithms in sleeping semi-bandits. Future work will focus on narrowing the gap between these bounds, and studying the relationship between the number of random variables and their variances.

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## **187 A** Numerical Experiments

#### 188 A.1 Algorithm Description for CTS-G and CL-SG

<sup>189</sup> The algorithm descriptions for CTS-G and CL-SG are presented in Algs. 1 and 2, respectively.

Algorithm 1 Combinatorial Thompson Sampling with Gaussian Priors (CTS-G)

**Require:** arm set [N], exploration rate  $\gamma$ Initialize  $n_{a,1} = 0$  and  $\hat{r}_{a,n_{a,1}} = 0$  for all base arms  $a \in [N]$ for  $t = 1, 2, \ldots$  do Observe feasible set  $\Theta_t$ Draw  $w_{a,t} \sim \mathcal{N}(\hat{r}_{a,n_{a,t}}, \frac{\gamma m \ln t}{n_{a,t}+1})$  for each base arm  $a \in [N]$ Play super arm  $A_t = \underset{A \in \Theta_t}{\arg \max} \sum_{a \in A} w_{a,t}$ Observe  $r_{a,t} \sim p_a$  for all base arms  $a \in A_t$  and update  $n_{a,t}$  and  $\hat{r}_{a,n_{a,t}}$  for all  $a \in A_t$ . end for

#### Algorithm 2 Combinatorial Learning with Single Gaussian Seed (CL-SG)

**Require:** arm set [N], exploration rate  $\gamma$ Initialize  $n_{a,1} = 0$  and  $\hat{r}_{a,0} = 0$  for all base arms  $a \in [N]$ for  $t = 1, \dots$  do Observe decision set  $\Theta_t$ Draw  $w_t \sim \mathcal{N}(0, 1)$ Construct  $\bar{r}_{a,t} = \hat{r}_{a,n_{a,t}} + w_t \cdot \sqrt{\frac{\gamma \ln t}{n_{a,t}+1}}$  for all base arms  $a \in [N]$ Play super arm  $A_t = \underset{A \in \Theta_t}{\arg \max} \sum_{a \in A} \bar{r}_{a,t}$ Observe  $r_{a,t} \sim p_a$  for all base arms  $a \in A_t$  and update  $n_{a,t}$  and  $\hat{r}_{a,n_{a,t}}$  for all  $a \in A_t$ . end for

## 190 A.2 Combinatorial Learning with Least Gaussian Seed (CL-LG)

We aim to explore whether further reducing the number of Gaussian samples in the algorithm can enhance the practical performance. To this end, we propose the *Combinatorial Learning with Least Gaussian Seed (CL-LG)* algorithm, as shown in Alg. 3. Different from CL-SG (see Alg. 2), which requires an independent Gaussian sample in each round, our approach only draws a single Gaussian sample  $w \sim \mathcal{N}(0, 1)$  at the beginning of the game.

Algorithm 3 Combinatorial Learning with Least Gaussian Seed (CL-LG)

**Require:** arm set [N], exploration rate  $\gamma$ Initialize  $n_{a,1} = 0$  and  $\hat{r}_{a,0} = 0$  for all base arms  $a \in [N]$ Draw  $w \sim \mathcal{N}(0, 1)$ for  $t = 1, \dots$  do Observe feasible set  $\Theta_t$ Construct  $\bar{r}_{a,t} = \hat{r}_{a,n_{a,t}} + w \cdot \sqrt{\frac{\gamma \ln t}{n_{a,t}+1}}$  for all base arms  $a \in [N]$ Play super arm  $A_t = \underset{A \in \Theta_t}{\arg \max} \sum_{a \in A} \bar{r}_{a,t}$ Observe  $r_{a,t} \sim p_a$  for all base arms  $a \in A_t$  and update  $n_{a,t}$  and  $\hat{r}_{a,n_{a,t}}$  for all  $a \in A_t$ . end for

#### 196 A.3 Experiment Settings

We conduct experiments in two settings to show the performance of the proposed algorithms with  $\gamma = 0.1$  to study the number of Gaussian seeds and the impact of different  $\gamma$ , which can be found in Appendix A.4 and A.5. All the experiment results are the average of 100 independent experiments conducted on a MacBook Pro with M1 Max and 32GB RAM using Numpy.

In Setting 1, we consider a simple environment with N = 10 arms, and at most m = 3 arms can be played in each round. The actual rewards for all the arms follow the Bernoulli distributions, while the first three arms have a mean reward of 0.9, and the rest of the arms have a mean reward of 0.8. In Setting 2, we consider a more complicated setting where N = 50 and m = 15. In this setting, rewards are again based on Bernoulli distributions, where the first five arms have mean rewards generated uniformly from [0.725, 0.75], and the rest of the arms have mean rewards generated uniformly from [0.7, 0.725]. For both settings, the availability of each arm is determined by a Bernoulli distribution with a mean of 0.5. The reason we chose Bernoulli distributions for the rewards is that we want to compare with the following CTS-B (which requires Bernoulli rewards) and CombUCB algorithms. Both algorithms play arms  $A_t := \arg \max_{A \in \Theta_t} \sum_{a \in A} \theta_{a,t}$ , where  $\theta_{a,t}$  is defined differently as follows.

• CTS-B (Wang & Chen, 2018): In each round t, CTS-B draws random samples from Beta distributions for each available arm  $\theta_{a,t} \sim \mathbf{Beta}(\hat{r}_{a,n_{a,t}}n_{a,t} + 1, n_{a,t} - n_{a,t}\hat{r}_{a,n_{a,t}} + 1)$ , and plays arms  $A_t := \arg \max_{A \in \Theta_t} \sum_{a \in A} \theta_{a,t}$ .

• CombUCB (Kveton et al., 2015): In each rount t, CombUCB estimates the UCB values for each arm  $\theta_{a,t} = \hat{r}_{a,n_{a,t}} + \sqrt{\frac{1.5 \ln t}{n_{a,t}}}$  in each round t.

#### 217 A.4 Impact of Number of Gaussian Seed

The regret results over  $T = 10^5$  rounds are shown in Fig. 1 with 97.5% confidence intervals. In both settings, CTS-G performs worse than others, suffering the highest regret, because of the algorithm's reliance on Gaussian random samples, which are unbounded and result in an excessive exploration rate. This overemphasis on exploration, at the expense of exploiting known rewarding arms, fundamentally undermines the algorithm's efficiency.

On the other hand, CL-SG demonstrates comparable performance to CL-LG in Setting 1, both outperforming CTS-B. In Setting 2, CL-SG maintains its advantage, whereas CL-LG falls behind CTS-G. This highlights the effectiveness of CL-SG's design in optimizing the exploration-exploitation trade-off more efficiently than its counterparts.

Notably, in both settings, CL-LG with  $\gamma = 0.1$  outperforms CombUCB, suggesting that the initial

randomness incorporated in CL-LG helps balance the trade-off between exploration and exploitation.

It remains an open question of how initial randomness helps.



(a) Setting 1 (N = 10 and m = 3) (b) Setting 2 (N = 50 and m = 15)

Figure 1: The comparison of regret for both settings with  $\gamma = 0.1$ .

## 230 A.5 Impact of Different $\gamma$

We performed experiments with the CTS-G, CL-SG, and CL-LG algorithms under Settings 1 and 2. The experiments utilized  $\gamma$  values of 0.01, 0.1, 0.5, and 1. The results are illustrated in Figs. 2 and 3.

Regarding Setting 1, CTS-G performs worse as  $\gamma$  increases, as shown in Fig. 2a, because a higher  $\gamma$ corresponds to a higher exploration rate, which will over-explore the simple scenario. For CL-SG, the performance with  $\gamma = 0.1$  is better than that with other  $\gamma$  values. CL-LG achieves the best performance with 0.5, which indicates the performance of algorithms is not necessarily linear with  $\gamma$ .

<sup>237</sup> When comparing the algorithms at their optimal  $\gamma$  values (see Fig. 2d), CTS-G shows the worst <sup>238</sup> performance, whereas CL-SG performs comparably to CL-LG.



Figure 2: The comparison of different  $\gamma$  for CTS-G, CL-SG and CL-LG in Setting 1.

Additionally, CTS-G is very sensitive to the change of  $\gamma$ , and the performance of CTS-G with  $\gamma = 1$ is about 200 times worse than that of CTS-G with  $\gamma = 0.01$ . In contrast, CL-SG and CL-LG demonstrate greater robustness to changes in  $\gamma$ , showing that fewer Gaussian samples may prevent over-exploration.

Regarding the more complicated Setting 2, we can observe a change in CL-LG, where  $\gamma = 1$  leads to the worst performance, while  $\gamma = 0.5$  achieves the best performance. This indicates that CL-LG with  $\gamma = 1$  will over-explore. When comparing all the algorithms with their optimal  $\gamma$  values, we can see that CL-SG with  $\gamma = 0.1$  achieves the best performance. More interestingly, we can observe that algorithms with fewer Gaussian samples require higher  $\gamma$  to achieve better performance.

From this experiment, we can see that different Gaussian samples react differently to different exploration rates. This observation raises an intriguing question for future research: what is the relationship between the number of random variables and their variance, and what is the optimal combination to achieve the best results?

## 252 A.6 Tightness of regret bound

We consider a setting of 100 arms, and at most 10 arms can be played in each round. The mean rewards for the first 10 arms are 0.925, and the mean rewards for the rest suboptimal arms are 0.9.

We compare the regret of CTS-G with the lower regret bound  $0.1\sqrt{mNT \ln(\frac{N}{m})}$  in Fig. 4a. As we

can see, there are still gaps between the actual performance and the theoretical lower bound, and the

257 increasing rate of CTS-G is larger than the lower bound, which indicates that the lower bound may 258 still have room to be improved.

Similarly, we compared CT-SG with the lower bound of  $0.1\sqrt{mNT}$ , and we can see that the regret of CL-SG increases faster than the lower bound, indicating that the lower bound can be improved.



Figure 3: The comparison of different  $\gamma$  for CTS-G, CL-SG and CL-LG in Setting 2.



(a) Tightness of the lower bound for CTS-G (b) Tightness of the lower bound for CS-SG

Figure 4: Tightness of Regret Bound for both CTS-G and CL-SG.

## 261 **B** Notations and Facts

Notations: Let  $\mathcal{F}_{t-1}$  denote by the history of past actions and rewards until the end of round t-1. Recall that  $\mathbf{E}_{\Theta_t}[\cdot] := \mathbf{E}[\cdot | \Theta_t]$  and  $\operatorname{Pr}_{\Theta_t}(\cdot) := \operatorname{Pr}(\cdot | \Theta_t)$ . Denote by  $\mathcal{E}_t :=$  $\{\forall a \in [N] : |r_a - \hat{r}_{a,n_{a,t}}| \leq \sqrt{\frac{3 \ln Nt}{n_{a,t}+1}}\}$  the high-probability event that the empirical mean is close to the true mean reward for arm a, and by  $\overline{\mathcal{E}}_t$  the complementary event of  $\mathcal{E}_t$ . Recall that  $\tilde{w}_{a,t} \sim \mathcal{N}(\hat{r}_{a,n_{a,t}}, \frac{\gamma m \ln t}{n_{a,t}+1})$  is i.i.d. of  $w_{a,t}$  for CTS-G, and  $\tilde{r}_t := \hat{r}_{a,n_{a,t}} + \tilde{w}_t \sqrt{\frac{\gamma \ln t}{n_{a,t}+1}}$ , where  $\tilde{w}_t \sim \mathcal{N}(0, 1)$  is i.i.d. of  $w_t$  for CL-SG.

