

UCB with clustering and improved exploration

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Abstract

In this paper, we present a novel algorithm for the stochastic multi-armed bandit (MAB) problem. Our proposed Efficient Clustered UCB method, referred to as EClusUCB partitions the arms into clusters and then follows the UCB-Improved strategy with aggressive exploration factors to eliminate sub-optimal arms, as well as entire clusters. Through a theoretical analysis, we establish that EClusUCB achieves a better gap-dependent regret upper bound than UCB-Improved (Auer & Ortner, 2010) and MOSS (Audibert & Bubeck, 2009) algorithms. Further, numerical experiments on test-cases with small gaps between optimal and sub-optimal mean rewards show that EClusUCB results in lower cumulative regret than several popular UCB variants as well as MOSS, OCUCB (Lattimore, 2015), Thompson sampling and Bayes-UCB (Kaufmann et al., 2012). We also present another algorithm called Adaptive Clustered UCB or AClusUCB which is intended to look at the effect of using more traditional approaches, like hierarchical clustering, for the grouping of arms.

1. Introduction

In this paper, we consider the stochastic multi-armed bandit problem, a classical problem in sequential decision making. In this setting, a learning algorithm is provided with a set of decisions (or arms) with reward distributions unknown to the algorithm. The learning proceeds in an iterative fashion, where in each round, the algorithm chooses an arm and receives a stochastic reward that is drawn from a stationary distribution specific to the arm selected. Given the goal of maximizing the cumulative reward, the learning algorithm faces the exploration-exploitation dilemma, i.e., in each round should the algorithm select the arm which has the highest observed mean reward so far (*exploitation*), or should the algorithm choose a new arm to gain more knowledge of the true mean reward of the arms and thereby avert a sub-optimal greedy decision (*exploration*).

Let r_i , $i = 1, \dots, K$ denote the mean reward of the i th arm out of the K arms and $r^* = \max_i r_i$ the optimal mean

reward. The objective in the stochastic bandit problem is to minimize the cumulative regret, which is defined as follows:

$$R_T = r^*T - \sum_{i \in A} r_i N_i(T),$$

where T is the number of rounds, $N_i(T) = \sum_{m=1}^T I(I_m = i)$ is the number of times the algorithm has chosen arm i up to round T . The expected regret of an algorithm after T rounds can be written as

$$\mathbb{E}[R_T] = \sum_{i=1}^K \mathbb{E}[N_i(T)] \Delta_i,$$

where $\Delta_i = r^* - r_i$ denotes the gap between the means of the optimal arm and the i -th arm.

An early work involving a bandit setup is Thompson (1933), where the author deals the problem of choosing between two treatments to administer on patients who come in sequentially. Following the seminal work of Robbins (1952), bandit algorithms have been extensively studied in a variety of applications. From a theoretical standpoint, an asymptotic lower bound for the regret was established in Lai & Robbins (1985). In particular, it was shown that for any consistent allocation strategy, we have $\liminf_{T \rightarrow \infty} \frac{\mathbb{E}[R_T]}{\log T} \geq \sum_{\{i: r_i < r^*\}} \frac{(r^* - r_i)}{D(p_i || p^*)}$, where $D(p_i || p^*)$ is the Kullback-Leibler divergence between the reward densities p_i and p^* , corresponding to arms with mean r_i and r^* , respectively.

There have been several algorithms with strong regret guarantees. For further reference we point the reader to Bubeck et al. (2012). The foremost among them is UCB1 (Auer et al., 2002a), which has a regret upper bound of $O\left(\frac{K \log T}{\Delta}\right)$, where $\Delta = \min_{i: \Delta_i > 0} \Delta_i$. This result is asymptotically order-optimal for the class of distributions considered. However, the worst case gap independent regret bound of UCB1 can be as bad as $O(\sqrt{TK \log T})$. In Audibert & Bubeck (2009), the authors propose the MOSS algorithm and establish that the worst case regret of MOSS is $O(\sqrt{TK})$ which improves upon UCB1 by a factor of order $\sqrt{\log T}$. However, the gap-dependent regret of MOSS is $O\left(\frac{K^2 \log(T \Delta^2 / K)}{\Delta}\right)$ and in certain regimes, this can be worse than even UCB1 (see (Audibert & Bubeck,

2009), (Lattimore, 2015)). The UCB-Improved algorithm, proposed in Auer & Ortner (2010), is a round-based algorithm¹ variant of UCB1 that has a gap-dependent regret bound of $O\left(\frac{K \log T \Delta^2}{\Delta}\right)$, which is better than that of UCB1. On the other hand, the worst case regret of UCB-Improved is $O(\sqrt{TK \log K})$. Recently in Lattimore (2015), the algorithm OCUCB achieves order-optimal gap-dependent regret bound of $O\left(\sum_{i=2}^K \frac{\log(T/H_i)}{\Delta_i}\right)$ where $H_i = \sum_{j=1}^K \min\{\frac{1}{\Delta_i^2}, \frac{1}{\Delta_j^2}\}$ and gap-independent regret bound of $O(\sqrt{KT})$. In certain environments, for a larger number of arms and uniform gaps, OCUCB does not perform well.

The idea of clustering in the bandit framework is not entirely new. In particular, the idea of clustering has been extensively studied in the contextual bandit setup, an extension of the MAB where side information or features are attached to each arm (see Auer (2002); Langford & Zhang (2008); Li et al. (2010); Beygelzimer et al. (2011); Slivkins (2014)). The clustering in this case is typically done over the feature space (Bui et al., 2012; Cesa-Bianchi et al., 2013; Gentile et al., 2014), however, in our work we cluster or group the arms directly.

1.1. Our Contribution

We propose a variant of UCB algorithm, henceforth referred to as EClusUCB, that incorporates clustering and an improved exploration scheme. EClusUCB starts with partitioning of arms into small clusters, each having same number of arms. The clustering is done at the start with a pre-specified number of clusters. Each timestep of EClusUCB involves both (individual) arm elimination as well as cluster elimination.

The clustering of arms provides two benefits. First, it creates a context where a UCB-Improved like algorithm can be run in parallel on smaller sets of arms with limited exploration, which could lead to fewer pulls of sub-optimal arms with the help of more aggressive elimination of sub-optimal arms. Second, the cluster elimination leads to whole sets of sub-optimal arms being simultaneously eliminated when they are found to yield poor results. These two simultaneous criteria for arm elimination can be seen as borrowing the strengths of UCB-Improved as well as other popular round based approaches.

While EClusUCB does not achieve the gap-dependent regret bound of OCUCB, the theoretical analysis establishes that the gap-dependent regret of EClusUCB is always better than that of UCB-Improved and better than that of

¹An algorithm is *round-based* if it pulls all the arms equal number of times in each round and then proceeds to eliminate one or more arms that it identifies to be sub-optimal.

Table 1: Comparison of different algorithms against EClusUCB. The \checkmark indicates that EClusUCB outperforms the respective baseline. E1, E2 and E3 correspond to experiments 1, 2 and 3 in Section 5

| Algorithm | Gap-Dep | Gap-Ind | E1 | E2 | E3 |
|-----------|--------------|--------------|--------------|--------------|--------------|
| UCB1 | \checkmark | \checkmark | \checkmark | \checkmark | N/A |
| UCB-Imp | \checkmark | \checkmark | \checkmark | \checkmark | N/A |
| MOSS | \checkmark | \times | \checkmark | \checkmark | \checkmark |
| OCUCB | \times | \times | \checkmark | \checkmark | \checkmark |

MOSS when $\sqrt{\frac{K}{14T}} \leq \Delta \leq 1$ (see Table 1, Table 2 in Appendix A). Moreover, the gap-independent bound of EClusUCB is of the same order as UCB-Improved, i.e., $O(\sqrt{KT \log K})$. However, EClusUCB is not able to match the gap-independent bound of $O(\sqrt{KT})$ for MOSS and OCUCB. We also establish the exact values for the exploration parameters and the number of clusters required for optimal behavior in the corollaries. On four synthetic setups with small gaps, we observe empirically that EClusUCB outperforms UCB-Improved (Auer & Ortner, 2010), MOSS (Audibert & Bubeck, 2009) and OCUCB (Lattimore, 2015) as well as other popular stochastic bandit algorithms such as DMED (Honda & Takemura, 2010), UCB-V (Audibert et al., 2009), Median Elimination (Even-Dar et al., 2006), Thompson Sampling (Agrawal & Goyal, 2011), Bayes-UCB (Kaufmann et al., 2012) and KL-UCB (Garivier & Cappé, 2011). Adaptive ClusUCB (AclucUCB) which estimates the clusters based on hierarchical clustering is introduced in Appendix G. An empirical study comparing its performance to EClusUCB is presented in experiment 4.

The rest of the paper is organized as follows: In Section 2 we introduce EClusUCB. In Section 3, we present the associated regret bounds and prove the main theorem on the regret upper bound for EClusUCB in Section 4. In Section 5, we present the numerical experiments and provide concluding remarks in Section 6. Further proofs of corollaries, theorems and proposition presented in Section 4 are provided in the appendices. The algorithm Adaptive ClusUCB is presented in Appendix G and more experiments are presented in Appendix H.

2. Algorithm: Efficient Clustered UCB

2.1 Notations: We denote the set of arms by A , with the individual arms labeled $i, i = 1, \dots, K$. We denote an arbitrary round of EClusUCB by m . We denote an arbitrary cluster by s_k , the subset of arms within the cluster s_k by A_{s_k} and the set of clusters by S with $|S| = p \leq K$. Here p is a pre-specified limit for the number of clusters. For simplicity, we assume that the optimal arm is unique and denote it by $*$, with s^* denoting the corresponding cluster. The true best arm in a cluster s_k is denoted by $a_{max_{s_k}}$.

Algorithm 1 EClusUCB

Input: Number of clusters p , time horizon T , exploration parameters ρ_a, ρ_s and ψ .

Initialization: Set $m := 0$, $B_0 := A$, $S_0 = S$, $\epsilon_0 := 1$, $M = \lfloor \frac{1}{2} \log_2 \frac{14T}{K} \rfloor$, $n_0 = \left\lceil \frac{2 \log(\psi T \epsilon_0^2)}{\epsilon_0} \right\rceil$ and $N_0 = K n_0$.

Create a partition S_0 of the arms at random into p clusters of size up to $\ell = \left\lceil \frac{K}{p} \right\rceil$ each.

Pull each arm once

for $t = K + 1, \dots, T$ **do**

Pull arm $i \in \arg \max_{j \in B_m} \left\{ \hat{r}_j + \sqrt{\frac{\rho_s \log(\psi T \epsilon_m^2)}{2z_j}} \right\}$,

where z_j is the number of times arm j has been pulled
 $t := t + 1$

Arm Elimination

For each cluster $s_k \in S_m$, delete arm $i \in s_k$ from B_m if

$$\hat{r}_i + \sqrt{\frac{\rho_a \log(\psi T \epsilon_m^2)}{2n_m}} < \max_{j \in s_k} \left\{ \hat{r}_j - \sqrt{\frac{\rho_a \log(\psi T \epsilon_m^2)}{2n_m}} \right\}$$

Cluster Elimination

Delete cluster $s_k \in S_m$ and remove all arms $i \in s_k$ from B_m if

$$\begin{aligned} & \max_{i \in s_k} \left\{ \hat{r}_i + \sqrt{\frac{\rho_s \log(\psi T \epsilon_m^2)}{2n_m}} \right\} \\ & < \max_{j \in B_m} \left\{ \hat{r}_j - \sqrt{\frac{\rho_s \log(\psi T \epsilon_m^2)}{2n_m}} \right\}. \end{aligned}$$

if $t \geq N_m$ and $m \leq M$ **then**

$$\epsilon_{m+1} := \frac{\epsilon_m}{2}$$

$$B_{m+1} := B_m$$

$$n_{m+1} := \left\lceil \frac{2 \log(\psi T \epsilon_{m+1}^2)}{\epsilon_{m+1}} \right\rceil$$

$$N_{m+1} := t + |B_{m+1}| n_{m+1}$$

$$m := m + 1$$

Stop if $|B_m| = 1$ and pull $i \in B_m$ till T is reached.

end if

end for

We denote the sample mean of the rewards seen so far for arm i by \hat{r}_i and for the true best arm within a cluster s_k by $\hat{r}_{a_{\max s_k}}$. z_i is the number of times an arm i has been pulled. We assume the rewards of all arms are bounded in $[0, 1]$.