**Fact 1.** For a Gaussian distributed random variable Z with mean  $\mu$  and variance  $\delta^2$ , for any z, we have that

$$\frac{1}{4\sqrt{\pi}} \cdot e^{-7z^2/2} \le \Pr(|Z - \mu| > z\sigma) \le \frac{1}{2}e^{-z^2/2}, \tag{6}$$

270 and for any z > 0,

$$\Pr(Z - \mu > z\sigma) \ge \frac{1}{\sqrt{2\pi}} \frac{z}{z^2 + 1} e^{-\frac{z^2}{2}}.$$
(7)

Fact 2. Let  $X_1, \ldots, X_N$  be N real random variables with  $X_i \sim \text{subG}(\sigma^2)$ ,  $i = 1, \ldots, N$ , not necessarily independent. Then,

$$\mathbb{E}\left[\max_{i=1,\ldots,N} |X_i|\right] \leq \sigma \sqrt{2\log(2N)}$$

# 273 C Proofs for Theorem 1

## 274 C.1 Proof of Lemma 1

**Lemma 1.** In any round  $t \ge \max{\sqrt{m}, 4}$ , the optimism part in CTS-G satisfies that

$$\mathbf{E}\left[\sum_{t=\max\{\sqrt{m},4\}}^{T}\left(\sum_{a\in A_{t}^{*}}r_{a}-\sum_{a\in A_{t}}w_{a,t}\right)\right] \leq 8\sqrt{3\gamma}\Phi(-\sqrt{4/\gamma})^{-1}m\ln T\sqrt{NT}.$$
 (8)

Proof. For each  $a \in [N]$ , we let  $\tilde{w}_{a,t} \sim \mathcal{N}\left(\hat{r}_{a,n_{a,t}}, \frac{m\gamma \ln t}{n_{a,t}+1}\right)$  be an independent copy of  $w_{a,t}$ . Let  $(\cdot)^+ := \max\{\cdot, 0\}$ . Let w collect all the Gaussian random variables  $w_{a,t}$  for all  $a \in [N]$ . Recall that  $\mathbf{E}_{\Theta_t}[\cdot] := \mathbf{E}[\cdot | \Theta_t]$ . There are three steps for the proofs.

279 Step 1: we show that in each round  $t \ge \max{\sqrt{m}, 4}$ , we have

$$\mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t^*} r_a - \sum_{a \in A_t} w_{a,t} \right] \leq 2\Phi (-\sqrt{4/\gamma})^{-1} \mathbf{E}_{\Theta_t} \left[ \left( \sum_{a \in A_t} w_{a,t} - \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} w_{a,t} \right] \right)^+ \right].$$
(9)

**Step 2**: we further bound the expectation term in the RHS of (9) as follows.

$$\mathbf{E}_{\Theta_t} \left[ \left( \sum_{a \in A_t} w_{a,t} - \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} w_{a,t} \right] \right)^+ \right] \leq \mathbf{E}_{\Theta_t} \left[ \left| \sum_{a \in A_t} w_{a,t} - \sum_{a \in A_t} \tilde{w}_{a,t} \right| \right].$$
(10)

**Step 3**: summing over T, we show that (10) is upper bounded as follows.

$$\mathbf{E}\left[\sum_{t=1}^{T}\left|\sum_{a\in A_{t}}w_{a,t}-\sum_{a\in A_{t}}\tilde{w}_{a,t}\right|\right] \leq 4m\ln T\sqrt{3\gamma NT}$$
(11)

282 Combining these three steps, we have

$$\mathbf{E} \left[ \sum_{t=\max\{\sqrt{m},4\}}^{T} \left( \sum_{a \in A_{t}^{*}} r_{a} - \sum_{a \in A_{t}} w_{a,t} \right) \right] \\
\leq 2\Phi(-\sqrt{4/\gamma})^{-1} \mathbf{E} \left[ \sum_{t=\max\{\sqrt{m},4\}}^{T} \left| \sum_{a \in A_{t}} w_{a,t} - \sum_{a \in A_{t}} \tilde{w}_{a,t} \right| \right] \\
\leq 2\Phi(-\sqrt{4/\gamma})^{-1} \mathbf{E} \left[ \sum_{t=1}^{T} \left| \sum_{a \in A_{t}} w_{a,t} - \sum_{a \in A_{t}} \tilde{w}_{a,t} \right| \right] \\
\leq 8\sqrt{3\gamma}\Phi(-\sqrt{4/\gamma})^{-1}m \ln T\sqrt{NT}.$$
(12)

- Now, we give the details for these three steps.
- 284 Let  $\alpha := \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t^*} r_a \sum_{a \in A_t} w_{a,t} \right].$

Step 1 proof. If  $\alpha = \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t^*} r_a - \sum_{a \in A_t} w_{a,t} \right] \leq 0$ , the proof is trivial as the RHS of (9) is non-negative. Note that  $2\Phi(-\sqrt{4/\gamma})^{-1} < +\infty$ 

For the case where  $\alpha > 0$ , we view  $\left(\sum_{a \in A_t} w_{a,t} - \mathbf{E}_{\Theta_t} \left[\sum_{a \in A_t} w_{a,t}\right]\right)^+ \ge 0$  as a nonnegative random variable and use Markov's inequality. We have

$$\mathbf{E}_{\Theta_t} \left[ \left( \sum_{a \in A_t} w_{a,t} - \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} w_{a,t} \right] \right)^+ \right] \ge \alpha \operatorname{Pr}_{\Theta_t} \left( \sum_{a \in A_t} w_{a,t} - \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} w_{a,t} \right] \ge \alpha \right),$$
(13)

289 which gives

$$\alpha \leq \frac{\mathbf{E}_{\Theta_{t}}\left[\left(\sum_{a \in A_{t}} w_{a,t} - \mathbf{E}_{\Theta_{t}}\left[\sum_{a \in A_{t}} w_{a,t}\right]\right)^{+}\right]}{\Pr_{\Theta_{t}}\left(\sum_{a \in A_{t}} w_{a,t} - \mathbf{E}_{\Theta_{t}}\left[\sum_{a \in A_{t}} w_{a,t}\right] \geq \alpha\right)}$$

$$= \frac{\mathbf{E}_{\Theta_{t}}\left[\left(\sum_{a \in A_{t}} w_{a,t} - \mathbf{E}_{\Theta_{t}}\left[\sum_{a \in A_{t}} w_{a,t}\right]\right)^{+}\right]}{\Pr_{\Theta_{t}}\left(\sum_{a \in A_{t}} w_{a,t} - \mathbf{E}_{\Theta_{t}}\left[\sum_{a \in A_{t}} w_{a,t}\right]\right) \geq \mathbf{E}_{\Theta_{t}}\left[\sum_{a \in A_{t}^{*}} r_{a} - \sum_{a \in A_{t}} w_{a,t}\right]\right)}{\frac{\mathbf{E}_{\Theta_{t}}\left[\left(\sum_{a \in A_{t}} w_{a,t} - \mathbf{E}_{\Theta_{t}}\left[\sum_{a \in A_{t}} w_{a,t}\right]\right)^{+}\right]}{\Pr_{\Theta_{t}}\left(\sum_{a \in A_{t}} w_{a,t} \geq \sum_{a \in A_{t}^{*}} r_{a}\right)} \leq \frac{\mathbf{E}_{\Theta_{t}}\left[\left(\sum_{a \in A_{t}} w_{a,t} - \mathbf{E}_{\Theta_{t}}\left[\sum_{a \in A_{t}} w_{a,t}\right]\right)^{+}\right]}{\frac{\mathbf{P}_{\Theta_{t}}\left(\sum_{a \in A_{t}} w_{a,t} \geq \sum_{a \in A_{t}^{*}} r_{a}\right)} \leq \frac{\mathbf{E}_{\Theta_{t}}\left[\left(\sum_{a \in A_{t}} w_{a,t} - \mathbf{E}_{\Theta_{t}}\left[\sum_{a \in A_{t}^{*}} w_{a,t}\right]\right)^{+}\right]}{\frac{\mathbf{P}_{\Theta_{t}}\left(\sum_{a \in A_{t}} w_{a,t} \geq \sum_{a \in A_{t}^{*}} r_{a}\right)}{\left(\sum_{a \in A_{t}} w_{a,t} - \mathbf{E}_{\Theta_{t}}\left[\left(\sum_{a \in A_{t}} w_{a,t}\right)\right)^{+}\right]},$$

$$(14)$$

where step (a) is due to that  $A_t$  is the optimal super arm, and thus, we have  $\sum_{a \in A_t^*} w_{a,t} \leq \sum_{a \in A_t} w_{a,t}$  and step (b) uses the result shown in Lemma 4.

**Step 2 proof.** Recall that  $w_{a,t}$  and  $\tilde{w}_{a,t}$  are i.i.d. according to  $\mathcal{N}\left(\hat{r}_{a,n_{a,t}}, \frac{m\gamma \ln t}{n_{a,t}+1}\right)$ , and  $A_t$  is the optimal super arm based on  $\Theta_t$  and  $\mathbf{w}$ . We have  $\mathbf{E}_{\Theta_t}\left[\sum_{a\in A_t} w_{a,t}\right] = \mathbf{E}_{\Theta_t}\left[\max_{A\in\Theta_t}\sum_{a\in A} \tilde{w}_{a,t}\right] \geq \mathbf{E}_{\Theta_t}\left[\sum_{a\in A_t} \tilde{w}_{a,t} \mid A_t\right] = \mathbf{E}_{\Theta_t}\left[\sum_{a\in A_t} \tilde{w}_{a,t} \mid A_t, \mathbf{w}\right]$ . Then, we have

$$\mathbf{E}_{\Theta_{t}} \left[ \left( \sum_{a \in A_{t}} w_{a,t} - \mathbf{E}_{\Theta_{t}} \left[ \sum_{a \in A_{t}} w_{a,t} \right] \right)^{+} \right] \leq \mathbf{E}_{\Theta_{t}} \left[ \left( \sum_{a \in A_{t}} w_{a,t} - \mathbf{E}_{\Theta_{t}} \left[ \sum_{a \in A_{t}} \tilde{w}_{a,t} \mid A_{t}, \mathbf{w} \right] \right)^{+} \right] \\
= \mathbf{E}_{\Theta_{t}} \left[ \left( \mathbf{E}_{\Theta_{t}} \left[ \left( \sum_{a \in A_{t}} w_{a,t} - \sum_{a \in A_{t}} \tilde{w}_{a,t} \right) \mid A_{t}, \mathbf{w} \right] \right)^{+} \right] \\
\leq \mathbf{E}_{\Theta_{t}} \left[ \left| \mathbf{E}_{\Theta_{t}} \left[ \left( \sum_{a \in A_{t}} w_{a,t} - \sum_{a \in A_{t}} \tilde{w}_{a,t} \right) \mid A_{t}, \mathbf{w} \right] \right|^{+} \right] \\
\leq \mathbf{E}_{\Theta_{t}} \left[ \left| \mathbf{E}_{\Theta_{t}} \left[ \left( \sum_{a \in A_{t}} w_{a,t} - \sum_{a \in A_{t}} \tilde{w}_{a,t} \right) \mid A_{t}, \mathbf{w} \right] \right| \\
\leq \mathbf{E}_{\Theta_{t}} \left[ \mathbf{E}_{\Theta_{t}} \left[ \left| \sum_{a \in A_{t}} w_{a,t} - \sum_{a \in A_{t}} \tilde{w}_{a,t} \right| \mid A_{t}, \mathbf{w} \right] \right] \\
= \mathbf{E}_{\Theta_{t}} \left[ \left| \sum_{a \in A_{t}} w_{a,t} - \sum_{a \in A_{t}} \tilde{w}_{a,t} \right| \right],$$
(15)

## where the last inequality is due to Jensen's inequality.

Step 3 proof. Since  $w_{a,t} - \tilde{w}_{a,t} \sim \mathcal{N}\left(0, \frac{2\gamma m \ln t}{n_{a,t}+1}\right)$ , we can express  $w_{a,t} - \tilde{w}_{a,t}$  as  $\sqrt{2}\zeta_{a,t}\delta_{a,t}$ , where  $\zeta_{a,t} \sim \mathcal{N}(0, 1)$  and  $\delta_{a,t} = \sqrt{\frac{\gamma m \ln t}{n_{a,t}+1}}$ . Thus, we have

$$\mathbf{E}\left[\sum_{t=1}^{T}\left|\sum_{a\in A_{t}}w_{a,t}-\sum_{a\in A_{t}}\tilde{w}_{a,t}\right|\right] \leq \sqrt{2}\mathbf{E}\left[\sum_{t=1}^{T}\sum_{a\in A_{t}}\left|\zeta_{a,t}\delta_{a,t}\right|\right]$$

$$\stackrel{(a)}{\leq}\sqrt{2}\mathbf{E}\left[\max_{t\in[T],a\in[N]}\left|\zeta_{a,t}\right|\sum_{t=1}^{T}\sum_{a\in A_{t}}\left|\delta_{a,t}\right|\right]$$

$$=\sqrt{2}\mathbf{E}\left[\max_{t\in[T],a\in[N]}\left|\zeta_{a,t}\right|\sum_{t=1}^{T}\sum_{a\in A_{t}}\sqrt{\frac{\gamma m \ln t}{n_{a,t}+1}}\right] \quad (16)$$

$$\stackrel{(b)}{\leq}2m\sqrt{2\gamma NT \ln T}\mathbf{E}\left[\max_{t\in[T],a\in[N]}\zeta_{a,t}\right]$$

$$\stackrel{(c)}{\leq}2m\sqrt{2\gamma NT \ln T}\cdot\sqrt{6 \ln T}$$

$$\leq 4m \ln T\sqrt{3\gamma NT}.$$

where step (a) is due to Hölder's inequality. Step (b) is due to Lemma 5 such that  $\sum_{t=1}^{T} \sum_{a \in A_t} \sqrt{\frac{1}{n_{a,t}+1}} \leq 2\sqrt{mNT}.$  Step (c) is due to the maximal inequality for Gaussian variables (Fact 2) such that  $\mathbf{E} \left[ \max_{t \in [T], a \in [N]} \zeta_{a,t} \right] \leq \sqrt{2 \ln 2NT} \leq \sqrt{6 \ln T}$  because  $2 \leq N \leq T.$ 

## 303 C.2 Proof of Lemma 2

**Lemma 2.** Let  $\mathcal{E}_t := \left\{ \forall a \in [N], \hat{r}_{a,n_{a,t}} - r_a \leq \sqrt{\frac{3 \ln Nt}{n_{a,t}+1}} \right\}$ . In CTS-G, the regret of the deviation part is

$$\mathbf{E}\left[\sum_{t=1}^{T}\left(\sum_{a\in A_{t}}w_{a,t}-\sum_{a\in A_{t}}r_{a}\right)\mathbf{1}[\mathcal{E}_{t}]\right] \leq 2m\ln T\sqrt{6\gamma NT}+2\sqrt{6mNT\ln T}.$$

304 *Proof.* We can do decomposition as follows.

$$\mathbf{E} \left[ \sum_{t=1}^{T} \left( \sum_{a \in A_{t}} w_{a,t} - \sum_{a \in A_{t}} r_{a} \right) \mathbf{1}[\mathcal{E}_{t}] \right] \\
= \mathbf{E} \left[ \sum_{t=1}^{T} \left( \sum_{a \in A_{t}} w_{a,t} - \sum_{a \in A_{t}} \hat{r}_{a,n_{a,t}} + \sum_{a \in A_{t}} \hat{r}_{a,n_{a,t}} - \sum_{a \in A_{t}} r_{a} \right) \mathbf{1}[\mathcal{E}_{t}] \right] \\
= \mathbf{E} \left[ \sum_{t=1}^{T} \left( \sum_{a \in A_{t}} w_{a,t} - \sum_{a \in A_{t}} \hat{r}_{a,n_{a,t}} \right) \mathbf{1}[\mathcal{E}_{t}] \right] + \mathbf{E} \left[ \sum_{t=1}^{T} \left( \sum_{a \in A_{t}} \hat{r}_{a,n_{a,t}} - \sum_{a \in A_{t}} r_{a} \right) \mathbf{1}[\mathcal{E}_{t}] \right] \\
\overset{(a)}{\leq} \mathbf{E} \left[ \sum_{t=1}^{T} \sum_{a \in A_{t}} \left( w_{a,t} - \hat{r}_{a,n_{a,t}} \right) \right] + \mathbf{E} \left[ \sum_{t=1}^{T} \sum_{a \in A_{t}} \sqrt{\frac{6 \ln T}{n_{a,t} + 1}} \right] \\
\overset{(b)}{\leq} \mathbf{E} \left[ \sum_{t=1}^{T} \sum_{a \in A_{t}} \left( w_{a,t} - \hat{r}_{a,n_{a,t}} \right) \right] + 2\sqrt{6mNT \ln T},$$
(17)

where step (a) is because event  $\mathcal{E}_t$  is true and  $\ln NT \leq 2 \ln T$  because of  $N \leq T$ , and step (b) is due to Lemma 5 such that  $\sum_{t=1}^T \sum_{a \in A_t} \sqrt{\frac{1}{n_{a,t}+1}} \leq 2\sqrt{mNT}$ .

We can represent each  $w_{a,t} - \hat{r}_{a,n_{a,t}}$  by  $\zeta_{a,t}\delta_{a,t}$ , where  $\zeta_{a,t} \sim \mathcal{N}(0, 1)$  and  $\delta_{a,t} = \sqrt{\frac{\gamma m \ln t}{n_{a,t}+1}}$ . Then, we can bound the first term on the RHS of the above equation as follows:

$$\mathbf{E}\left[\sum_{t=1}^{T}\sum_{a\in A_{t}}\left(w_{a,t} - \hat{r}_{a,n_{a,t}}\right)\right] \leq \mathbf{E}\left[\sum_{t=1}^{T}\sum_{a\in A_{t}}\zeta_{a,t}\delta_{a,t}\right] \\
\stackrel{(a)}{\leq} \mathbf{E}\left[\max_{t\in[T],a\in[N]}|\zeta_{a,t}| \cdot \sum_{t=1}^{T}\sum_{a\in A_{t}}|\delta_{a,t}|\right] \\
= \mathbf{E}\left[\max_{t\in[T],a\in[N]}|\zeta_{a,t}| \cdot \sum_{t=1}^{T}\sum_{a\in A_{t}}\sqrt{\frac{\gamma m \ln t}{n_{a,t}+1}}\right],$$
(18)

<sup>309</sup> where (a) is due to Hölder's inequality. By invoking Lemma 5 again, we have that

$$\sum_{t=1}^{T} \sum_{a \in A_t} \sqrt{\frac{\gamma m \ln t}{n_{a,t} + 1}} \le \sqrt{\gamma m \ln T} \sum_{t=1}^{T} \sum_{a \in A_t} \sqrt{\frac{1}{n_{a,t} + 1}} \le 2m\sqrt{\gamma NT \ln T}.$$
 (19)

Then, using the maximal inequality (Fact 2), we have  $\mathbf{E} \left[ \max_{t \in [T], a \in [N]} |\zeta_{a,t}| \right] \leq \sqrt{2 \ln 2NT} \leq \sqrt{6 \ln T}$ , where the last inequality is due to that  $2 \leq N \leq T$ . Thus, we have

$$\mathbf{E}\left[\sum_{t=1}^{T}\sum_{a\in A_{t}}\left(w_{a,t}-\hat{r}_{a,n_{a,t}}\right)\right] \leq 2m\ln T\sqrt{6\gamma NT}.$$
(20)

<sup>312</sup> Finally, by substituting (20) into (17), we complete the proof.

## 313 C.3 Proof of Lemma 3

**Lemma 3.** The probability that event  $\overline{\mathcal{E}_t}$  to happen satisfies that

$$\sum_{t=1}^{T} \Pr(\overline{\mathcal{E}_t}) \leq \frac{\pi^2}{3}.$$

<sup>314</sup> *Proof.* By a union bound and Hoeffding's inequality, we have that

$$\sum_{t=1}^{T} \Pr\left(\exists a \in [N] : |r_{a} - \hat{r}_{a,n_{a,t}}| > \sqrt{\frac{3 \ln Nt}{n_{a,t} + 1}}\right)$$

$$\leq \sum_{t=1}^{T} \sum_{a \in [N]} \sum_{s=0}^{t-1} \Pr\left(|\hat{r}_{a,s} - r_{a}| > \sqrt{\frac{3 \ln Nt}{s + 1}}\right)$$

$$= \sum_{a \in [N]} \sum_{t=1}^{T} \left(\Pr\left(r_{a} > \sqrt{3 \ln Nt}\right) + \sum_{s=1}^{t-1} \Pr\left(|\hat{r}_{a,s} - r_{a}| > \sqrt{\frac{3 \ln Nt}{s + 1}}\right)\right) \quad (21)$$

$$\stackrel{(a)}{\leq} \sum_{a \in [N]} \left(0 + \sum_{t=1}^{T} \sum_{s=1}^{t-1} \Pr\left(|\hat{r}_{a,s} - r_{a}| > \sqrt{\frac{3 \ln Nt}{2s}}\right)\right)$$

$$\leq N \sum_{t=1}^{\infty} \sum_{s=1}^{t-1} \frac{2}{(Nt)^{3}} = \frac{\pi^{2}}{3N^{2}},$$

s15 where step (a) is due to  $r_a \in [0, 1], \forall a \in [N]$  and  $3 \ln Nt > 1$  because  $N \ge 2$ , and that 316  $s + 1 \le 2s$  for any  $s \ge 1$ .