2.2 The algorithm. As mentioned in a recent work (Liu & Tsuruoka, 2016), UCB-Improved has two shortcomings:

(i) A significant number of pulls are spent in early exploration, since each round m of UCB-Improved involves pulling every arm an identical $n_m = \left\lceil \frac{2 \log(T \epsilon_m^2)}{\epsilon_m^2} \right\rceil$ number of times. The quantity ϵ_m is initialized to 1 and halved after every round.

(ii) In UCB-Improved, arms are eliminated conservatively, i.e., only after $\epsilon_m < \frac{\Delta_i}{2}$, the sub-optimal arm i is discarded with high probability. This is disadvantageous when K is large and the gaps are identical ($r_1 = r_2 = \dots = r_{K-1} < r^*$) and small.

To reduce early exploration, the number of pulls n_m allocated to each arm per round in EClusUCB is lower than that of UCB-Improved and also that of Median-Elimination, which used $n_m = \frac{4}{\epsilon^2} \log\left(\frac{3}{\delta}\right)$, where ϵ, δ are confidence parameters. To handle the second problem mentioned above, EClusUCB partitions the larger problem into several small sub-problems using clustering and then performs local exploration aggressively to eliminate sub-optimal arms within each clusters with high probability.

As described in the pseudocode in Algorithm 1, EClusUCB begins with an initial clustering of arms that is performed by random uniform allocation. The set of clusters S thus obtained satisfies $|S| = p$, with individual clusters having a size that is bounded above by $\ell = \left\lceil \frac{K}{p} \right\rceil$. Each timestep of EClusUCB involves both individual arm as well as cluster elimination conditions. These elimination conditions are inspired by UCB-Improved. Notice that, unlike UCB-Improved, there is no longer a single point of reference based on which we are eliminating arms. Instead we now have as many reference points to eliminate arms as number of clusters formed. In EClusUCB we also introduce the idea of optimistic greedy sampling similar to Liu & Tsuruoka (2016) which they used to modify the UCB-Improved algorithm. In optimistic greedy sampling, we only sample the arm with the highest upper confidence bound in each timestep. We further modify the idea by introducing clustering and arm elimination parameters. EClusUCB checks arm and cluster elimination conditions in every timestep and update parameters when a round is complete. It divides each round into $|B_m| n_m$ timesteps so that each surviving arms can be allocated atmost n_m pulls. The exploration regulatory factor ψ governing the arm and cluster elimination conditions in EClusUCB is more aggressive than that in UCB-Improved. With appropriate choices of ψ, ρ_a and ρ_s , we can achieve aggressive elimination even when the gaps Δ_i are small and K is large. Also we use different exploration regulatory factor than Liu & Tsuruoka (2016) and we come up with a cumulative regret bound whereas Liu & Tsuruoka (2016) only gives simple regret bound for the CCB algorithm.

In Liu & Tsuruoka (2016), the authors recommend incorporating a factor of d_i inside the log-term of the UCB val-

ues, i.e., $\max\{\hat{r}_i + \sqrt{\frac{d_i \log T \epsilon_m^2}{2n_m}}\}$. The authors there examine the following choices for d_i : $\frac{T}{z_i}$, $\frac{\sqrt{T}}{z_i}$ and $\frac{\log T}{z_i}$, where z_i is the number of times an arm i has been sampled. Unlike Liu & Tsuruoka (2016), we employ cluster as well as arm elimination and establish from a theoretical analysis that the choice $\psi = \frac{T}{196 \log(K)}$ helps in achieving a better gap-dependent regret upper bound for EClusUCB as compared to UCB-Improved and MOSS (Corollary 1).

2.3 Adaptive Clustered UCB: One of the disadvantages of EClusUCB is that it requires the knowledge of the number of clusters p . To counter this we introduce Adaptive Clustered UCB or AClusUCB which employs hierarchical clustering to estimate the clusters on-the-fly and is shown in Appendix G.

3. Main results

We now state the main result that upper bounds the expected regret of EClusUCB.

Theorem 1 (Regret bound). *The regret R_T of EClusUCB satisfies*

$$\begin{aligned} \mathbb{E}[R_T] \leq & \sum_{\substack{i \in A_{s^*}, \\ \Delta_i > b}} \left\{ \frac{C_1(\rho_a)T^{1-\rho_a}}{\Delta_i^{4\rho_a-1}} + \Delta_i \right. \\ & + \left. \frac{32\rho_a \log(\psi T \frac{\Delta_i^4}{16\rho_a^2})}{\Delta_i} \right\} + \sum_{\substack{i \in A, \\ \Delta_i > b}} \left\{ 2\Delta_i + \frac{C_1(\rho_s)T^{1-\rho_s}}{\Delta_i^{4\rho_s-1}} \right. \\ & + \left. \frac{32\rho_a \log(\psi T \frac{\Delta_i^4}{16\rho_a^2})}{\Delta_i} + \frac{32\rho_s \log(\psi T \frac{\Delta_i^4}{16\rho_s^2})}{\Delta_i} \right\} \\ & + \sum_{\substack{i \in A_{s^*}, \\ \Delta_i > b}} \frac{C_2(\rho_a)T^{1-\rho_a}}{\Delta_i^{4\rho_a-1}} + \sum_{\substack{i \in A_{s^*}, \\ 0 < \Delta_i \leq b}} \frac{C_2(\rho_a)T^{1-\rho_a}}{b^{4\rho_a-1}} \\ & + \sum_{\substack{i \in A \setminus A_{s^*}, \\ \Delta_i > b}} \frac{2C_2(\rho_s)T^{1-\rho_s}}{\Delta_i^{4\rho_s-1}} + \sum_{\substack{i \in A \setminus A_{s^*}, \\ 0 < \Delta_i \leq b}} \frac{2C_2(\rho_s)T^{1-\rho_s}}{b^{4\rho_s-1}} \\ & + \max_{i: \Delta_i \leq b} \Delta_i T, \end{aligned}$$

where $b \geq \sqrt{\frac{K}{14T}}$, $C_1(x) = \frac{2^{1+4x}x^{2x}}{\psi^x}$, $C_2(x) = \frac{2^{2x+\frac{3}{2}}x^{2x}}{\psi^x}$, and A_{s^*} is the subset of arms in cluster s^* containing optimal arm a^* .

Proof. See Section 4. \square

We now specialize the result in the theorem above by substituting specific values for the exploration constants ρ_s, ρ_a and ψ .

Corollary 1 (Gap-dependent bound). *With $\psi = \frac{T}{196 \log(K)}$, $\rho_a = \frac{1}{2}$, and $\rho_s = \frac{1}{2}$, we have the following*

gap-dependent bound for the regret of EClusUCB:

$$\begin{aligned} \mathbb{E}[R_T] \leq & \sum_{\substack{i \in A_{s^*}, \\ \Delta_i > b}} \left\{ \frac{96\sqrt{\log(K)}}{\Delta_i} + \Delta_i + \right. \\ & \left. \frac{32 \log(T \frac{\Delta_i^2}{\sqrt{\log(K)}})}{\Delta_i} \right\} + \sum_{i \in A: \Delta_i > b} \left\{ \frac{56\sqrt{\log(K)}}{\Delta_i} + 2\Delta_i \right. \\ & + \left. \frac{64 \log(T \frac{\Delta_i^2}{\sqrt{\log(K)}})}{\Delta_i} \right\} + \sum_{\substack{i \in A_{s^*}, \\ 0 < \Delta_i \leq b}} \frac{40\sqrt{\log(K)}}{\Delta_i} \\ & + \sum_{\substack{i \in A \setminus A_{s^*}, \\ \Delta_i > b}} \frac{80\sqrt{\log(K)}}{\Delta_i} + \sum_{\substack{i \in A \setminus A_{s^*}, \\ 0 < \Delta_i \leq b}} \frac{80\sqrt{\log(K)}}{\Delta_i} \\ & + \max_{i \in A: \Delta_i \leq b} \Delta_i T, \quad \text{for all } b \geq \sqrt{\frac{K}{14T}}. \end{aligned}$$

Proof. See Appendix C. \square

The most significant term in the bound above is $\sum_{i \in A: \Delta_i \geq b} \frac{64 \log(T \frac{\Delta_i^2}{\sqrt{\log(K)}})}{\Delta_i}$ and hence, the regret upper bound for EClusUCB is of the order $O\left(\frac{K \log\left(\frac{T \Delta^2}{\sqrt{\log(K)}}\right)}{\Delta}\right)$.

Since Corollary 1 holds for all $\Delta \geq \sqrt{\frac{K}{14T}}$, it can be clearly seen that for all $\sqrt{\frac{K}{14T}} \leq \Delta \leq 1$ and $K \geq 2$, the gap-dependent bound is better than that of UCB1, UCB-Improved and MOSS (see Table 2).

Corollary 2 (Gap-independent bound). *Considering the same gap of $\Delta_i = \Delta = \sqrt{\frac{K \log K}{T}}$ for all $i: i \neq *$ and with $\psi = \frac{T}{196 \log K}$, $p = \left\lceil \frac{K}{\log K} \right\rceil$, $\rho_a = \frac{1}{2}$ and $\rho_s = \frac{1}{2}$, we have the following gap-independent bound for the regret of EClusUCB:*

$$\begin{aligned} \mathbb{E}[R_T] \leq & 270 \frac{\sqrt{T} \log K}{\sqrt{K}} + \frac{32\sqrt{T} \log K \log(\log K)}{\sqrt{K}} \\ & + 56\sqrt{KT} + 128\sqrt{KT} \log K \\ & + \frac{64\sqrt{KT} \log(\log K)}{\sqrt{\log K}} + 150\sqrt{\frac{T \log K}{e}} \\ & + 300\sqrt{\frac{T}{e}} (\log K)^{\frac{3}{2}} + 300 \frac{K}{K + \log K} \sqrt{KT} \end{aligned}$$

Proof. See Appendix D. \square

From the above result, we observe that the order of the regret upper bound of EClusUCB is $O(\sqrt{KT} \log K)$, and this matches the order of UCB-Improved. However, this

is not as low as the order $O(\sqrt{KT})$ of MOSS or OCUCB. Also, the gap-independent bound of UCB-Improved holds for $\sqrt{\frac{e}{T}} \leq \Delta \leq 1$ while in our case the gap independent bound holds for $\sqrt{\frac{K}{14T}} \leq \Delta \leq 1$.

Analysis of elimination error (Why Clustering?)

Let \tilde{R}_T denote the contribution to the expected regret in the case when the optimal arm $*$ gets eliminated during one of the rounds of EClusUCB. This can happen if a sub-optimal arm eliminates $*$ or if a sub-optimal cluster eliminates the cluster s^* that contains $*$ – these correspond to cases b2 and b3 in the proof of Theorem 1 (see Section 4). We shall denote variant of EClusUCB that includes arm elimination condition only as EClusUCB-AE while EClusUCB corresponds to Algorithm 1, which uses both arm and cluster elimination conditions. The regret upper bound for EClusUCB-AE is given in Proposition 1 in Appendix B.