#### 318 C.4 Proof of Lemma 4

317

319 **Lemma 4.** In each round  $t \ge \max{\sqrt{m}, 4}$ , given any  $\Theta_t$ , we have

$$\frac{1}{\Pr_{\Theta_t} \left( \sum_{a \in A_t^*} w_{a,t} \geq \sum_{a \in A_t^*} r_a \right)} \leq 2\Phi \left( -\sqrt{4/\gamma} \right)^{-1},$$

where  $\Phi(\cdot)$  is the cdf of the standard Gaussian distribution.

<sup>321</sup> Proof. Given  $\Theta_t$ ,  $A_t^*$  is determined. Define  $\mathcal{H}_t := \left\{ \forall a \in A_t^* : |r_a - \hat{r}_{a,n_{a,t}}| \le \sqrt{\frac{4 \ln t}{n_{a,t}+1}} \right\}$ . <sup>322</sup> Since  $t \ge \max\{\sqrt{m}, 4\}$ , we have that

$$\Pr_{\Theta_{t}} (\mathcal{H}_{t}) \geq 1 - \sum_{a \in A_{t}^{*}} \sum_{s_{a}=0}^{t-1} \Pr_{\Theta_{t}} \left( |r_{a} - \hat{r}_{a,s_{a}}| \geq \sqrt{\frac{4 \ln t}{s_{a} + 1}} \right) \\
= 1 - \sum_{a \in A_{t}^{*}} \sum_{s_{a}=1}^{t-1} \Pr_{\Theta_{t}} \left( |r_{a} - \hat{r}_{a,s_{a}}| \geq \sqrt{\frac{4 \ln t}{s_{a} + 1}} \right) \\
\geq 1 - \sum_{a \in A_{t}^{*}} \sum_{s_{a}=1}^{t-1} \Pr_{\Theta_{t}} \left( |r_{a} - \hat{r}_{a,s_{a}}| \geq \sqrt{\frac{4 \ln t}{2s_{a}}} \right) \\
\geq 1 - mt \cdot 2 \cdot e^{-2 \cdot s_{a} \cdot 4 \ln t / (2s_{a})} \\
= 1 - \frac{2mt}{t^{4}} \\
\geq 0.5 .$$
(22)

323 We have

$$\Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}^{*}} w_{a,t} \geq \sum_{a \in A_{t}^{*}} r_{a} \right) \geq \Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}^{*}} w_{a,t} \geq \sum_{a \in A_{t}^{*}} r_{a}, \mathcal{H}_{t} \right) \\
= \Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}^{*}} w_{a,t} - \hat{r}_{a,n_{a,t}} \geq \sum_{a \in A_{t}^{*}} r_{a} - \hat{r}_{a,n_{a,t}}, \mathcal{H}_{t} \right) \\
= \Pr_{\Theta_{t}} (\mathcal{H}_{t}) \cdot \Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}^{*}} w_{a,t} - \hat{r}_{a,n_{a,t}} \geq \sum_{a \in A_{t}^{*}} r_{a} - \hat{r}_{a,n_{a,t}} \mid \mathcal{H}_{t} \right) \\
\stackrel{(a)}{\geq} 0.5 \cdot \Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}^{*}} w_{a,t} - \hat{r}_{a,n_{a,t}} \geq \sum_{a \in A_{t}^{*}} \sqrt{\frac{4 \ln t}{n_{a,t} + 1}} \right) \\
\stackrel{(b)}{\geq} 0.5 \cdot \Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}^{*}} w_{a,t} - \hat{r}_{a,n_{a,t}} \geq \sqrt{m \sum_{a \in A_{t}^{*}} \frac{4 \ln t}{n_{a,t} + 1}} \right) \\
= 0.5 \cdot \Phi \left( -\sqrt{4/\gamma} \right) ,$$
(23)

where step (a) is due to (22) and the fact that event  $\mathcal{E}_t$  is true. Step (b) uses the Cauchy–Schwarz inequality, i.e., we have  $\sum_{a \in A_t^*} \sqrt{\frac{4 \ln t}{n_{a,t}+1}} \leq \sqrt{m \cdot \sum_{a \in A_t^*} \frac{4 \ln t}{n_{a,t}+1}}$ . The last equality is due to the standardization of Gaussian distribution.

#### 327 C.5 Proof of Lemma 5

**Lemma 5.** We have  $\sum_{t=1}^{T} \sum_{a \in A_t} \sqrt{\frac{1}{n_{a,t}+1}} \leq 2\sqrt{mNT}$ .

*Proof.* Note that the LHS of the above inequality is a random variable. We provide an upper bound
 for this random variable.

Recall  $n_{a,t} := \sum_{\tau=1}^{t-1} \mathbf{1} [a \in A_{\tau}]$  is the number of times that arm a has been played at the beginning of round t. Let  $\tau_a(n)$  denote the round for arm a to be played for the n-th time, and thus  $n_{a,\tau_a(n)} = n - 1$ .

$$\sum_{t=1}^{T} \sum_{a \in A_{t}} \sqrt{\frac{1}{n_{a,t} + 1}} = \sum_{t=1}^{T} \sum_{a \in [N]} \sqrt{\frac{1}{n_{a,t} + 1}} \mathbf{1} [a \in A_{t}] 
\stackrel{(a)}{=} \sum_{a \in [N]} \sum_{n=1}^{n_{a,T+1}} \sum_{t=\tau_{a}(n)}^{\tau_{a}(n+1)-1} \sqrt{\frac{1}{n_{a,t} + 1}} \mathbf{1} [a \in A_{t}] 
\stackrel{(b)}{=} \sum_{a \in [N]} \sum_{n=1}^{n_{a,T+1}} \sqrt{\frac{1}{n}} \leq \sum_{a \in [N]} \int_{0}^{n_{a,T+1}} \sqrt{\frac{1}{n}} dn 
= 2 \sum_{a \in [N]} \sqrt{n_{a,T+1}} \stackrel{(c)}{\leq} 2 \sqrt{N} \sum_{a \in [N]} n_{a,T+1} 
\stackrel{(d)}{=} 2\sqrt{mNT},$$
(24)

where step (a) partitions all T rounds into multiple intervals based on the arrivals of observations from arm a. Step (b) uses the fact that  $\sum_{t=\tau_a(n)}^{\tau_a(n+1)-1} \mathbf{1}[a \in A_t] \cdot \sqrt{\frac{1}{n_{a,t}+1}} = \sqrt{\frac{1}{n-1+1}} = \sqrt{\frac{1}{n}}$ , because  $n_{a,\tau_a(n)} = n - 1$  and  $\mathbf{1}[a \in A_t] = 0$  for all  $t \in \{\tau_a(n) + 1, \ldots, \tau_a(n + 1) - 1\}$ . Step (c) uses Cauchy-Schwarz inequality. Step (d) uses the fact that  $\sum_{a \in [N]} n_{a,T+1} \leq mT$ .

338

#### 339 C.6 Proof of Upper bound

340 Upper Bound Proof of Theorem 1. Denote by  $\mathcal{E}_t := \left\{ \forall a \in [N] : |r_a - \hat{r}_{a,n_{a,t}}| \leq \sqrt{\frac{3 \ln Nt}{n_{a,t+1}}} \right\}$ 341 the high-probability event that the empirical mean reward is close to the true mean reward for arm a, 342 and by  $\overline{\mathcal{E}_t}$  the complementary event of  $\mathcal{E}_t$ .

Let  $t' = \max{\sqrt{m}, 4}$ . We first decompose the regret as follows:

$$\mathcal{R}(T) = \sum_{t=1}^{t'-1} \mathbf{E} \left[ \sum_{a \in A_t^*} r_a - \sum_{a \in A_t} r_a \right] + \sum_{t=t'}^T \mathbf{E} \left[ \sum_{a \in A_t^*} r_a - \sum_{a \in A_t} r_a \right]$$

$$\stackrel{(a)}{\leq} m \max\{\sqrt{m}, 4\} + \mathbf{E} \left[ \sum_{t=t'}^T \left( \sum_{a \in A_t^*} r_a - \sum_{a \in A_t} r_a \right) \mathbf{1}[\mathcal{E}_t] \right] + \mathbf{E} \left[ \sum_{t=t'}^T \left( \sum_{a \in A_t^*} r_a - \sum_{a \in A_t} r_a \right) \mathbf{1}[\mathcal{E}_t] \right]$$

$$\stackrel{(b)}{\leq} m \max\{\sqrt{m}, 4\} + \mathbf{E} \left[ \sum_{t=t'}^T \left( \sum_{a \in A_t^*} r_a - \sum_{a \in A_t} w_{a,t} + \sum_{a \in A_t} w_{a,t} - \sum_{a \in A_t} r_a \right) \mathbf{1}[\mathcal{E}_t] \right] + m \frac{\pi^2}{3N^2}$$

$$\leq \underbrace{\sum_{t=t'}^T \mathbf{E} \left[ \left( \sum_{a \in A_t^*} r_a - \sum_{a \in A_t} w_{a,t} \right) \right]}_{=:I_1, \text{ optimism part}} + \underbrace{\sum_{t=t'}^T \mathbf{E} \left[ \sum_{a \in A_t} (w_{a,t} - r_a) \mathbf{1}[\mathcal{E}_t] \right]}_{=:I_2, \text{ deviation part}} + m \max\{\sqrt{m}, 4\} + \frac{\pi^2}{3},$$

where step (a) is due to the fact that  $\sum_{a \in A_t^*} r_a - \sum_{a \in A_t} r_a \leq m$  by the definition of  $r_a$  and mand step (b) is due to Lemma 3.

Now, invoking Lemma 1 with proofs in Appendix C.1, we have term  $I_1$  bounded as follows:

$$I_1 \leq 8\sqrt{3\gamma}\Phi(-\sqrt{4/\gamma})^{-1}m\ln T\sqrt{NT},$$
(26)

and  $I_2$  can be bounded by using Lemma 2 with proofs in Appendix C.2:

$$I_2 \leq 2m \ln T \sqrt{6\gamma NT} + 2\sqrt{6mNT} \ln T.$$
(27)

348 Thus, we have that

$$\mathcal{R}(T) \leq \left(2\sqrt{6\gamma} + 8\sqrt{3\gamma}\Phi(-\sqrt{4/\gamma})^{-1}\right) m \ln T\sqrt{NT} + 2\sqrt{6mNT} \ln T + m \left(\max\{\sqrt{m}, 4\} + \frac{\pi^2}{3}\right).$$
(28)

Using numerical optimization methods searching from  $\gamma = 0.0001$  to  $\gamma = 100$ , we can find that when  $\gamma = 6.4$ , the coefficient for the first item can achieve a minimum value of 175.74.

351

#### 352 C.7 Proof of Lower Bound



Figure 5: Problem instance for the lower-bound proof. Nodes S and T are the starting and ending points for each path.

- Lower bound Proof in Theorem 1. Our proof uses similar ideas to the proofs of Theorem 1.4 in Agrawal & Goyal (2017b).
- We construct a path selection problem involving N links (each link corresponds to a base arm) and K
- paths (each path corresponds to a super arm), as illustrated in Fig. 5. Each path consists of m links,

and thus, the total number of base arms N = mK. We consider a fixed availability set throughout all T rounds, i.e.,  $\Theta_t = \Theta := \{A_1, A_2, \dots, A_K\}$  for all rounds  $t \in [T]$  with each super arm  $A_k$  being a feasible path. We assume the first path  $A_1$  is the unique optimal one.

We construct the following Bernoulli reward distributions for each base arm. Let  $\Delta := \sqrt{K \ln K/T}$ . For any base arm in the optimal super arm  $A_1$ , we use a degenerate distribution putting mass 1 on a single point  $\sqrt{\gamma}\Delta$ , i.e., if  $A_1$  is played, for any base arm in it, we always observe  $\sqrt{\gamma}\Delta$  as the random reward. Similarly, for the remaining base arms in the sub-optimal super arms, we put mass 1 on a single point 0, i.e., the random reward is always 0 for any base arm in a sub-optimal super arm.

Let  $Q_A(t)$  denote the number of times that super arm  $A \in \Theta$  has been played at the beginning of round t. Since there are no overlapping base arms between two distinct super arms, we have  $Q_A(t) = n_{a,t}$  for all  $a \in A$ . Let  $c \in (0, 1)$  be some universal constant that will be tuned later. Define  $B_t^* := \{Q_{A_1}(t) > t - cT\}$  as the event that the optimal super arm  $A_1$  has been observed at least (t - cT) times by the beginning of round t.

We lower bound the total regret from round 1 to the end of round T by analyzing two cases that are exhaustive and mutually exclusive based on events  $B_t^*$  for all rounds  $t \in [T]$ .

If  $B_t^*$  is not true for some  $t \in [T]$ , we have the total number of times of playing suboptimal super arms by the beginning of round t is  $\sum_{A \in \Theta \setminus A_1} Q_A(t) = t - Q_{A_1}(t) \ge t - (t - CT) \ge cT$ , which implies the total regret by the end of round T is at least  $cT \cdot m \cdot \sqrt{\gamma}\Delta = \Omega(m\sqrt{KT \ln K}) = \Omega(\sqrt{mNT \ln(N/m)})$ . Note that the total regret from round 1 to round t is a lower bound for the total regret over all T rounds.

If  $B_t^*$  is true for all  $t \in [T]$ , we have the total number of times  $\sum_{A \in \Theta \setminus A_1} Q_A(t)$  of playing sub-optimal super arms by the beginning of round t is upper bounded by

$$\sum_{A \in \Theta \setminus A_1} Q_A(t) = t - Q_{A_1}(t) \le t - (t - cT) = cT \quad .$$
(29)

<sup>380</sup> Due to the spread of a sub-optimal super arm's posterior distribution, the learning agent will make <sup>381</sup> mistakes when deciding which super arm to play. Formally, we show that with at least a constant <sup>382</sup> probability, the learning agent will play a sub-optimal super arm. Note that whether event  $B_t^*$  is true <sup>383</sup> or not is determined by the history information  $\mathcal{F}_{t-1}$ .

Recall  $w_{a,t} \sim \mathcal{N}\left(\hat{r}_{a,n_{a,t}}, \frac{\gamma m \ln t}{n_{a,t}+1}\right)$ . Now, we construct a lower bound for the probability of selecting a sub-optimal arm in round t conditioned on instantiations  $F_{t-1}$  of  $\mathcal{F}_{t-1}$  such that  $B_t^*$  is true. We have

$$\Pr \left(\exists A \in \Theta \setminus A_{1} : A_{t} = A \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$\geq \Pr(\exists A \in \Theta \setminus A_{1} : \sum_{a \in A} w_{a,t} > \sum_{a \in A_{1}} w_{a,t} \mid \mathcal{F}_{t-1} = F_{t-1})$$

$$\stackrel{(a)}{\geq} \Pr(\exists A \in \Theta \setminus A_{1} : \sum_{a \in A} w_{a,t} \geq m\sqrt{\gamma}\Delta \mid \mathcal{F}_{t-1} = F_{t-1})$$

$$\cdot \Pr(\sum_{a \in A_{1}} w_{a,t} < m\sqrt{\gamma}\Delta \mid \mathcal{F}_{t-1} = F_{t-1})$$

$$\stackrel{(b)}{=} \Pr(\exists A \in \Theta \setminus A_{1} : \sum_{a \in A} w_{a,t} \geq m\sqrt{\gamma}\Delta \mid \mathcal{F}_{t-1} = F_{t-1}) \cdot \frac{1}{2} ,$$

$$(30)$$

where step (a) uses the fact that all super arms are independent based on our construction of the path selection problem. Step (b) uses the fact that the sum of multiple independent Gaussian random variables is still Gaussian and  $(\sum_{a \in A_1} w_{a,t} - m\sqrt{\gamma}\Delta)$  is a zero-mean Gaussian distribution. Note that the empirical mean of each base arm in the optimal super arm is exactly  $\sqrt{\gamma}\Delta$ . Now, we construct a lower bound for (30) by using Gaussian anti-concentration bounds. We have

$$\Pr\left(\exists A \in \Theta \setminus A_{1} : \sum_{a \in A} w_{a,t} \geq m\sqrt{\gamma}\Delta \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$\geq \Pr\left(\exists A \in \Theta \setminus A_{1} : \sum_{a \in A} w_{a,t} \geq m\sqrt{\gamma}\Delta\sqrt{\ln t} \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$= 1 - \Pr\left(\sum_{a \in A} w_{a,t} < m\Delta\sqrt{\gamma \ln t}, \forall A \in \Theta \setminus A_{1} \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$= 1 - \prod_{A \in \Theta \setminus A_{1}} \left(1 - \Pr\left(\sum_{a \in A} w_{a,t}\sqrt{(Q_{A}(t) + 1)} \geq m\Delta\sqrt{(Q_{A}(t) + 1)\gamma \ln t} \mid \mathcal{F}_{t-1} = F_{t-1}\right)\right)\right)$$

$$= 1 - \prod_{A \in \Theta \setminus A_{1}} \left(1 - \Pr\left(\frac{\sum_{a \in A} w_{a,t}\sqrt{(Q_{A}(t) + 1)}}{m\sqrt{\gamma \ln t}} \geq \Delta\sqrt{(Q_{A}(t) + 1)} \mid \mathcal{F}_{t-1} = F_{t-1}\right)\right)$$

$$\geq 1 - \prod_{A \in \Theta \setminus A_{1}} \left(1 - \frac{1}{8\sqrt{\pi}}e^{-\frac{\tau}{2}\Delta^{2}(Q_{A}(t)+1)}\right) ,$$
(31)

where the last inequality uses the fact that  $\frac{\sum_{a \in A} w_{a,t} \sqrt{Q_A(t)+1}}{m \sqrt{\gamma \ln t}} \sim \mathcal{N}(0, 1)$  and then the one-sided anti-concentration inequality shown in (6).

Tune constant c = 0.001. Then, we use the upper bound constructed in (29) to continue lower bounding (31). We have

$$1 - \prod_{A \in \Theta \setminus A_{1}} \left( 1 - \frac{1}{8\sqrt{\pi}} e^{-\frac{7}{2}\Delta^{2}(Q_{A}(t)+1)} \right)$$

$$\stackrel{(a)}{\geq} 1 - \prod_{A \in \Theta \setminus A_{1}} \left( 1 - \frac{1}{8\sqrt{\pi}} e^{-\frac{7c}{2}\Delta^{2}\frac{\sqrt{KT \ln K}}{(K-1)\Delta} - \frac{7\Delta^{2}}{2}} \right)$$

$$= 1 - \prod_{A \in \Theta \setminus A_{1}} \left( 1 - \frac{1}{8\sqrt{\pi}} e^{-\frac{7c}{2}\frac{K \ln K}{(K-1)} - \frac{7K \ln K}{2}} \right)$$

$$= 1 - \prod_{A \in \Theta \setminus A_{1}} \left( 1 - \frac{1}{8\sqrt{\pi}} e^{-(\frac{7c}{2}\frac{K}{K-1} + \frac{7K}{2T}) \ln K} \right)$$

$$\stackrel{(b)}{\geq} 1 - \prod_{A \in \Theta \setminus A_{1}} \left( 1 - \frac{1}{8\sqrt{\pi}} e^{-\ln K} \right)$$

$$= 1 - \left( 1 - \frac{1}{8\sqrt{\pi}K} \right)^{K-1}$$

$$\stackrel{(c)}{\geq} 1 - \left( e^{-\frac{1}{8\sqrt{\pi}K}} \right)^{K-1}$$

$$\geq 1 - e^{-\frac{1}{16\sqrt{\pi}}},$$
(32)

where step (a) is due to the fact that, constrained on (29), i.e.,  $\sum_{A \in \Theta \setminus A_1} Q_A(t) \leq cT = c \frac{\sqrt{KT \ln K}}{\Delta}$ , the quantity  $\prod_{A \in \Theta \setminus A_1} \left(1 - \frac{1}{4\sqrt{\pi}}e^{-\frac{7c}{2}\Delta^2 \frac{\sqrt{KT \ln K}}{(K-1)\Delta} - \frac{7\Delta^2}{2}}\right)$  is maximized when  $Q_A(t) = \frac{c\sqrt{KT \ln K}}{(K-1)\Delta}$  for all  $A \in \Theta \setminus A_1$ . Step (b) uses the fact that, when c = 0.001, we have  $\frac{7c}{2} \frac{K}{K-1} + \frac{7K}{2T} \leq 1$  when T is sufficiently large, e.g., T > 5K. Step (c) uses  $1 - x \leq e^{-x}$ . Now, we are ready to complete the proof. Let  $p := \frac{1}{2} \left( 1 - e^{-\frac{1}{16\sqrt{\pi}}} \right)$ . By plugging the lower bound constructed in (32) into (30), we have  $\Pr(\exists A \in \Theta \setminus A_1 : A_t = A \mid \mathcal{F}_{t-1} = F_{t-1}) \ge p$ , which implies the total regret by the end of round T is at least  $Tpm\sqrt{\gamma}\Delta = \Omega(\sqrt{mNT \ln(N/m)})$ .

# 404 **D Proofs for Theorem 2**

#### 405 D.1 Proof of Lemma 6

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406 Lemma 6. The optimism part in CL-SG satisfies that

$$\mathbf{E}\left[\sum_{t=\max\{m,4\}}^{T} \left(\sum_{a\in A_t^*} r_a - \sum_{a\in A_t} \bar{r}_{a,t}\right)\right] \leq 8\sqrt{2\gamma} \Phi(-\sqrt{4/\gamma})^{-1} \ln T\sqrt{mNT}.$$
 (33)

407 *Proof.* Similar to the proof of Lemma 1. There are three steps for the proofs.