For EClusUCB-AE, the quantity \tilde{R}_T can be extracted from the proofs (in particular, case b2 in Appendix B) and simplified using the values $\rho_a = \frac{1}{2}$ and $\psi = \frac{T}{196 \log K}$, to obtain $\tilde{R}_T = 150\sqrt{KT \log K} + 150\sqrt{KT}$. Finally, for EClusUCB, the relevant terms from Theorem 1 that corresponds to \tilde{R}_T can be simplified with $\rho_a = \frac{1}{2}$, $\rho_s = \frac{1}{2}$, $p = \lceil \frac{K}{\log K} \rceil$ and $\psi = \frac{T}{196 \log K}$ (as in Corollary 2 to obtain $\tilde{R}_T = \frac{150\sqrt{T \log K}^{\frac{3}{2}}}{\sqrt{K}} + \frac{150\sqrt{T \log K}}{\sqrt{K}} + 300\frac{K}{K+\log K}\sqrt{KT \log K} + 300\frac{K}{K+\log K}\sqrt{KT}$. Hence, in comparison to EClusUCB-AE which has an elimination regret bound of $O(\sqrt{KT \log K})$, the elimination error contribution to regret is lower in EClusUCB which has a bound of $O(\frac{K}{K+\log K}\sqrt{KT \log K})$. Thus, we observe that clustering in conjunction with improved exploration via ρ_a, ρ_s, p and ψ helps in reducing the factor associated with $\sqrt{KT \log K}$ for the gap-independent error regret bound for EClusUCB. Also in section 5, in experiment 4 we show that EClusUCB outperforms EClusUCB-AE. A table containing the regret error bound is shown in Appendix E and further experiment showing that the performance of EClusUCB against CCB(Liu & Tsuruoka, 2016) is shown in Appendix H.

4. Proof of Theorem 1

Proof. Let $A' = \{i \in A, \Delta_i > b\}$, $A'' = \{i \in A, \Delta_i > 0\}$, $A'_{s_k} = \{i \in A_{s_k}, \Delta_i > b\}$ and $A''_{s_k} = \{i \in A_{s_k}, \Delta_i > 0\}$. C_g is the cluster set containing max payoff arm from each cluster in g -th round. The arm having the true highest payoff in a cluster s_k is denote by $a_{\max_{s_k}}$. Let for each sub-optimal arm $i \in A$, $m_i = \min \{m | \sqrt{\rho_a \epsilon_m} < \frac{\Delta_i}{2}\}$ and let for each cluster $s_k \in S$, $g_{s_k} = \min \{g | \sqrt{\rho_s \epsilon_g} < \frac{\Delta_{a_{\max_{s_k}}}}{2}\}$. Let $\check{A} = \{i \in A' | i \in s_k, \forall s_k \in S\}$. Also z_i denotes total number of times an arm i has been pulled. In the m -th round, n_m denotes the number of pulls allocated to the surviving arms in B_m . The analysis proceeds by considering the contribution to the re-

gret in each of the following cases:

Case a: Some sub-optimal arm i is not eliminated in round $\max(m_i, g_{s_k})$ or before, with the optimal arm $*$ $\in C_{\max(m_i, g_{s_k})}$. We consider an arbitrary sub-optimal arm i and analyze the contribution to the regret when i is not eliminated in the following exhaustive sub-cases:

Case a1: In round $\max(m_i, g_{s_k})$, $i \in s^*$.

Similar to case (a) of Auer & Ortner (2010), observe that when the following two conditions hold, arm i gets eliminated:

$$\hat{r}_i \leq r_i + c_{m_i} \text{ and } \hat{r}^* \geq r^* - c_{m_i}, \quad (1)$$

where $c_{m_i} = \sqrt{\frac{\rho_a \log(\psi T \epsilon_{m_i}^2)}{2n_{m_i}}}$. As arm elimination condition is being checked in every timestep, for any $z_i \geq n_{m_i}$, the arm i gets eliminated because

$$\begin{aligned} \hat{r}_i + c_{m_i} &\leq r_i + 2c_{m_i} < r_i + \Delta_i - 2c_{m_i} \\ &\leq r^* - 2c_{m_i} \leq \hat{r}^* - c_{m_i}. \end{aligned}$$

In the above, we have used the fact that

$c_{m_i} = \sqrt{\rho_a \epsilon_{m_i+1}} < \frac{\Delta_i}{4}$, since $n_{m_i} = \frac{2 \log(\psi T \epsilon_{m_i}^2)}{\epsilon_{m_i}}$ and $\rho_a \in (0, 1]$. From the foregoing, we have to bound the events complementary to that in (1) for an arm i to not get eliminated. Considering Chernoff-Hoeffding bound this is done as follows:

$$\begin{aligned} \mathbb{P}(\hat{r}_i \geq r_i + c_{m_i}) &\leq \exp(-2c_{m_i}^2 n_{m_i}) \\ &\leq \exp(-2 * \frac{\rho_a \log(\psi T \epsilon_{m_i}^2)}{2n_{m_i}} * n_{m_i}) \leq \frac{1}{(\psi T \epsilon_{m_i}^2)^{\rho_a}} \end{aligned}$$

Along similar lines, we have $\mathbb{P}(\hat{r}^* \leq r^* - c_{m_i}) \leq \frac{1}{(\psi T \epsilon_{m_i}^2)^{\rho_a}}$. Thus, the probability that a sub-optimal arm i is not eliminated in any round on or before m_i is bounded above by $\left(\frac{2}{(\psi T \epsilon_{m_i}^2)^{\rho_a}}\right)$. Summing up over all arms in A'_{s^*} in conjunction with a simple bound of $T\Delta_i$ for each arm, we obtain

$$\begin{aligned} \sum_{i \in A'_{s^*}} \left(\frac{2T\Delta_i}{(\psi T \epsilon_{m_i}^2)^{\rho_a}} \right) &\leq \sum_{i \in A'_{s^*}} \left(\frac{2T\Delta_i}{(\psi T \frac{\Delta_i^4}{16\rho_a^2})^{\rho_a}} \right) \\ &= \sum_{i \in A'_{s^*}} \left(\frac{C_1(\rho_a)T^{1-\rho_a}}{\Delta_i^{4\rho_a-1}} \right), \text{ where } C_1(x) = \frac{2^{1+4x}x^{2x}}{\psi^x} \end{aligned}$$

Case a2: In round $\max(m_i, g_{s_k})$, $i \in s_k$ for some $s_k \neq s^*$.

Following a parallel argument like in Case a1, as cluster elimination condition is being checked at every timestep, we have to bound the following two events of arm $a_{\max_{s_k}}$ not getting eliminated on or before g_{s_k} -th round for any $z_{a_{\max_{s_k}}} \geq n_{g_{s_k}}$,

$$\hat{r}_{a_{\max_{s_k}}} \geq r_{a_{\max_{s_k}}} + c_{g_{s_k}} \text{ and } \hat{r}^* \leq r^* - c_{g_{s_k}}$$

We can prove using Chernoff-Hoeffding bounds and considering independence of events mentioned above, that for $c_{g_{s_k}} = \sqrt{\frac{\rho_s \log(\psi T \epsilon_{g_{s_k}}^2)}{2n_{g_{s_k}}}}$ and $n_{g_{s_k}} = \frac{2 \log(\psi T \epsilon_{g_{s_k}}^2)}{\epsilon_{g_{s_k}}}$ the probability of the above two events is bounded by $\left(\frac{2}{(\psi T \epsilon_{g_{s_k}}^2)^{\rho_s}}\right)$. Now, for any round g_{s_k} , all the elements of $C_{\max(m_i, g_{s_k})}$ are the respective maximum payoff arms of their cluster s_k , $\forall s_k \in S$, and since clusters are fixed so we can bound the maximum probability that a sub-optimal arm $i \in A'$ and $i \in s_k$ such that $a_{\max s_k} \in C_{g_{s_k}}$ is not eliminated on or before the g_{s_k} -th round by the same probability as above. Summing up over all p clusters and bounding the regret for each arm $i \in A'_{s_k}$ trivially by $T\Delta_i$,

$$\begin{aligned} \sum_{k=1}^p \sum_{i \in A'_{s_k}} \left(\frac{2T\Delta_i}{(\psi T \frac{\Delta_i^4}{16\rho_s^2})^{\rho_s}} \right) &= \sum_{i \in A'} \left(\frac{2T\Delta_i}{(\psi T \frac{\Delta_i^4}{16\rho_s^2})^{\rho_s}} \right) \\ &\leq \sum_{i \in A'} \left(\frac{2^{1+4\rho_s} \rho_s^{2\rho_s} T^{1-\rho_s}}{\psi^{\rho_s} \Delta_i^{4\rho_s-1}} \right) = \sum_{i \in A'} \frac{C_1(\rho_s) T^{1-\rho_s}}{\Delta_i^{4\rho_s-1}} \end{aligned}$$

Summing the bounds in Cases $a1 - a2$ and observing that the bounds in the aforementioned cases hold for any round $C_{\max\{m_i, g_{s_k}\}}$, we obtain the following contribution to the expected regret from case a:

$$\sum_{i \in A_{s^*}} \frac{C_1(\rho_a) T^{1-\rho_a}}{\Delta_i^{4\rho_a-1}} + \sum_{i \in A'} \left(\frac{C_1(\rho_s) T^{1-\rho_s}}{\Delta_i^{4\rho_s-1}} \right)$$

Case b: For each arm i , either i is eliminated in round $\max(m_i, g_{s_k})$ or before or there is no optimal arm $*$ in $C_{\max(m_i, g_{s_k})}$.

Case b1: $*$ $\in C_{\max(m_i, g_{s_k})}$ for each arm $i \in A'$ and cluster $s_k \in \tilde{A}$. The condition in the case description above implies the following:

- (i) each sub-optimal arm $i \in A'$ is eliminated on or before $\max(m_i, g_{s_k})$ and hence pulled not more than $z_i < n_{m_i}$ number of times.
- (ii) each sub-optimal cluster $s_k \in \tilde{A}$ is eliminated on or before $\max(m_i, g_{s_k})$ and hence pulled not more than $z_{a_{\max s_k}} < n_{g_{s_k}}$ number of times.

Hence, the maximum regret suffered due to pulling of a sub-optimal arm or a sub-optimal cluster is no more than the following:

$$\begin{aligned} \sum_{i \in A'} \Delta_i \left\lceil \frac{2 \log(\psi T \epsilon_{m_i}^2)}{\epsilon_{m_i}} \right\rceil + \sum_{k=1}^p \sum_{i \in A'_{s_k}} \Delta_i \left\lceil \frac{2 \log(\psi T \epsilon_{g_{s_k}}^2)}{\epsilon_{g_{s_k}}} \right\rceil \\ \leq \sum_{i \in A'} \Delta_i \left(1 + \frac{32\rho_a \log\left(\psi T \left(\frac{\Delta_i}{2\sqrt{\rho_a}}\right)^4\right)}{\Delta_i^2} \right) \end{aligned}$$

$$\begin{aligned} &+ \sum_{i \in A'} \Delta_i \left(1 + \frac{32\rho_s \log\left(\psi T \left(\frac{\Delta_i}{2\sqrt{\rho_s}}\right)^4\right)}{\Delta_i^2} \right) \\ &\leq \sum_{i \in A'} \left[2\Delta_i + \frac{32(\rho_a \log(\psi T \frac{\Delta_i^4}{16\rho_a^2}) + \rho_s \log(\psi T \frac{\Delta_i^4}{16\rho_s^2}))}{\Delta_i} \right] \end{aligned}$$

In the above, the first inequality follows since $\sqrt{\rho_a \epsilon_{m_i}} < \frac{\Delta_i}{2}$ and $\sqrt{\rho_s \epsilon_{n_{g_{s_k}}}} < \frac{\Delta_{a_{\max s_k}}}{2}$.