Step 1: Let  $t' = \max{\sqrt{m}, 4}$  we show that the following inequality holds for each round t conditioned on  $\Theta_t$ :

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$$\mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t^*} r_a - \sum_{a \in A_t} \bar{r}_{a,t} \right] \leq 2\Phi(-\sqrt{4/\gamma})^{-1} \cdot \mathbf{E}_{\Theta_t} \left[ \left( \sum_{a \in A_t} \bar{r}_{a,t} - \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} \bar{r}_{a,t} \right] \right)^+ \right].$$
(34)

Step 2: Let  $\tilde{r}_{a,t} = \hat{r}_{a,t} + \tilde{w}_t \sqrt{\frac{\gamma \ln t}{n_{a,t}+1}}$ , where  $\tilde{w}_t \sim \mathcal{N}(0, 1)$  is an independent copy of  $w_t$ . With  $\tilde{r}_{a,t}$ , we can further bound the last term in (34) as follows.

$$\mathbf{E}_{\Theta_t} \left[ \left( \sum_{a \in A_t} \bar{r}_{a,t} - \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} \bar{r}_{a,t} \right] \right)^+ \right] \leq \mathbf{E}_{\Theta_t} \left[ \left| \sum_{a \in A_t} \bar{r}_{a,t} - \sum_{a \in A_t} \tilde{r}_{a,t} \right| \right].$$
(35)

412 Step 3: Summing over T rounds, we have that

$$\mathbf{E}\left[\sum_{t=1}^{T} \left|\sum_{a \in A_{t}} \bar{r}_{a,t} - \sum_{a \in A_{t}} \tilde{r}_{a,t}\right|\right] \leq 4 \ln T \sqrt{2\gamma m N T}$$
(36)

413 Combining these three steps, we have

$$\mathbf{E}\left[\sum_{t=\max\{\sqrt{m},4\}}^{T}\left(\sum_{a\in A_{t}^{*}}r_{a}-\sum_{a\in A_{t}}\bar{r}_{a,t}\right)\right] \leq 2\Phi(-\sqrt{4/\gamma})^{-1}\mathbf{E}\left[\sum_{t=\max\{\sqrt{m},4\}}^{T}\left|\sum_{a\in A_{t}}\bar{r}_{a,t}-\sum_{a\in A_{t}}\tilde{r}_{a,t}\right|\right] \\ \leq 2\Phi(-\sqrt{4/\gamma})^{-1}\mathbf{E}\left[\sum_{t=1}^{T}\left|\sum_{a\in A_{t}}\bar{r}_{a,t}-\sum_{a\in A_{t}}\tilde{r}_{a,t}\right|\right] \\ \leq 8\sqrt{2\gamma}\Phi(-\sqrt{4/\gamma})^{-1}\ln T\sqrt{mNT}.$$
(37)

414 Now, we give the details for these three steps.

415 **Step 1 proof.** If  $\mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t^*} r_a - \sum_{a \in A_t} \bar{r}_{a,t} \right] \leq 0$ , the proof is trivial as the RHS in (34) is 416 non-negative. 417 Recall  $(\cdot)^+ := \max \{\cdot, 0\}$ . For the case where  $\alpha := \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t^*} r_a - \sum_{a \in A_t} \bar{r}_{a,t} \right] > 0$ , we use 418 Markov's inequality and have

$$\mathbf{E}_{\Theta_{t}}\left[\left(\sum_{a\in A_{t}}\bar{r}_{a,t} - \mathbf{E}_{\Theta_{t}}\left[\sum_{a\in A_{t}}\bar{r}_{a,t}\right]\right)^{+}\right] \geq \alpha \cdot \Pr_{\Theta_{t}}\left(\left(\sum_{a\in A_{t}}\bar{r}_{a,t} - \mathbf{E}_{\Theta_{t}}\left[\sum_{a\in A_{t}}\bar{r}_{a,t}\right]\right)^{+} \geq \alpha\right) \\ \geq \alpha \cdot \Pr_{\Theta_{t}}\left(\sum_{a\in A_{t}}\bar{r}_{a,t} - \mathbf{E}_{\Theta_{t}}\left[\sum_{a\in A_{t}}\bar{r}_{a,t}\right] \geq \alpha\right),$$
(38)

419 which gives

$$\begin{aligned} \alpha &= \mathbf{E}_{\Theta_{t}} \left[ \sum_{a \in A_{t}^{*}} r_{a} - \sum_{a \in A_{t}} \bar{r}_{a,t} \right] \\ &\leq \frac{\mathbf{E}_{\Theta_{t}} \left[ \left( \sum_{a \in A_{t}} \bar{r}_{a,t} - \mathbf{E}_{\Theta_{t}} \left[ \sum_{a \in A_{t}} \bar{r}_{a,t} \right] \right)^{+} \right]}{\Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}} \bar{r}_{a,t} - \mathbf{E}_{\Theta_{t}} \left[ \sum_{a \in A_{t}} \bar{r}_{a,t} \right] \right)^{+} \right] \\ &= \frac{\mathbf{E}_{\Theta_{t}} \left[ \left( \sum_{a \in A_{t}} \bar{r}_{a,t} - \mathbf{E}_{\Theta_{t}} \left[ \sum_{a \in A_{t}} \bar{r}_{a,t} \right] \right)^{+} \right]}{\Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}} \bar{r}_{a,t} - \mathbf{E}_{\Theta_{t}} \left[ \sum_{a \in A_{t}} \bar{r}_{a,t} \right] \right)^{+} \right]} \\ &= \frac{\mathbf{E}_{\Theta_{t}} \left[ \left( \sum_{a \in A_{t}} \bar{r}_{a,t} - \mathbf{E}_{\Theta_{t}} \left[ \sum_{a \in A_{t}} \bar{r}_{a,t} \right] \right)^{+} \right]}{\Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}} \bar{r}_{a,t} \right]} \\ &\leq \frac{\mathbf{E}_{\Theta_{t}} \left[ \left( \sum_{a \in A_{t}} \bar{r}_{a,t} - \mathbf{E}_{\Theta_{t}} \left[ \sum_{a \in A_{t}} \bar{r}_{a,t} \right] \right)^{+} \right]}{\Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}} \bar{r}_{a,t} \right]} \\ &= 2\Phi(-\sqrt{4/\gamma})^{-1} \cdot \mathbf{E}_{\Theta_{t}} \left[ \left( \sum_{a \in A_{t}} \bar{r}_{a,t} - \mathbf{E}_{\Theta_{t}} \left[ \sum_{a \in A_{t}} \bar{r}_{a,t} \right] \right)^{+} \right]. \end{aligned}$$

$$\tag{39}$$

420 Step 2 proof. Since 
$$w_t$$
 and  $\tilde{w}_t$  are i.i.d., we have  $\mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} \bar{r}_{a,t} \right] =$   
421  $\mathbf{E}_{\Theta_t} \left[ \max_{A \in \Theta_t} \sum_{a \in A} \bar{r}_{a,t} \right] = \mathbf{E}_{\Theta_t} \left[ \max_{A \in \Theta_t} \sum_{a \in A} \tilde{r}_{a,t} \right] \ge \mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} \tilde{r}_{a,t} \mid A_t \right] =$   
422  $\mathbf{E}_{\Theta_t} \left[ \sum_{a \in A_t} \tilde{r}_{a,t} \mid A_t, w_t \right]$ . Then, we have

$$\mathbf{E}_{\Theta_{t}}\left[\left(\sum_{a\in A_{t}}\bar{r}_{a,t}-\mathbf{E}_{\Theta_{t}}\left[\sum_{a\in A_{t}}\bar{r}_{a,t}\right]\right)^{+}\right] \leq \mathbf{E}_{\Theta_{t}}\left[\left(\sum_{a\in A_{t}}\bar{r}_{a,t}-\mathbf{E}_{\Theta_{t}}\left[\sum_{a\in A_{t}}\bar{r}_{a,t}\mid A_{t}\right]\right)^{+}\right] \\
= \mathbf{E}_{\Theta_{t}}\left[\left(\sum_{a\in A_{t}}\bar{r}_{a,t}-\mathbf{E}_{\Theta_{t}}\left[\sum_{a\in A_{t}}\bar{r}_{a,t}\mid A_{t},w_{t}\right]\right)^{+}\right] \\
= \mathbf{E}_{\Theta_{t}}\left[\left(\mathbf{E}_{\Theta_{t}}\left[\left(\sum_{a\in A_{t}}\bar{r}_{a,t}-\sum_{a\in A_{t}}\bar{r}_{a,t}\right)\mid A_{t},w_{t}\right]\right)^{+}\right] \\
\leq \mathbf{E}_{\Theta_{t}}\left[\left|\mathbf{E}_{\Theta_{t}}\left[\left(\sum_{a\in A_{t}}\bar{r}_{a,t}-\sum_{a\in A_{t}}\bar{r}_{a,t}\right)\mid A_{t},w_{t}\right]\right]\right] \\
\leq \mathbf{E}_{\Theta_{t}}\left[\mathbf{E}_{\Theta_{t}}\left[\left|\sum_{a\in A_{t}}\bar{r}_{a,t}-\sum_{a\in A_{t}}\bar{r}_{a,t}\right|\mid A_{t},w_{t}\right]\right] \\
\leq \mathbf{E}_{\Theta_{t}}\left[\left|\sum_{a\in A_{t}}\bar{r}_{a,t}-\sum_{a\in A_{t}}\bar{r}_{a,t}\right|\mid A_{t},w_{t}\right]\right]$$
(40)

423 Step 3 proof. By Hölder's inequality, we have that

$$\mathbf{E}\left[\sum_{t=1}^{T}\left|\sum_{a\in A_{t}}\bar{r}_{a,t}-\sum_{a\in A_{t}}\tilde{r}_{a,t}\right|\right] \leq \mathbf{E}\left[\sum_{t=1}^{T}\left|w_{t}-\tilde{w}_{t}\right|\sum_{a\in A_{t}}\sqrt{\frac{\gamma\ln t}{n_{a,t}+1}}\right] \\ \leq \mathbf{E}\left[\max_{t\in[T]}\left|w_{t}-\tilde{w}_{t}\right|\sum_{t=1}^{T}\sum_{a\in A_{t}}\sqrt{\frac{\gamma\ln t}{n_{a,t}+1}}\right] \\ \stackrel{(a)}{\leq} \mathbf{E}\left[\max_{t\in[T]}\left|w_{t}-\tilde{w}_{t}\right|\right] \cdot 2\sqrt{\gamma mNT\ln T} \\ \stackrel{(b)}{\leq} 2\sqrt{\ln 2T} \cdot 2\sqrt{\gamma mNT\ln T} \\ \leq 4\ln T\sqrt{2\gamma mNT},$$
(41)

where step (a) is due to Lemma 5, and step (b) is due to Fact 2 and  $w_t - \tilde{w}_t$  is a Gaussian variable with variance 2.