Case b2: $*$ is eliminated by some sub-optimal arm in s^* . Optimal arm a^* can get eliminated by some sub-optimal arm i only if arm elimination condition holds, i.e.,

$$\hat{r}_i - c_{m_i} > \hat{r}^* + c_{m_i},$$

where, as mentioned before, $c_{m_i} = \sqrt{\frac{\rho_a \log(\psi T \epsilon_{m_i}^2)}{2n_{m_i}}}$. From analysis in Case $a1$, notice that, if (1) holds in conjunction with the above, arm i gets eliminated. Also, recall from Case $a1$ that the events complementary to (1) have low-probability and can be upper bounded by $\frac{2}{(\psi T \epsilon_{m_i}^2)^{\rho_a}}$. Moreover, a sub-optimal arm that eliminates $*$ has to survive until round m_* . In other words, all arms $j \in s^*$ such that $m_j < m_*$ are eliminated on or before m_* (this corresponds to case b1). Let, the arms surviving till m_* round be denoted by A'_{s^*} . This leaves any arm a_b such that $m_b \geq m_*$ to still survive and eliminate arm $*$ in round m_* . Let, such arms that survive $*$ belong to A'_{s^*} . Also maximal regret per step after eliminating $*$ is the maximal Δ_j among the remaining arms in A'_{s^*} with $m_j \geq m_*$. Let $m_b = \min\{m | \sqrt{\rho_a \epsilon_m} < \frac{\Delta_b}{2}\}$. Let $C_2(x) = \frac{2^{2x+\frac{3}{2}} x^{2x}}{\psi^x}$. Hence, the maximal regret after eliminating the arm $*$ is upper bounded by,

$$\begin{aligned} &\max_{j \in A'_{s^*}} m_j \sum_{m_*=0} \sum_{\substack{i \in A'_{s^*}: \\ m_i \geq m_*}} \left(\frac{2}{(\psi T \epsilon_{m_*}^2)^{\rho_a}} \right) \cdot T \max_{\substack{j \in A'_{s^*}: \\ m_j \geq m_*}} \Delta_j \\ &\leq \sum_{m_*=0}^{\max_{j \in A'_{s^*}} m_j} \sum_{i \in A'_{s^*}: m_i \geq m_*} \left(\frac{2}{(\psi T \epsilon_{m_*}^2)^{\rho_a}} \right) \cdot T \cdot 2\sqrt{\rho_a \epsilon_{m_*}} \\ &\leq \sum_{m_*=0}^{\max_{j \in A'_{s^*}} m_j} \sum_{i \in A'_{s^*}: m_i \geq m_*} 4 \left(\frac{T^{1-\rho_a}}{\psi^{\rho_a} \epsilon_{m_*}^{2\rho_a - \frac{1}{2}}} \right) \\ &\leq \sum_{i \in A'_{s^*}: m_i \geq m_*} \sum_{m_*=0}^{\min\{m_i, m_b\}} \left(\frac{4T^{1-\rho_a}}{\psi^{\rho_a} 2^{-(2\rho_a - \frac{1}{2})m_*}} \right) \\ &\leq \sum_{i \in A'_{s^*}} \frac{4T^{1-\rho_a}}{\psi^{\rho_a} 2^{-(2\rho_a - \frac{1}{2})m_*}} + \sum_{i \in A'_{s^*} \setminus A'_{s^*}} \frac{4T^{1-\rho_a}}{\psi^{\rho_a} 2^{-(2\rho_a - \frac{1}{2})m_b}} \end{aligned}$$

$$\begin{aligned}
 &\leq \sum_{i \in A'_{s^*}} \frac{T^{1-\rho_a} \rho_a^{2\rho_a} 2^{2\rho_a + \frac{3}{2}}}{\psi^{\rho_a} \Delta_i^{4\rho_a - 1}} + \sum_{i \in A''_{s^*} \setminus A'_{s^*}} \frac{T^{1-\rho_a} \rho_a^{2\rho_a} 2^{2\rho_a + \frac{3}{2}}}{\psi^{\rho_a} b^{4\rho_a - 1}} \\
 &= \sum_{i \in A'_{s^*}} \frac{C_2(\rho_a) T^{1-\rho_a}}{\Delta_i^{4\rho_a - 1}} + \sum_{i \in A''_{s^*} \setminus A'_{s^*}} \frac{C_2(\rho_a) T^{1-\rho_a}}{b^{4\rho_a - 1}}.
 \end{aligned}$$

Case b3: s^* is eliminated by some sub-optimal cluster. Let $C'_g = \{a_{\max_{s_k}} \in A' \mid \forall s_k \in S\}$ and $C''_g = \{a_{\max_{s_k}} \in A'' \mid \forall s_k \in S\}$. A sub-optimal cluster s_k will eliminate s^* in round g_* only if the cluster elimination condition of Algorithm 1 holds, which is the following when $* \in C_{g_*}$:

$$\hat{r}_{a_{\max_{s_k}}} - c_{g_*} > \hat{r}^* + c_{g_*}. \quad (2)$$

Notice that when $* \notin C_{g_*}$, since $r_{a_{\max_{s_k}}} > r^*$, the inequality in (2) has to hold for cluster s_k to eliminate s^* . As in case b2, the probability that a given sub-optimal cluster s_k eliminates s^* is upper bounded by $\frac{2}{(\psi T \epsilon_{g_*}^2)^{\rho_s}}$ and all sub-optimal clusters with $g_{s_j} < g_*$ are eliminated before round g_* . This leaves any arm $a_{\max_{s_b}}$ such that $g_{s_b} \geq g_*$ to still survive and eliminate arm $*$ in round g_* . Let, such arms that survive $*$ belong to C''_g . Hence, following the same way as case b2, the maximal regret after eliminating $*$ is,

$$\sum_{g_*=0}^{\max_{a_{\max_{s_j}} \in C'_g} g_{s_j}} \sum_{\substack{a_{\max_{s_k}} \in C''_g: \\ g_{s_k} \geq g_*}} \left(\frac{2}{(\psi T \epsilon_{g_*}^2)^{\rho_s}} \right) T \max_{\substack{a_{\max_{s_j}} \in C'_g: \\ g_{s_j} \geq g_*}} \Delta_{a_{\max_{s_j}}}$$

Using $A' \supset C'_g$ and $A'' \supset C''_g$, we can bound the regret contribution from this case in a similar manner as Case b2 as follows:

$$\begin{aligned}
 &\sum_{i \in A' \setminus A'_{s^*}} \frac{T^{1-\rho_s} \rho_s^{2\rho_s} 2^{2\rho_s + \frac{3}{2}}}{\psi^{\rho_s} \Delta_i^{4\rho_s - 1}} + \sum_{i \in A'' \setminus A' \cup A'_{s^*}} \frac{T^{1-\rho_s} \rho_s^{2\rho_s} 2^{2\rho_s + \frac{3}{2}}}{\psi^{\rho_s} b^{4\rho_s - 1}} \\
 &= \sum_{i \in A' \setminus A'_{s^*}} \frac{C_2(\rho_s) T^{1-\rho_s}}{\Delta_i^{4\rho_s - 1}} + \sum_{i \in A'' \setminus A' \cup A'_{s^*}} \frac{C_2(\rho_s) T^{1-\rho_s}}{b^{4\rho_s - 1}}
 \end{aligned}$$

Case b4: $*$ is not in $C_{\max(m_i, g_{s_k})}$, but belongs to $B_{\max(m_i, g_{s_k})}$.

In this case the optimal arm $* \in s^*$ is not eliminated, also s^* is not eliminated. So, for all sub-optimal arms i in A'_{s^*} which gets eliminated on or before $\max\{m_i, g_{s_k}\}$ will get pulled no less than $z_i < \left\lceil \frac{2 \log(\psi T \epsilon_{m_i}^2)}{\epsilon_{m_i}} \right\rceil$ number of times, which leads to the following bound the contribution to the expected regret, as in Case b1:

$$\sum_{i \in A'_{s^*}} \left\{ \Delta_i + \frac{32 \rho_a \log(\psi T \frac{\Delta_i^4}{16 \rho_a^2})}{\Delta_i} \right\}$$

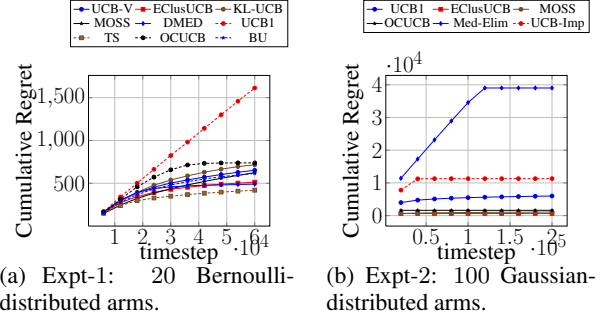


Figure 1: Cumulative regret for various bandit algorithms on two stochastic K-armed bandit environments.

For arms $a_i \notin s^*$, the contribution to the regret cannot be greater than that in Case b3. So the regret is bounded by,

$$\sum_{i \in A' \setminus A'_{s^*}} \frac{C_2(\rho_s) T^{1-\rho_s}}{\Delta_i^{4\rho_s - 1}} + \sum_{i \in A'' \setminus A' \cup A'_{s^*}} \frac{C_2(\rho_s) T^{1-\rho_s}}{b^{4\rho_s - 1}}$$

The main claim follows by summing the contributions to the expected regret from each of the cases above. \square

The regret upper bound for EClusUCB-AE is given in Proposition 1 in Appendix B. Also the simple regret guarantee of EClusUCB is weaker than CCB(Liu & Tsuruoka, 2016) which is shown in Theorem 2 and Corollary 3 in Appendix F. But, this is expected as EClusUCB is geared towards minimizing cumulative regret whereas CCB is made for minimizing simple regret. Also we know from Bubeck et al. (2009) that algorithms that tend to minimize cumulative regret necessarily ends up having a poorer simple regret guarantee.

5. Simulation experiments

We conduct an empirical performance using cumulative regret as the metric. We implement the following algorithms: KL-UCB(Garivier & Cappé, 2011), DMED(Honda & Takemura, 2010), MOSS(Audibert & Bubeck, 2009), UCB1(Auer et al., 2002a), UCB-Improved(Auer & Ortner, 2010), Median Elimination(Even-Dar et al., 2006), Thompson Sampling(TS)(Agrawal & Goyal, 2011), OCUCB(Lattimore, 2015), Bayes-UCB(BU)(Kaufmann et al., 2012) and UCB-V(Audibert et al., 2009)². The parameters of EClusUCB algorithm for all the experiments are set as follows: $\psi = \frac{T}{196 \log K}$, $\rho_s = 0.5$, $\rho_a = 0.5$ and $p = \lceil \frac{K}{\log K} \rceil$ (as in Corollary 2).

First experiment: This is conducted over a testbed of 20 arms in an environment involving Bernoulli reward distributions with expected rewards of the arms $r_{i \neq *} = 0.07$ and

²The implementation for KL-UCB, Bayes-UCB and DMED were taken from (Cappé et al., 2012)

$r^* = 0.1$. These type of cases are frequently encountered in web-advertising domain. The horizon T is set to 60000. The regret is averaged over 100 independent runs and is shown in Figure 1(a). EClusUCB, MOSS, UCB1, UCB-V, KL-UCB, TS, BU and DMED are run in this experimental setup and we observe that EClusUCB performs better than all the aforementioned algorithms except TS. Because of the small gaps and short horizon T , we do not implement UCB-Improved and Median Elimination on this test-case.

Second experiment: This is conducted over a testbed of 100 arms involving Gaussian reward distributions with expected rewards of the arms $r_{i \neq *:1-33} = 0.1$, $r_{i \neq *:34-99} = 0.6$ and $r_{i=100}^* = 0.9$ with variance set at $\sigma_i^2 = 0.3, \forall i \in A$. The horizon T is set for a large duration of 2×10^5 and the regret is averaged over 100 independent runs and is shown in Figure 1(b). From the results in Figure 1(b), we observe that EClusUCB outperforms MOSS, UCB1, UCB-Improved and Median-Elimination($\epsilon = 0.1, \delta = 0.1$). Also the performance of UCB-Improved is poor in comparison to other algorithms, which is probably because of pulls wasted in initial exploration whereas EClusUCB with the choice of ψ, ρ_a and ρ_s performs much better.