## 426 D.2 Proof of Lemma 7

Lemma 7. In CL-SG, the regret of the deviation part is

$$\mathbf{E}\left[\sum_{t=1}^{T}\left(\sum_{a\in A_{t}}\bar{r}_{a,t} - \sum_{a\in A_{t}}r_{a}\right)\mathbf{1}[\mathcal{E}_{t}]\right] \leq 4\ln T\sqrt{\gamma mNT} + 2\sqrt{6mNT\ln T}.$$

427 *Proof.* Recall that  $\bar{r}_{a,t} = \hat{r}_{a,n_{a,t}} + w_t \sqrt{\frac{\gamma \ln t}{n_{a,t}+1}}$ . When  $\mathcal{E}_t$  happens, we have that

$$\mathbf{E}\left[\sum_{t=1}^{T}\left(\sum_{a\in A_{t}}\bar{r}_{a,t}-\sum_{a\in A_{t}}r_{a}\right)\mathbf{1}[\mathcal{E}_{t}]\right] = \mathbf{E}\left[\sum_{t=1}^{T}\sum_{a\in A_{t}}\left(\hat{r}_{a,n_{a,t}}+w_{t}\sqrt{\frac{\gamma\ln t}{n_{a,t}+1}}-\hat{r}_{a,n_{a,t}}+\sqrt{\frac{3\ln Nt}{n_{a,t}+1}}\right)\mathbf{1}[\mathcal{E}_{t}]\right] \\ \leq \sqrt{\gamma\ln T}\mathbf{E}\left[\sum_{t=1}^{T}w_{t}\left(\sum_{a\in A_{t}}\sqrt{\frac{1}{n_{a,t}+1}}\right)\right]+\sqrt{6\ln T}\mathbf{E}\left[\sum_{t=1}^{T}\sum_{a\in A_{t}}\sqrt{\frac{1}{n_{a,t}+1}}\right], \tag{42}$$

where the last inequality is due to that  $N \leq T$ . Regarding the first item in RHS of (42), we can apply Hölder's inequality to have that

$$\mathbf{E}\left[\sum_{t=1}^{T} w_t \left(\sum_{a \in A_t} \sqrt{\frac{1}{n_{a,t} + 1}}\right)\right] \leq \mathbf{E}\left[\max_{1 \leq t \leq T} |w_t| \cdot \left|\sum_{t=1}^{T} \sum_{a \in A_t} \sqrt{\frac{1}{n_{a,t} + 1}}\right|\right] \\
\leq \mathbf{E}\left[\max_{1 \leq t \leq T} |w_t| \cdot 2\sqrt{mNT}\right] \\
\leq 4\sqrt{mNT \ln T},$$
(43)

where the second inequality is due to Lemma 5, and the last inequality is due to the maximal inequality (Fact 2) for Gaussian variables such that  $\mathbf{E} \left[ \max_{1 \le t \le T} |w_t| \right] \le \sqrt{2 \ln 2T} \le 2\sqrt{T}$ .

Regarding the second term in RHS of (42), we can invoke Lemma 5 again to give a bound of  $2\sqrt{6mNT \ln T}$ .

#### 435 D.3 Proof of Lemma 8

434

436 **Lemma 8.** In each round  $t > \max{\sqrt{m}, 4}$ , given any  $\Theta_t$ , we have that for CL-SG:

$$\frac{1}{\Pr_{\Theta_t} \left( \sum_{a \in A_t^*} \bar{r}_{a,t} \ge \sum_{a \in A_t^*} r_a \right)} \le 2\Phi \left( -\sqrt{4/\gamma} \right)^{-1}.$$
(44)

$$\Pr_{\Theta_{t}} (\mathcal{H}_{t}) \geq 1 - \sum_{a \in A_{t}^{*}} \sum_{s_{a}=0}^{t-1} \Pr_{\Theta_{t}} \left( |r_{a} - \hat{r}_{a,s_{a}}| \geq \sqrt{\frac{4 \ln t}{s_{a}+1}} \right) \\ = 1 - \sum_{a \in A_{t}^{*}} \sum_{s_{a}=1}^{t-1} \Pr_{\Theta_{t}} \left( |r_{a} - \hat{r}_{a,s_{a}}| \geq \sqrt{\frac{4 \ln t}{s_{a}+1}} \right) \\ \geq 1 - \sum_{a \in A_{t}^{*}} \sum_{s_{a}=1}^{t-1} \Pr_{\Theta_{t}} \left( |r_{a} - \hat{r}_{a,s_{a}}| \geq \sqrt{\frac{4 \ln t}{s_{a}+1}} \right) \\ \geq 1 - mt \cdot 2 \cdot e^{-2 \cdot s_{a} \cdot 4 \ln t / (2s_{a})} \\ = 1 - \frac{2mt}{t} \\ \geq 0.5 , \qquad (45)$$

439 where the last two inequalities are due to that  $t > \max\{\sqrt{m}, 4\}$ .

440 We have

$$\Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}^{*}} \bar{r}_{a,t} \geq \sum_{a \in A_{t}^{*}} r_{a} \right) \geq \Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}^{*}} \bar{r}_{a,t} \geq \sum_{a \in A_{t}^{*}} r_{a}, \mathcal{H}_{t} \right) \\
= \Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}^{*}} \bar{r}_{a,t} - \hat{r}_{a,n_{a,t}} \geq \sum_{a \in A_{t}^{*}} r_{a} - \hat{r}_{a,n_{a,t}}, \mathcal{H}_{t} \right) \\
= \Pr_{\Theta_{t}} (\mathcal{H}_{t}) \cdot \Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}^{*}} \bar{r}_{a,t} - \hat{r}_{a,n_{a,t}} \geq \sum_{a \in A_{t}^{*}} r_{a} - \hat{r}_{a,n_{a,t}} | \mathcal{H}_{t} \right) \\
\stackrel{(a)}{\geq} 0.5 \cdot \Pr_{\Theta_{t}} \left( \sum_{a \in A_{t}^{*}} w_{t} \sqrt{\frac{\gamma \ln t}{n_{a,t} + 1}} \geq \sum_{a \in A_{t}^{*}} \sqrt{\frac{4 \ln t}{n_{a,t} + 1}} \right) \\
= 0.5 \cdot \Pr_{\Theta_{t}} \left( w_{t} \geq \sqrt{4/\gamma} \right) \\
= 0.5 \cdot \Phi \left( -\sqrt{4/\gamma} \right) ,$$
(46)

where step (a) is due to (45) and the fact that event  $\mathcal{E}_t$  is true.

# 442 **D.4 Proof of Upper Bound**

443 *Proof.* Recall that  $\mathcal{E}_t := \left\{ \forall a \in [N] : |r_a - \hat{r}_{a,n_{a,t}}| \leq \sqrt{\frac{3 \ln Nt}{n_{a,t}+1}} \right\}$  is the high-probability 444 event that the empirical mean reward is close to the true mean reward for arm a, and  $\overline{\mathcal{E}}_t$  is the 445 complementary event of  $\mathcal{E}_t$ .

Similar to the proof of the upper bound for CTS-G, we first let  $t' = \max{\sqrt{m}, 4}$ , and then decompose the regret as follows:

$$\mathcal{R}(T) \leq \underbrace{\sum_{t=t'}^{T} \mathbf{E}\left[\left(\sum_{a \in A_t^*} r_a - \sum_{a \in A_t} \bar{r}_{a,t}\right)\right]}_{=:I_1, \text{ optimism part}} + \underbrace{\sum_{t=t'}^{T} \mathbf{E}\left[\sum_{a \in A_t} (\bar{r}_{a,t} - r_a) \mathbf{1}[\mathcal{E}_t]\right]}_{=:I_2, \text{ deviation part}} + m\left(\max\{\sqrt{m}, 4\} + \frac{\pi^2}{3}\right),$$

$$(47)$$

<sup>448</sup> Now, invoking Lemma 6 with proofs in Appendix D.1, we have term  $I_1$  bounded as follows:

$$I_1 \leq 8\sqrt{2\gamma}\Phi(-\sqrt{4/\gamma})^{-1} \ln T\sqrt{mNT}, \tag{48}$$

and  $I_2$  can be bounded by using Lemma 7 with proofs in Appendix D.2:

$$I_2 \leq 4 \ln T \sqrt{\gamma m N T} + 2\sqrt{6m N T \ln T}.$$
(49)

<sup>450</sup> Therefore, we have the regret bounded as follows:

$$\mathcal{R}(T) \leq \left(4\sqrt{\gamma} + 8\sqrt{2\gamma}\Phi(-\sqrt{4/\gamma})^{-1}\right)\ln T\sqrt{mNT} + 2\sqrt{6mNT\ln T} + m\left(\max\{\sqrt{m}, 4\} + \frac{\pi^2}{3}\right),$$

where the coefficient of the first term can be minimized to 144.43 at  $\gamma = 4.57$ .

#### 452 D.5 Proof of Lower Bound

*Lower bound Proof in Theorem 2.* The main challenge in the proofs arises from the fact that all base arms share a single random Gaussian seed, creating dependencies between paths that are no longer independent. However, the lower-bound proof for Theorem 1 relies on the independence of each super arm. Therefore, this proof must manage these dependencies effectively.

$$t = 1 \qquad t = cT \qquad t = \alpha T \qquad t = T$$

Figure 6: The regret of CL-SG is lower bounded by the regret from rounds  $\alpha T$  to T.

We construct a path selection problem involving N links (i.e., each link corresponds to a base arm) and K paths (i.e., each path corresponds to a super arm). Each path consists of m links as illustrated in Fig. 5 and the total number of base arms is N = mK. We use a fixed availability set throughout all T rounds, i.e.,  $\Theta_t = \Theta := \{A_1, A_2, \ldots, A_K\}$  for all rounds  $t \in [T]$  with each  $A_k$  being a feasible path. We assume the first path is the unique optimal one.

We construct the following Bernoulli reward distributions for each base arm. Let  $\Delta := \sqrt{K/T}$ . For any base arm in the optimal super arm  $A_1$ , we use a degenerate distribution putting mass 1 on a single point  $\sqrt{\gamma}\Delta$ , i.e., if  $A_1$  is played, for each base arm in it, the observed random reward is always  $\sqrt{\gamma}\Delta$ . Similarly, for the remaining base arms in the sub-optimal super arms, we put mass 1 on a single point 0, i.e., the random reward is always 0 for any base arm in a sub-optimal super arm.

Let  $Q_A(t)$  denote the total number of times that super arm  $A \in \Theta$  has been played at the beginning of round t. Since there are no overlapping base arms between two distinct super arms, we have  $Q_A(t) = n_{a,t}$  for all  $a \in A$ , i.e., all base arms in a super arm have the same amount of observations.

Let  $c := \frac{1}{6}$ . Define  $B_t^* := \{Q_{A_1}(t) > t - cT\}$  as the event that the optimal super arm  $A_1$  has been observed enough times at the beginning of round t.