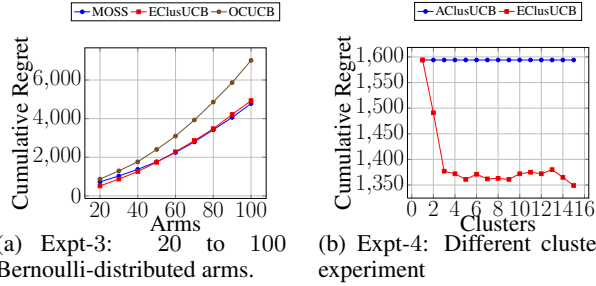


Figure 2: Cumulative regret and choice of parameter p

Third experiment: This is conducted over a testbed of 20 – 100 (interval of 10) arms with Bernoulli reward distributions, where the expected rewards of the arms are $r_{i \neq *} = 0.05$ and $r^* = 0.1$. For each of these testbeds of 20 – 100 arms, we report the cumulative regret over a large horizon $T = 10^5 + K_{20:100}^3$ timesteps averaged over 100 independent runs. We report the performance of MOSS, OCUCB and EClusUCB only over this setup. From the results in Figure 2(a), it is evident that the growth of regret for EClusUCB is lower than that of OCUCB and nearly same as MOSS. This corroborates the finding of Lattimore (2015) which states that MOSS breaks down only when the number of arms are exceptionally large or the horizon is unreasonably high and gaps are very small.

Fourth experiment: This is conducted to show that our choice of $p = \lceil \frac{K}{\log K} \rceil$ which we use to reduce the elimination error, is indeed close to optimal. The experiment is performed over a testbed having 30 Bernoulli-distributed

arms with $r_{i \neq *} = 0.07, \forall i \in A$ and $r^* = 0.1$ averaged over 100 independent runs for each cluster. In Figure 2(b), we report the cumulative regret over $T = 80000$ timesteps averaged over 100 independent runs plotted against the number of clusters $p = 1$ to $\frac{K}{2}$ (so that each cluster have exactly two arms). We see that for $p = \lceil \frac{K}{\log K} \rceil = 9$, the cumulative regret of EClusUCB is almost the lowest over the entire range of clusters considered. The lowest is reached for $\frac{K}{2} = 15$, but this would increase the elimination error of EClusUCB in our theoretical analysis. So, the choice of $p = \lceil \frac{K}{\log K} \rceil$ helps to balance both theoretical and empirical performance of EClusUCB. Also, we show cumulative regret for AClusUCB (which does not have p as an input parameter) as a straight line, constant over the number of clusters. AClusUCB performs poorly as compared to EClusUCB. We conjecture that this happens because AClusUCB conducts a significant amount of initial exploration to find the number of clusters or waits till the optimal arm settles in its own cluster which will eliminate all the other clusters by cluster elimination condition, as opposed to EClusUCB which has an uniform clustering scheme from the very start. Also $p = 1$ gives us EClusUCB-AE and we can clearly see that its cumulative regret is the highest among all the clusters considered showing clearly that clustering indeed has some benefits. More experiments are shown in Appendix H.

6. Conclusions and future work

From a theoretical viewpoint, we conclude that the gap-dependent regret bound of EClusUCB is lower than MOSS and UCB-Improved. From the numerical experiments on settings with small gaps between optimal and sub-optimal mean rewards, we observed that EClusUCB outperforms several popular bandit algorithms, including OCUCB. Also EClusUCB is remarkably stable for a large horizon and large number of arms and performs well across different types of distributions. While we exhibited better regret bounds for EClusUCB, it would be interesting future research to improve the theoretical analysis of EClusUCB to achieve the gap-independent regret bound of MOSS and OCUCB. This is also one of the first papers to apply clustering in stochastic MAB and another future direction is to use this in contextual or in distributed bandits.

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Appendix

The Appendix is organized as follows. In Appendix A we show the regret bound Table. In Appendix B we prove Proposition 1. In Appendix C we prove Corollary 1 and in Appendix D we prove Corollary 2. Appendix E deals with the idea of why we do clustering. The simple regret bound of EClusUCB and its associated Corollary is proved in F. Algorithm 2, Adaptive Clustered UCB is shown in Appendix G. More experiments are shown in Appendix H.

A. Regret Bound Table

Table 2: Gap-dependent regret bounds for different bandit algorithms

| Algorithm | Upper bound |
|--------------|--|
| UCB1 | $O\left(\frac{K \log T}{\Delta}\right)$ |
| UCB-Improved | $O\left(\frac{K \log(T\Delta^2)}{\Delta}\right)$ |
| MOSS | $O\left(\frac{K^2 \log(T\Delta^2/K)}{\Delta}\right)$ |
| EClusUCB | $O\left(\frac{K \log\left(\frac{T\Delta^2}{\sqrt{\log(K)}}\right)}{\Delta}\right)$ |

B. Proof of Proposition 1

Proposition 1. *The regret R_T for EClusUCB-AE satisfies*

$$\mathbb{E}[R_T] \leq \sum_{\substack{i \in A \\ \Delta_i > b}} \left\{ \frac{C_1(\rho_a)T^{1-\rho_a}}{\Delta_i^{4\rho_a-1}} + \Delta_i + \frac{32\rho_a \log\left(\frac{\psi T \Delta_i^4}{16\rho_a^2}\right)}{\Delta_i} + \frac{C_2(\rho_a)T^{1-\rho_a}}{\Delta_i^{4\rho_a-1}} \right\} + \sum_{\substack{i \in A \\ \Delta_i \leq b}} \frac{C_2(\rho_a)T^{1-\rho_a}}{b^{4\rho_a-1}} + \max_{\substack{i \in A: \\ \Delta_i \leq b}} \Delta_i T,$$

for all $b \geq \sqrt{\frac{K}{14T}}$. In the above, C_1, C_2 are as defined in Theorem 1.

Proof. Let $p = 1$ such that all the arms in A belongs to a single cluster. Hence, in EClusUCB-AE there is only arm elimination and no cluster elimination. Let, for each sub-optimal arm i , $m_i = \min\{m | \sqrt{\rho_a \epsilon_m} < \frac{\Delta_i}{2}\}$. Also $\rho_a \in (0, 1]$ is a constant in this proof. Let $A' = \{i \in A : \Delta_i > b\}$ and $A'' = \{i \in A : \Delta_i > 0\}$. Also z_i denotes total number of times an arm i has been pulled. In the m -th round, n_m denotes the number of pulls allocated to the surviving arms in B_m .

Case a: Some sub-optimal arm i is not eliminated in round m_i or before and the optimal arm $* \in B_{m_i}$

Following the steps of Theorem 1 Case a1, an arbitrary sub-optimal arm $i \in A'$ can get eliminated only when the event,

$$\hat{r}_i \leq r_i + c_{m_i} \text{ and } \hat{r}^* \geq r^* - c_{m_i} \quad (3)$$

takes place. So to bound the regret we need to bound the probability of the complementary event of these two conditions.

Note that $c_{m_i} = \sqrt{\frac{\rho_a \log(\psi T \epsilon_{m_i}^2)}{2n_{m_i}}}$. As arm elimination condition is being checked in every timestep, any arm i cannot be pulled more than $z_i \geq n_{m_i}$ times or it will get eliminated. This is because in the m_i -th round $n_{m_i} = \frac{2 \log(\psi T \epsilon_{m_i}^2)}{\epsilon_{m_i}}$.

Putting this in c_{m_i} we get, $c_{m_i} = \sqrt{\frac{\rho_a \epsilon_{m_i} \log(\psi T \epsilon_{m_i}^2)}{2 * 2 \log(\psi T \epsilon_{m_i}^2)}} = \frac{\sqrt{\rho_a \epsilon_{m_i}}}{2} \leq \sqrt{\rho_a \epsilon_{m_i+1}} < \frac{\Delta_i}{4}$, as $\rho_a \in (0, 1]$. Again, for $i \in A'$,

$$\hat{r}_i + c_{m_i} \leq r_i + 2c_{m_i} < r_i + \Delta_i - 2c_{m_i} \leq r^* - 2c_{m_i} \leq \hat{r}^* - c_{m_i}$$

Applying Chernoff-Hoeffding bound and considering independence of complementary of the two events in 3,

$$\mathbb{P}\{\hat{r}_i \geq r_i + c_{m_i}\} \leq \exp(-2c_{m_i}^2 n_{m_i}) \leq \exp(-2 * \frac{\rho_a \log(\psi T \epsilon_{m_i}^2)}{2n_{m_i}} * n_{m_i}) \leq \frac{1}{(\psi T \epsilon_{m_i}^2)^{\rho_a}}$$

Similarly, $\mathbb{P}\{\hat{r}^* \leq r^* - c_{m_i}\} \leq \frac{1}{(\psi T \epsilon_{m_i}^2)^{\rho_a}}$. Summing the two up, the probability that a sub-optimal arm i is not eliminated on or before m_i -th round is $\left(\frac{2}{(\psi T \epsilon_{m_i}^2)^{\rho_a}}\right)$.

Summing up over all arms in A' and bounding the regret for each arm $i \in A'$ trivially by $T\Delta_i$, we obtain

$$\begin{aligned} \sum_{i \in A'} \left(\frac{2T\Delta_i}{(\psi T \epsilon_{m_i}^2)^{\rho_a}} \right) &\leq \sum_{i \in A'} \left(\frac{2T\Delta_i}{(\psi T \frac{\Delta_i^4}{16\rho_a^2})^{\rho_a}} \right) \leq \sum_{i \in A'} \left(\frac{2^{1+4\rho_a} T^{1-\rho_a} \rho_a^{2\rho_a} \Delta_i}{\psi^{\rho_a} \Delta_i^{4\rho_a}} \right) \leq \sum_{i \in A'} \left(\frac{2^{1+4\rho_a} \rho_a^{2\rho_a} T^{1-\rho_a}}{\psi^{\rho_a} \Delta_i^{4\rho_a-1}} \right) \\ &= \sum_{i \in A'} \left(\frac{C_1(\rho_a) T^{1-\rho_a}}{\Delta_i^{4\rho_a-1}} \right), \text{ where } C_1(x) = \frac{2^{1+4x} x^{2x}}{\psi^x} \end{aligned}$$

Case b: Either an arm i is eliminated in round m_i or before or else there is no optimal arm $*$ $\in B_{m_i}$

CASE b1: $*$ $\in B_{m_i}$ and each $i \in A'$ is eliminated on or before m_i

Since we are eliminating a sub-optimal arm i on or before round m_i , it is pulled no longer than,

$$z_i < \left\lceil \frac{2 \log(\psi T \epsilon_{m_i}^2)}{\epsilon_{m_i}} \right\rceil$$

So, the total contribution of i till round m_i is given by,

$$\begin{aligned} \Delta_i \left\lceil \frac{2 \log(\psi T \epsilon_{m_i}^2)}{\epsilon_{m_i}} \right\rceil &\leq \Delta_i \left\lceil \frac{2 \log(\psi T (\frac{\Delta_i}{2\sqrt{\rho_a}})^4)}{(\frac{\Delta_i}{2\sqrt{\rho_a}})^2} \right\rceil, \text{ since } \sqrt{\rho_a \epsilon_{m_i}} < \frac{\Delta_i}{2} \\ &\leq \Delta_i \left(1 + \frac{32\rho_a \log(\psi T (\frac{\Delta_i}{2\sqrt{\rho_a}})^4)}{\Delta_i^2} \right) \leq \Delta_i \left(1 + \frac{32\rho_a \log(\psi T \frac{\Delta_i^4}{16\rho_a^2})}{\Delta_i^2} \right) \end{aligned}$$

Summing over all arms in A' the total regret is given by,

$$\sum_{i \in A'} \Delta_i \left(1 + \frac{32\rho_a \log(\psi T \frac{\Delta_i^4}{16\rho_a^2})}{\Delta_i^2} \right)$$

CASE b2: Optimal arm $*$ is eliminated by a sub-optimal arm

Firstly, if conditions of Case a holds then the optimal arm $*$ will not be eliminated in round $m = m_*$ or it will lead to the contradiction that $r_i > r^*$. In any round m_* , if the optimal arm $*$ gets eliminated then for any round from 1 to m_j all arms j such that $m_j < m_*$ were eliminated according to assumption in Case a . Let the arms surviving till m_* round be denoted by A' . This leaves any arm a_b such that $m_b \geq m_*$ to still survive and eliminate arm $*$ in round m_* . Let such arms that survive $*$ belong to A'' . Also maximal regret per step after eliminating $*$ is the maximal Δ_j among the remaining arms j with $m_j \geq m_*$. Let $m_b = \min\{m | \sqrt{\rho_a \epsilon_m} < \frac{\Delta_b}{2}\}$. Hence, the maximal regret after eliminating the arm $*$ is upper bounded by,

$$\sum_{m_*=0}^{max_{j \in A'} m_j} \sum_{i \in A'' : m_i > m_*} \left(\frac{2}{(\psi T \epsilon_{m_*}^2)^{\rho_a}} \right) \cdot T \max_{j \in A'' : m_j \geq m_*} \Delta_j$$

$$\begin{aligned}
 &\leq \sum_{m_*=0}^{\max_{j \in A'} m_j} \sum_{i \in A'' : m_i > m_*} \left(\frac{2}{(\psi T \epsilon_{m_*}^2)^{\rho_a}} \right) \cdot T \cdot 2\sqrt{\rho_a \epsilon_{m_*}} \\
 &\leq \sum_{m_*=0}^{\max_{j \in A'} m_j} \sum_{i \in A'' : m_i > m_*} 4 \left(\frac{T^{1-\rho_a}}{\psi^{\rho_a} \epsilon_{m_*}^{2\rho_a - \frac{1}{2}}} \right) \\
 &\leq \sum_{i \in A'' : m_i > m_*} \sum_{m_*=0}^{\min\{m_i, m_b\}} \left(\frac{4T^{1-\rho_a}}{\psi^{\rho_a} 2^{-(2\rho_a - \frac{1}{2})m_*}} \right) \\
 &\leq \sum_{i \in A'} \left(\frac{4T^{1-\rho_a}}{\psi^{\rho_a} 2^{-(2\rho_a - \frac{1}{2})m_*}} \right) + \sum_{i \in A'' \setminus A'} \left(\frac{4T^{1-\rho_a}}{\psi^{\rho_a} 2^{-(2\rho_a - \frac{1}{2})m_b}} \right) \\
 &\leq \sum_{i \in A'} \left(\frac{4\rho_a^{2\rho_a} T^{1-\rho_a} * 2^{2\rho_a - \frac{1}{2}}}{\psi^{\rho_a} \Delta_i^{4\rho_a - 1}} \right) + \sum_{i \in A'' \setminus A'} \left(\frac{4\rho_a^{2\rho_a} T^{1-\rho_a} * 2^{2\rho_a - \frac{1}{2}}}{\psi^{\rho_a} b^{4\rho_a - 1}} \right) \\
 &\leq \sum_{i \in A'} \left(\frac{T^{1-\rho_a} \rho_a^{2\rho_a} 2^{2\rho_a + \frac{3}{2}}}{\psi^{\rho_a} \Delta_i^{4\rho_a - 1}} \right) + \sum_{i \in A'' \setminus A'} \left(\frac{T^{1-\rho_a} \rho_a^{2\rho_a} 2^{2\rho_a + \frac{3}{2}}}{\psi^{\rho_a} b^{4\rho_a - 1}} \right) \\
 &= \sum_{i \in A'} \left(\frac{C_2(\rho_a) T^{1-\rho_a}}{\Delta_i^{4\rho_a - 1}} \right) + \sum_{i \in A'' \setminus A'} \left(\frac{C_2(\rho_a) T^{1-\rho_a}}{b^{4\rho_a - 1}} \right), \text{ where } C_2(x) = \frac{2^{2x + \frac{3}{2}} x^{2x}}{\psi^x}
 \end{aligned}$$

Summing up **Case a** and **Case b**, the total regret till round m is given by,

$$\begin{aligned}
 R_T &\leq \sum_{i \in A : \Delta_i > b} \left\{ \left(\frac{C_1(\rho_a) T^{1-\rho_a}}{\Delta_i^{4\rho_a - 1}} \right) + \left(\Delta_i + \frac{32\rho_a \log(\psi T \frac{\Delta_i^4}{16\rho_a^2})}{\Delta_i} \right) + \left(\frac{C_2(\rho_a) T^{1-\rho_a}}{\Delta_i^{4\rho_a - 1}} \right) \right\} \\
 &\quad + \sum_{i \in A : 0 < \Delta_i \leq b} \left(\frac{C_2(\rho_a) T^{1-\rho_a}}{\psi^{\rho_a} b^{4\rho_a - 1}} \right) + \max_{i \in A : \Delta_i \leq b} \Delta_i T
 \end{aligned}$$

□

C. Proof of Corollary 1

Proof. Here we take $\psi = \frac{T}{196 \log(K)}$, $\rho_a = \frac{1}{2}$ and $\rho_s = \frac{1}{2}$. Taking into account Theorem 1 below for all $b \geq \sqrt{\frac{K}{14T}}$

$$\begin{aligned}
 \mathbb{E}[R_T] &\leq \sum_{\substack{i \in A_{s^*}, \\ \Delta_i > b}} \left\{ \frac{C_1(\rho_a) T^{1-\rho_a}}{\Delta_i^{4\rho_a - 1}} + \Delta_i + \frac{32\rho_a \log(\psi T \frac{\Delta_i^4}{16\rho_a^2})}{\Delta_i} \right\} + \sum_{\substack{i \in A, \\ \Delta_i > b}} \left\{ 2\Delta_i + \frac{C_1(\rho_s) T^{1-\rho_s}}{\Delta_i^{4\rho_s - 1}} \right. \\
 &\quad \left. + \frac{32\rho_a \log(\psi T \frac{\Delta_i^4}{16\rho_a^2})}{\Delta_i} + \frac{32\rho_s \log(\psi T \frac{\Delta_i^4}{16\rho_s^2})}{\Delta_i} \right\} + \sum_{\substack{i \in A_{s^*}, \\ \Delta_i > b}} \frac{C_2(\rho_a) T^{1-\rho_a}}{\Delta_i^{4\rho_a - 1}} + \sum_{\substack{i \in A_{s^*}, \\ 0 < \Delta_i \leq b}} \frac{C_2(\rho_a) T^{1-\rho_a}}{b^{4\rho_a - 1}} \\
 &\quad + \sum_{i \in A \setminus A_{s^*} : \Delta_i > b} \frac{2C_2(\rho_s) T^{1-\rho_s}}{\Delta_i^{4\rho_s - 1}} + \sum_{i \in A \setminus A_{s^*} : 0 < \Delta_i \leq b} \frac{2C_2(\rho_s) T^{1-\rho_s}}{b^{4\rho_s - 1}} + \max_{i : \Delta_i \leq b} \Delta_i T
 \end{aligned}$$

and putting the parameter values in the above Theorem 1 result,

$$\sum_{i \in A_{s^*} : \Delta_i > b} \left(\frac{T^{1-\rho_a} \rho_a^{2\rho_a} 2^{1+4\rho_a}}{\psi^{\rho_a} \Delta_i^{4\rho_a-1}} \right) = \sum_{i \in A_{s^*} : \Delta_i > b} \left(\frac{T^{1-\frac{1}{2}} \frac{1}{2} 2^{*\frac{1}{2}} 2^{1+4*\frac{1}{2}}}{\left(\frac{T}{196 \log(K)}\right)^{\frac{1}{2}} \Delta_i^{4*\frac{1}{2}-1}} \right) = \sum_{i \in A_{s^*} : \Delta_i > b} \frac{56\sqrt{\log(K)}}{\Delta_i}$$

Similarly for the term,

$$\sum_{i \in A : \Delta_i > b} \left(\frac{T^{1-\rho_s} \rho_s^{2\rho_s} 2^{1+4\rho_s}}{\psi^{\rho_s} \Delta_i^{4\rho_s-1}} \right) = \sum_{i \in A : \Delta_i > b} \frac{56\sqrt{\log(K)}}{\Delta_i}$$

For the term involving arm pulls,

$$\sum_{i \in A : \Delta_i > b} \frac{32\rho_s \log(\psi T \frac{\Delta_i^4}{16\rho_s^2})}{\Delta_i} = \sum_{i \in A : \Delta_i > b} \frac{16 \log(T^2 \frac{\Delta_i^4}{784 \log(K)})}{\Delta_i} \approx \sum_{i \in A : \Delta_i > b} \frac{32 \log(T \frac{\Delta_i^2}{\sqrt{\log(K)}})}{\Delta_i}$$

Similarly the term,

$$\sum_{i \in A : \Delta_i > b} \frac{32\rho_a \log(\psi T \frac{\Delta_i^4}{16\rho_a^2})}{\Delta_i} \approx \sum_{i \in A : \Delta_i > b} \frac{32 \log(T \frac{\Delta_i^2}{\sqrt{\log(K)}})}{\Delta_i}$$

Lastly we can bound the error terms as,

$$\sum_{i \in A_{s^*} : 0 < \Delta_i \leq b} \left(\frac{T^{1-\rho_a} \rho_a^{2\rho_a} 2^{2\rho_a+\frac{3}{2}}}{\psi^{\rho_a} \Delta_i^{4\rho_a-1}} \right) = \sum_{i \in A_{s^*} : 0 < \Delta_i \leq b} \frac{40\sqrt{\log(K)}}{\Delta_i}$$

Similarly for the term,

$$\sum_{i \in A \setminus A_{s^*} : 0 < \Delta_i \leq b} \left(\frac{T^{1-\rho_s} \rho_s^{2\rho_s} 2^{2\rho_s+\frac{3}{2}}}{(\psi^{\rho_s}) \Delta_i^{4\rho_s-1}} \right) = \sum_{i \in A \setminus A_{s^*} : 0 < \Delta_i \leq b} \frac{40\sqrt{\log(K)}}{\Delta_i}$$

So, the total gap dependent regret bound for using both arm and cluster elimination comes of as

$$\begin{aligned} & \sum_{i \in A_{s^*} : \Delta_i > b} \left\{ \frac{56\sqrt{\log(K)}}{\Delta_i} + \Delta_i + \frac{32 \log(T \frac{\Delta_i^2}{\sqrt{\log(K)}})}{\Delta_i} \right\} + \sum_{i \in A : \Delta_i > b} \left\{ \frac{56\sqrt{\log(K)}}{\Delta_i} + 2\Delta_i + \frac{64 \log(T \frac{\Delta_i^2}{\sqrt{\log(K)}})}{\Delta_i} \right\} \\ & + \sum_{i \in A_{s^*} : \Delta_i > b} \frac{40\sqrt{\log(K)}}{\Delta_i} + \sum_{i \in A_{s^*} : 0 < \Delta_i \leq b} \frac{40\sqrt{\log(K)}}{\Delta_i} + \sum_{i \in A \setminus A_{s^*} : \Delta_i > b} \frac{80\sqrt{\log(K)}}{\Delta_i} \\ & + \sum_{i \in A \setminus A \cup A_{s^*} : 0 < \Delta_i \leq b} \frac{80\sqrt{\log(K)}}{\Delta_i} + \max_{i \in A : \Delta_i \leq b} \Delta_i T \end{aligned}$$

□

D. Proof of Corollary 2

Proof. As stated in [Auer & Ortner \(2010\)](#), we can have a bound on regret of the order of $\sqrt{KT \log K}$ in non-stochastic MAB setting. This is shown in Exp4([Auer et al., 2002b](#)) algorithm. Also we know from [Bubeck et al. \(2011\)](#) that the function $x \in [0, 1] \mapsto x \exp(-Cx^2)$ is decreasing on $\left[\frac{1}{\sqrt{2C}}, 1\right]$ for any $C > 0$. So, taking $C = \left\lfloor \frac{14T}{K} \right\rfloor$ and similarly, by choosing $\Delta_i = \Delta = \sqrt{\frac{K \log K}{T}} > \sqrt{\frac{K}{14T}}$ for all $i : i \neq * \in A$, in the bound of UCB1([Auer et al., 2002a](#)) we get,

$$\sum_{i:r_i < r^*} \text{const} \frac{\log T}{\Delta_i} = \frac{\sqrt{KT} \log T}{\sqrt{\log K}}$$

So, this bound is worse than the non-stochastic setting and is clearly improvable and an upper bound regret of \sqrt{KT} is possible as shown in [Audibert & Bubeck \(2009\)](#) for MOSS which is consistent with the lower bound as proposed by Mannor and Tsitsiklis([Mannor & Tsitsiklis, 2004](#)).