We lower bound the total regret from round 1 to the end of round T by analyzing two cases that are exhaustive and mutually exclusive based on events  $B_t^*$  for all rounds  $t \in [T]$ .

If  $B_t^*$  is not true for some round  $t \in [T]$ , we have the total number of times of playing sub-optimal super arms until the beginning of round t is  $\sum_{A \in \Theta \setminus A_1} Q_A(t) = t - Q_{A_1}(t) \ge cT$ . This lower bound implies the total regret from round 1 to the end of round t - 1 is at least  $cT \cdot m \cdot \sqrt{\gamma}\Delta =$  $\Omega(Tm\sqrt{K/T}) = \Omega(Tm\sqrt{N/(mT)}) = \Omega(\sqrt{mNT})$ . Note that this lower bound is also a regret lower bound for the total regret from round 1 to the end of round T.

479 Let  $\alpha := \frac{5}{6}$ .

480 If  $B_t^*$  is true for all rounds  $t \in [T]$ , the total regret from round 1 to the end of round T is lower 481 bounded by the total regret from round  $t = \alpha T$  to the end of round T, as shown in Fig. 6. In each 482 round  $t \ge \alpha T$ , we have the following inequalities:

$$\sum_{A \in \Theta \setminus A_1} Q_A(t) = t - Q_{A_1}(t) \le t - (t - c \cdot T) = c \cdot T \quad , \tag{50}$$

483

$$Q_{A_1}(t) > t - c \cdot T \ge \alpha \cdot T - c \cdot T = (\alpha - c) \cdot T \quad , \tag{51}$$

484 and

$$Q_A(t) \le c \cdot T, \quad \forall A \in \Theta \setminus A_1 \quad . \tag{52}$$

From (51) and (52), for each sub-optimal super arm  $A \in \Theta \setminus A_1$ , we have

$$\sqrt{\frac{Q_A(t)+1}{Q_{A_1}(t)+1}} \le \sqrt{\frac{cT+1}{(\alpha-c)T+1}} = \sqrt{\frac{T/6+1}{4T/6+1}} \le \frac{1}{2} \quad , \tag{53}$$

486 which gives

$$1 - \sqrt{\frac{Q_A(t)+1}{Q_{A_1}(t)+1}} \ge \frac{1}{2} \quad . \tag{54}$$

Let  $p_0 := \frac{1}{8\sqrt{\pi}}e^{-\frac{28}{3}}$ . In the following, we prove that, with at least a constant probability  $p_0$ , a sub-optimal super arm is played in each round  $t \ge \alpha \cdot T$  conditioned on event  $B_t^*$  is true. Note that whether event  $B_t^*$  is true or not is determined by the history information  $\mathcal{F}_{t-1}$ . Conditioned on any instantiation  $F_{t-1}$  of  $\mathcal{F}_{t-1}$  such that event  $B_t^*$  is true, we have the probability of playing a sub-optimal super arm is

$$\Pr\left(\exists A \in \Theta \setminus A_{1} : A_{t} = A \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$\geq \Pr\left(\exists A \in \Theta \setminus A_{1} : \sum_{a \in A} \bar{r}_{a,t} > \sum_{b \in A_{1}} \bar{r}_{b,t} \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$= \Pr\left(\exists A \in \Theta \setminus A_{1} : \sum_{a \in A} \hat{r}_{a,n_{a,t}} + w_{t} \sqrt{\frac{\gamma \ln t}{n_{a,t} + 1}} > \sum_{b \in A_{1}} \hat{r}_{b,n_{b,t}} + w_{t} \sqrt{\frac{\gamma \ln t}{n_{b,t} + 1}} \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$\stackrel{(a)}{\cong} \Pr\left(\exists A \in \Theta \setminus A_{1} : \sum_{a \in A} w_{t} \sqrt{\frac{\gamma \ln t}{n_{a,t} + 1}} > \sum_{b \in A_{1}} \left(\sqrt{\gamma}\Delta + w_{t} \sqrt{\frac{\gamma \ln t}{n_{b,t} + 1}}\right) \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$\stackrel{(b)}{=} \Pr\left(\exists A \in \Theta \setminus A_{1} : \sum_{a \in A} w_{t} \sqrt{\frac{\gamma \ln t}{Q_{A}(t) + 1}} > \sum_{b \in A_{1}} \left(\sqrt{\gamma}\Delta + w_{t} \sqrt{\frac{\gamma \ln t}{Q_{A_{1}}(t) + 1}}\right) \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$= \Pr\left(\exists A \in \Theta \setminus A_{1} : w_{t} \sqrt{\frac{\ln t}{Q_{A}(t) + 1}} > \Delta + w_{t} \sqrt{\frac{\ln t}{Q_{A_{1}}(t) + 1}} \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$\geq \Pr\left(\exists A \in \Theta \setminus A_{1} : w_{t} \left(1 - \sqrt{\frac{Q_{A}(t) + 1}{Q_{A_{1}}(t) + 1}}\right) > \Delta \sqrt{Q_{A}(t) + 1} \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$\stackrel{(e)}{=} \Pr\left(\exists A \in \Theta \setminus A_{1} : w_{t} \cdot \frac{1}{2} > \Delta \sqrt{Q_{A}(t) + 1} \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$= 1 - \Pr\left(w_{t} \leq 2\Delta \sqrt{Q_{A}(t) + 1}, \forall A \in \Theta \setminus A_{1} \mid \mathcal{F}_{t-1} = F_{t-1}\right)$$

$$(55)$$

where step (a) uses the fact that for any base arm in a sub-optimal super arm, the empirical mean is 0, whereas for any base arm in the optimal super arm, the empirical mean is  $\sqrt{\gamma}\Delta$  based on our reward distribution construction. Step (b) uses the fact that all base arms in a super arm have the same number of observations. Step (c) uses the lower bound constructed in (54), i.e.,  $1 - \sqrt{\frac{Q_A(t)+1}{Q_{A_1}(t)+1}} \geq \frac{1}{2}$ . Note that for  $\lambda$ , the only randomness is  $w \sim \mathcal{N}(0, 1)$  as all  $Q_A(t)$  are determined by the history.

To construct an upper bound for  $\lambda$  above, we construct an optimization problem first using the constraint shown in (50). Recall (50) is  $\sum_{A \in \Theta \setminus A_1} Q_A(t) \leq cT$ . We construct the optimization problem with the objective function shown in the following (56)

$$\max_{x_1, x_2, \dots, x_{K-1}} \quad \Pr_{w \sim \mathcal{N}(0, 1)} \left( w \leq 2\Delta \sqrt{x_a + 1}, \, \forall a \in [K - 1] \right) \quad , \tag{56}$$

and constraints shown in (57)

$$x_a \ge 0, \forall a \in [K-1] \text{ and } \sum_{a=1}^{K-1} x_a \le c \cdot T$$
 (57)

Note that the optimal solution to (56) is the same as the optimal solution to the following objective function (58):

$$\max_{x_1, x_2, \dots, x_{K-1}} \quad \Pr_{w \sim \mathcal{N}(0, 1)} \left( w \leq \min_{a \in [K-1]} x_a \right) \quad .$$
(58)

It is not hard to verify that the objective function shown in (58) is maximized when  $x_a = \frac{cT}{K-1} = \frac{c\sqrt{KT}}{(K-1)\Delta}$  for all  $a \in [K-1]$ . Therefore,  $x_a = \frac{cT}{K-1} = \frac{c\sqrt{KT}}{(K-1)\Delta}$  for all  $a \in [K-1]$  is also the optimal solution to (56) and the maximum value of the objective function shown in (56) is  $\Pr_w \left(w \leq 2\Delta \sqrt{\frac{c\sqrt{KT}}{(K-1)\Delta}} + 1\right)$ .

Now, we are ready to construct an upper bound for  $\lambda$  and have

$$\lambda = \Pr_{w} \left( w \leq 2\Delta \sqrt{Q_{A}(t) + 1}, \forall A \in \Theta \setminus A_{1} \mid \mathcal{F}_{t-1} = F_{t-1} \right)$$

$$\leq \max_{x_{1}, x_{2}, \dots, x_{K-1}} \Pr_{w} \left( w \leq 2\Delta \sqrt{x_{a} + 1}, \forall a \in [K - 1] \mid \mathcal{F}_{t-1} = F_{t-1} \right)$$

$$= \max_{x_{1}, x_{2}, \dots, x_{K-1}} \Pr_{w} \left( w \leq 2\Delta \sqrt{x_{a} + 1}, \forall a \in [K - 1] \right)$$

$$\stackrel{(a)}{\leq} \Pr_{w} \left( w \leq 2\Delta \sqrt{\frac{c\sqrt{KT}}{(K - 1)\Delta} + 1} \right)$$

$$\stackrel{(a)}{\leq} 1 - \frac{1}{8\sqrt{\pi}} \cdot e^{-\frac{\tau}{2} \cdot 4\Delta^{2} \cdot \left(\frac{c\sqrt{KT}}{(K-1)\Delta} + 1\right)}$$

$$\stackrel{(c)}{\leq} 1 - \frac{1}{8\sqrt{\pi}} \cdot e^{-\frac{\tau}{2} \cdot 4\Delta^{2} \cdot \frac{2c\sqrt{KT}}{0.5K\Delta}}$$

$$= 1 - \frac{1}{8\sqrt{\pi}} \cdot e^{-\frac{\tau}{2} \cdot 8\sqrt{\frac{K}{T} \cdot \frac{1}{6} \cdot \frac{\sqrt{KT}}{0.5K}}$$

$$= 1 - \frac{1}{8\sqrt{\pi}} e^{-\frac{28}{3}}$$

$$= 1 - p_{0} ,$$
(59)

where step (a) uses the fact that  $\Pr_w\left(w \le 2\Delta\sqrt{\frac{c\sqrt{KT}}{(K-1)\Delta}} + 1\right)$  is the maximum value of the objective function shown in (56). Step (b) uses the one-sided anti-concentration inequality shown in (6). Step (c) uses the fact that K - 1 > 0.5K,  $\Delta = \sqrt{K/T}$ , and when T is large enough, we have  $\frac{c\sqrt{KT}}{(K-1)\Delta} \ge 1$ .

plugging By the upper bound for  $\lambda$ into (55), we have 512  $\Pr\left(\exists A \in \Theta \setminus A_1 : A_t = A \mid \mathcal{F}_{t-1} = F_{t-1}\right) \geq p_0, \text{ which concludes the proof for }$ 513 the statement that with at least a constant probability  $p_0$ , a sub-optimal super arm is played in round t. 514 To complete the proof, we use the fact that the total regret from round  $t = \alpha T$  to round T is 515 at least  $(1 - \alpha)T + p_0 + m + \sqrt{\gamma}\Delta = \Omega(Tm\Delta) = \Omega(Tm\sqrt{K/T}) = \Omega(Tm\sqrt{N/(mT)}) = \Omega(Tm\sqrt{N/(mT)})$ 516  $\Omega(\sqrt{mNT})$ , which is also a regret lower bound for the total regret from round 1 to round T. 517