Hence, we take $b \approx \sqrt{\frac{K \log K}{T}} > \sqrt{\frac{K}{14T}}$ (the minimum value for b), $\psi = \frac{T}{196 \log K}$, $\rho_a = \frac{1}{2}$ and $\rho_s = \frac{1}{2}$.

Taking into account Theorem 1 below,

$$\begin{aligned} \mathbb{E}[R_T] \leq & \sum_{\substack{i \in A_{s^*}, \\ \Delta_i > b}} \left\{ \frac{C_1(\rho_a)T^{1-\rho_a}}{\Delta_i^{4\rho_a-1}} + \Delta_i + \frac{32\rho_a \log(\psi T \frac{\Delta_i^4}{16\rho_a^2})}{\Delta_i} \right\} + \sum_{\substack{i \in A, \\ \Delta_i > b}} \left\{ 2\Delta_i + \frac{C_1(\rho_s)T^{1-\rho_s}}{\Delta_i^{4\rho_s-1}} \right. \\ & + \frac{32\rho_a \log(\psi T \frac{\Delta_i^4}{16\rho_a^2})}{\Delta_i} + \left. \frac{32\rho_s \log(\psi T \frac{\Delta_i^4}{16\rho_s^2})}{\Delta_i} \right\} + \sum_{\substack{i \in A_{s^*}, \\ \Delta_i > b}} \frac{C_2(\rho_a)T^{1-\rho_a}}{\Delta_i^{4\rho_a-1}} + \sum_{\substack{i \in A_{s^*}, \\ 0 < \Delta_i \leq b}} \frac{C_2(\rho_a)T^{1-\rho_a}}{b^{4\rho_a-1}} \\ & + \sum_{i \in A \setminus A_{s^*} : \Delta_i > b} \frac{2C_2(\rho_s)T^{1-\rho_s}}{\Delta_i^{4\rho_s-1}} + \sum_{i \in A \setminus A_{s^*} : 0 < \Delta_i \leq b} \frac{2C_2(\rho_s)T^{1-\rho_s}}{b^{4\rho_s-1}} + \max_{i: \Delta_i \leq b} \Delta_i T \end{aligned}$$

and putting the parameter values in the above Theorem 1 result,

$$\sum_{i \in A_{s^*} : \Delta_i > b} \left(\frac{T^{1-\rho_a} \rho_a^{2\rho_a} 2^{1+4\rho_a}}{\psi^{\rho_a} \Delta_i^{4\rho_a-1}} \right) = \left(K \frac{T^{1-\frac{1}{2}} \frac{1}{2}^{2\frac{1}{2}} 2^{1+4\frac{1}{2}}}{p \left(\frac{T}{196 \log K} \right)^{\frac{1}{2}} \Delta_i^{4\frac{1}{2}-1}} \right) = 56 \frac{\sqrt{KT}}{p}$$

Similarly, for the term,

$$\sum_{i \in A : \Delta_i > b} \left(\frac{T^{1-\rho_s} \rho_s^{2\rho_s} 2^{1+4\rho_s}}{\psi^{\rho_s} \Delta_i^{4\rho_s-1}} \right) = 56 \sqrt{KT}$$

For the term regarding number of pulls,

$$\begin{aligned} \sum_{i \in A : \Delta_i > b} \frac{32\rho_s \log(\psi T \frac{\Delta_i^4}{16\rho_s^2})}{\Delta_i} &= \frac{32K \sqrt{T}^{\frac{1}{2}} \log(T^2 \frac{K^4 (\log K)^2}{784 T^2 \log K})}{\sqrt{K \log K}} \leq \frac{32\sqrt{KT} \log(\frac{1}{28} K^2 (\sqrt{\log K}))}{\sqrt{\log K}} \\ &\leq 64\sqrt{KT \log K} + \frac{32\sqrt{KT} \log(\sqrt{\log K})}{\sqrt{\log K}} \end{aligned}$$

Similarly for the term,

$$\sum_{i \in A: \Delta_i > b} \frac{32\rho_a \log(\psi T \frac{\Delta_i^4}{16\rho_a^2})}{\Delta_i} \leq 64\sqrt{KT \log K} + \frac{32\sqrt{KT} \log(\sqrt{\log K})}{\sqrt{\log K}}$$

Lastly we can bound the error terms as,

$$\sum_{i \in A_{s^*}: 0 \leq \Delta_i \leq b} \left(\frac{T^{1-\rho_a} \rho_a^{2\rho_a} 2^{2\rho_a + \frac{3}{2}}}{\psi^{\rho_a} \Delta_i^{4\rho_a - 1}} \right) = \frac{K}{p} \left(\frac{T^{1-\frac{1}{2}} \frac{1}{2}^{2\frac{1}{2}} 2^{2\frac{1}{2} + \frac{3}{2}}}{(\frac{T}{196 \log K})^{\frac{1}{2}} (\Delta_i)^{4\frac{1}{2} - 1}} \right) < \frac{150\sqrt{KT \log K}}{p}$$

Similarly for the term,

$$\sum_{i \in A \setminus A_{s^*}: \Delta_i > b} \left(\frac{T^{1-\rho_s} \rho_s^{2\rho_s} 2^{2\rho_s + \frac{3}{2}}}{(\psi^{\rho_s}) \Delta_i^{4\rho_s - 1}} \right) < 150(K - \frac{K}{p}) \sqrt{\frac{T}{K \log K}}$$

Also, for all $b \geq \sqrt{\frac{K}{14T}}$,

$$\sum_{i \in A \setminus A_{s^*}: 0 < \Delta_i \leq b} \left(\frac{T^{1-\rho_s} \rho_s^{2\rho_s} 2^{2\rho_s + \frac{3}{2}}}{(\psi^{\rho_s}) b^{4\rho_s - 1}} \right) < 150(K - \frac{K}{p}) \sqrt{\frac{T \log K}{K}}$$

Now, $K - \frac{K}{p} = K \left(\frac{p-1}{p} \right) < K \left(\frac{\frac{K}{\log K} + 1 - 1}{\frac{K}{\log K} + 1} \right) < \frac{K^2}{K + \log K}$. So, after putting the value of $p = \left\lceil \frac{K}{\log K} \right\rceil$, we get,

$$\begin{aligned} \mathbb{E}[R_T] \leq & 56 \frac{\sqrt{T} \log K}{\sqrt{K}} + 64 \frac{\sqrt{T} \log K}{\sqrt{K}} + \frac{32\sqrt{T \log K} \log(\log K)}{\sqrt{K}} + 56\sqrt{KT} + 128\sqrt{KT \log K} \\ & + \frac{64\sqrt{KT} \log(\log K)}{\sqrt{\log K}} + \frac{150\sqrt{T} \log K^{\frac{3}{2}}}{\sqrt{K}} + \frac{150\sqrt{T} \log K}{\sqrt{K}} + 300 \frac{K}{K + \log K} \sqrt{KT \log K} + 300 \frac{K}{K + \log K} \sqrt{KT} \end{aligned}$$

So, the total bound for using both arm and cluster elimination cannot be worse than,

$$\begin{aligned} \mathbb{E}[R_T] \leq & 270 \frac{\sqrt{T} \log K}{\sqrt{K}} + \frac{32\sqrt{T \log K} \log(\log K)}{\sqrt{K}} + 56\sqrt{KT} + 128\sqrt{KT \log K} \\ & + \frac{64\sqrt{KT} \log(\log K)}{\sqrt{\log K}} + \frac{150\sqrt{T} \log K^{\frac{3}{2}}}{\sqrt{K}} + 300 \frac{K}{K + \log K} \sqrt{KT \log K} + 300 \frac{K}{K + \log K} \sqrt{KT} \end{aligned}$$

□

E. Why Clustering?

In this section we want to specify the apparent use of clustering. The error bounds are shown in Table 3.

While looking at the error terms in Table 3, we see that using just arm elimination (EClusUCB-AE) the elimination error bound is more than using both arm and cluster elimination simultaneously (EClusUCB).

Table 3: Error Bound

| Elim Type | Error Bound | Remarks |
|--------------------------------------|---|--|
| Only Arm Elimination (EClusUCB-AE) | $\underbrace{\sum_{i \in A: \Delta_i > b} \left(\frac{C_2(\rho_a) T^{1-\rho_a}}{\Delta_i^{4\rho_a-1}} \right)}_{\text{Case b2, Proposition 1}} + \underbrace{\sum_{i \in A: 0 < \Delta_i \leq b} \left(\frac{C_2(\rho_a) T^{1-\rho_a}}{b^{4\rho_a-1}} \right)}_{\text{Case b2, Proposition 1}}$ | With $\rho_a = \frac{1}{2}$, and $\psi = \frac{T}{196 \log K}$ this gives $150\sqrt{KT} + 150\sqrt{KT \log K}$. Hence, this has an order of $O(\sqrt{KT \log K})$. |
| Arm & Cluster Elimination (EClusUCB) | $\underbrace{\sum_{i \in A_{s^*}: \Delta_i > b} \left(\frac{C_2(\rho_a) T^{1-\rho_a}}{\Delta_i^{4\rho_a-1}} \right) + \sum_{i \in A_{s^*}: 0 \leq \Delta_i \leq b} \left(\frac{C_2(\rho_a) T^{1-\rho_a}}{b^{4\rho_a-1}} \right)}_{\text{Case b2, Arm Elim, Theorem 1}} + \underbrace{\sum_{i \in A \setminus A_{s^*}: \Delta_i > b} \left(\frac{2C_2(\rho_s) T^{1-\rho_s}}{\Delta_i^{4\rho_s-1}} \right) + \sum_{i \in A \setminus A_{s^*}: 0 \leq \Delta_i \leq b} \left(\frac{2C_2(\rho_s) T^{1-\rho_s}}{b^{4\rho_s-1}} \right)}_{\text{Case b3+b4, Clus Elim, Theorem 1}}$ | With $\rho_a = \frac{1}{2}$, $\rho_s = \frac{1}{2}$, $p = \lceil \frac{K}{\log K} \rceil$ and $\psi = \frac{T}{196 \log K}$ this gives $\frac{150\sqrt{T \log K}^{\frac{3}{2}}}{\sqrt{K}} + \frac{150\sqrt{T \log K}}{\sqrt{K}} + 300 \frac{K}{K+\log K} \sqrt{KT \log K} + 300 \frac{K}{K+\log K} \sqrt{KT}$. So we can reduce the error bound to $O(\frac{K}{K+\log K} \sqrt{KT \log K})$. |

F. Proof of Theorem 2

Theorem 2. For every $0 < \eta < 1$ and $\gamma > 1$, there exists τ such that for all $T > \tau$ the simple regret of EClusUCB is upper bounded by,

$$SR_{EClusUCB} \leq 4 \log_2 \left(\frac{14T}{K} \right) \gamma \sum_{i=1}^K \Delta_i \exp\left(-\frac{c_0 \sqrt{e}}{4}\right) \left\{ K^{\frac{3}{2}+2\rho_a} \left(\frac{\log(\psi T)}{T^{\frac{3}{2}}(\psi T^2)^{\rho_a}} \right) + K^{\frac{3}{2}+2\rho_s} \left(\frac{\log(\psi T)}{T^{\frac{3}{2}}(\psi T^2)^{\rho_s}} \right) \right\}$$

with probability at least $1 - \eta$, where $c_0 > 0$ is a constant.

Proof. We follow the same steps as in Theorem 2, (Liu & Tsuruoka, 2016). First we will state the two facts used by this proof.

- Fact 1:** From Theorem 1 we know that the probability of elimination of a sub-optimal arm in the $\max(m_i, g_{s_k})$ round is $\left(\frac{2}{(\psi T \epsilon_{m_i}^2)^{\rho_a}} \right)$ and of a sub-optimal cluster is $\left(\frac{2}{(\psi T \epsilon_{g_{s_k}}^2)^{\rho_s}} \right)$.
- Fact 2:** From Tolpin & Shimony (2012) we know that, for every $0 < \eta < 1$ and $\gamma > 1$, there exists τ such that for all $T > \tau$ the probability of a sub-optimal arm i being sampled in the m -th round is bounded by $Q_m \leq 2\gamma \exp(-c_m \frac{\sqrt{T}}{2})$, where $c_m = \frac{c_0}{2^m}$.

We start with an upper bound on the number of plays $\delta_{\max(m_i, g_{s_k})}$ in the $\max(m_i, g_{s_k})$ -th round divided by the total number of plays T . We know from Fact 1 that the total number of arms surviving in the $\max(m_i, g_{s_k})$ -th arm is

$$|B_{\max(m_i, g_{s_k})}| \leq \left(\frac{2K}{(\psi T \epsilon_{m_i}^2)^{\rho_a}} \right) + \left(\frac{2K}{(\psi T \epsilon_{g_{s_k}}^2)^{\rho_s}} \right)$$

Again in EClusUCB, we know that the number of pulls allocated for each surviving arm i in the $\max(m_i, g_{s_k})$ -th round is $n_{\max(m_i, g_{s_k})} = \frac{2 \log(\psi T \epsilon_{\max(m_i, g_{s_k})}^2)}{\epsilon_{\max(m_i, g_{s_k})}}$. Therefore, the proportion of plays $\delta_{\max(m_i, g_{s_k})}$ in the $\max(m_i, g_{s_k})$ -th round can be written as,

$$\begin{aligned} \delta_{\max(m_i, g_{s_k})} &= \frac{(|B_{\max(m_i, g_{s_k})}| \cdot n_{\max(m_i, g_{s_k})})}{T} \leq \left(\frac{1}{T} \cdot \frac{2K}{(\psi T \epsilon_{m_i}^2)^{\rho_a}} \cdot \frac{2 \log(\psi T \epsilon_{m_i}^2)}{\epsilon_{m_i}} \right) + \left(\frac{1}{T} \cdot \frac{2K}{(\psi T \epsilon_{g_{s_k}}^2)^{\rho_s}} \cdot \frac{2 \log(\psi T \epsilon_{g_{s_k}}^2)}{\epsilon_{g_{s_k}}} \right) \\ &\leq \left(\frac{4K \log(\psi T \epsilon_{m_i}^2)}{T \epsilon_{m_i} (\psi T \epsilon_{m_i}^2)^{\rho_a}} \right) + \left(\frac{4K \log(\psi T \epsilon_{g_{s_k}}^2)}{T \epsilon_{g_{s_k}} (\psi T \epsilon_{g_{s_k}}^2)^{\rho_s}} \right) \end{aligned}$$

Now, $\epsilon_{m_i} \geq \sqrt{\frac{K}{14T}}$ and $\epsilon_{g_{s_k}} \geq \sqrt{\frac{K}{14T}}$ for all rounds $m = 0, 1, 2, \dots, \lfloor \frac{1}{2} \log_2 \frac{14T}{K} \rfloor$.

$$\begin{aligned} \delta_{\max(m_i, g_{s_k})} &\leq \left(\frac{4K \log(\psi T \epsilon_{m_i}^2)}{T \epsilon_{m_i} (\psi T \epsilon_{m_i}^2)^{\rho_a}} \right) + \left(\frac{4K \log(\psi T \epsilon_{g_{s_k}}^2)}{T \epsilon_{g_{s_k}} (\psi T \epsilon_{g_{s_k}}^2)^{\rho_s}} \right) \leq \left(\frac{4K \log(\psi T)}{T \epsilon_M (\psi T \epsilon_M^2)^{\rho_a}} \right) + \left(\frac{4K \log(\psi T)}{T \epsilon_M (\psi T \epsilon_M^2)^{\rho_s}} \right) \\ &\leq \left(\frac{4K^{\frac{3}{2}+2\rho_a} \log(\psi T)}{T^{\frac{3}{2}} (\psi T^2)^{\rho_a}} \right) + \left(\frac{4K^{\frac{3}{2}+2\rho_s} \log(\psi T)}{T^{\frac{3}{2}} (\psi T^2)^{\rho_s}} \right) \end{aligned}$$

Now, applying the bound from Fact 2, we can show that the probability of the sub-optimal arm i being pulled is bounded above by,

$$\begin{aligned} P_i &= \sum_{m=0}^M \delta_m \cdot Q_m \leq \sum_{m=0}^M \left\{ \left(\frac{4K^{\frac{3}{2}+2\rho_a} \log(\psi T)}{T^{\frac{3}{2}} (\psi T^2)^{\rho_a}} \right) + \left(\frac{4K^{\frac{3}{2}+2\rho_s} \log(\psi T)}{T^{\frac{3}{2}} (\psi T^2)^{\rho_s}} \right) \right\} 2\gamma \exp\left(-\frac{c_m \sqrt{T}}{4}\right) \\ &\leq M \cdot \left\{ \left(\frac{4K^{\frac{3}{2}+2\rho_a} \log(\psi T)}{T^{\frac{3}{2}} (\psi T^2)^{\rho_a}} \right) + \left(\frac{4K^{\frac{3}{2}+2\rho_s} \log(\psi T)}{T^{\frac{3}{2}} (\psi T^2)^{\rho_s}} \right) \right\} 2\gamma \exp\left(-\frac{c_0 \sqrt{T}}{2M \cdot 4}\right) \\ &\leq \log_2 \frac{14T}{K} \gamma \exp\left(-\frac{c_0 \sqrt{e}}{4}\right) \left\{ \left(\frac{4K^{\frac{3}{2}+2\rho_a} \log(\psi T)}{T^{\frac{3}{2}} (\psi T^2)^{\rho_a}} \right) + \left(\frac{K^{\frac{3}{2}+2\rho_s} \log(\psi T)}{T^{\frac{3}{2}} (\psi T^2)^{\rho_s}} \right) \right\}, \text{ for } M = \lfloor \frac{1}{2} \log_2 \frac{14T}{K} \rfloor \end{aligned}$$

Hence, the simple regret of EClusUCB is upper bounded by,

$$\begin{aligned} SR_{EClusUCB} &= \sum_{i=1}^K \Delta_i \cdot P_i \leq \sum_{i=1}^K \Delta_i \cdot \log_2 \frac{14T}{K} \gamma \exp\left(-\frac{c_0 \sqrt{e}}{4}\right) \left\{ \left(\frac{4K^{\frac{3}{2}+2\rho_a} \log(\psi T)}{T^{\frac{3}{2}} (\psi T^2)^{\rho_a}} \right) + \left(\frac{4K^{\frac{3}{2}+2\rho_s} \log(\psi T)}{T^{\frac{3}{2}} (\psi T^2)^{\rho_s}} \right) \right\} \\ &\leq 4 \log_2 \frac{14T}{K} \gamma \sum_{i=1}^K \Delta_i \exp\left(-\frac{c_0 \sqrt{e}}{4}\right) \left\{ K^{\frac{3}{2}+2\rho_a} \left(\frac{\log(\psi T)}{T^{\frac{3}{2}} (\psi T^2)^{\rho_a}} \right) + K^{\frac{3}{2}+2\rho_s} \left(\frac{\log(\psi T)}{T^{\frac{3}{2}} (\psi T^2)^{\rho_s}} \right) \right\} \end{aligned}$$

□

Corollary 3. For $\psi = \frac{T}{196 \log(K)}$, $\rho_a = \frac{1}{2}$ and $\rho_s = \frac{1}{2}$, the simple regret of EClusUCB is given by,

$$SR_{EClusUCB} \leq 8 \log_2 \frac{14T}{K} K^{\frac{5}{2}} \gamma \sum_{i=1}^K \Delta_i \exp\left(-\frac{c_0 \sqrt{e}}{4}\right) \left(\frac{2 \sqrt{14 \log(K)} \log\left(\frac{T}{\sqrt{14 \log(K)}}\right)}{T^3} \right)$$

Proof. Putting $\psi = \frac{T}{196 \log(K)}$, $\rho_a = \frac{1}{2}$ and $\rho_s = \frac{1}{2}$ in the simple regret obtained in Theorem 2, we get

$$\begin{aligned} SR_{EClusUCB} &\leq 8 \log_2 \frac{7T}{K} K^{\frac{5}{2}} \gamma \sum_{i=1}^K \Delta_i \exp\left(-\frac{c_0 \sqrt{e}}{4}\right) \left(\frac{\log\left(\frac{T^2}{196 \log(K)}\right)}{T^{\frac{3}{2}} \left(\frac{T^3}{196 \log(K)}\right)^{\frac{1}{2}}} \right) \\ &\leq 8 \log_2 \frac{14T}{K} K^{\frac{5}{2}} \gamma \sum_{i=1}^K \Delta_i \exp\left(-\frac{c_0 \sqrt{e}}{4}\right) \left(\frac{2\sqrt{14 \log(K)} \log\left(\frac{T}{\sqrt{14 \log(K)}}\right)}{T^3} \right) \end{aligned}$$

Thus, we see that the simple regret of EClusUCB decreases at the rate of $O\left(\frac{\sqrt{\log K} (\log T)^2}{T^3}\right)$, while the simple regret of CCB decreases at the rate of $O\left(\frac{(\log T)^2}{T^4}\right)$. A table comparing the simple regret of CCB and EClusUCB is given in Table 4. \square

Table 4: Simple regret upper bounds for different bandit algorithms

| Algorithm | Upper bound |
|-----------|--|
| CCB | $O\left(\log_2\left(\frac{T}{e}\right) K \gamma \sum_{i=1}^K \Delta_i \exp\left(2 - \frac{c_0 \sqrt{e}}{4}\right) \frac{\log T}{T^4}\right)$ |
| EClusUCB | $O\left(\log_2\left(\frac{T}{K}\right) K^{\frac{5}{2}} \gamma \sum_{i=1}^K \Delta_i \exp\left(-\frac{c_0 \sqrt{e}}{4}\right) \left(\frac{\sqrt{\log(K)} \log\left(\frac{T}{\sqrt{\log(K)}}\right)}{T^3}\right)\right)$ |

G. Adaptive Clustered UCB

In Section 2, we saw that EClusUCB deals with too much early exploration through optimistic greedy sampling. This reduces the cumulative regret, but still one of the principal disadvantages that EClusUCB suffers from is the lack of knowledge of the number of clusters p . One way to handle this is to estimate the number of clusters on the fly. In Algorithm 2, named Adaptive Clustered UCB, hence referred to as AClusUCB, we explore this idea. AClusUCB uses *hierarchical clustering* (see Friedman et al. (2001)) to find the number of clusters present. AClusUCB is similar to EClusUCB with two major differences. The first difference is the call to procedure CreateClusters at every timestep. CreateClusters subroutine first creates a singleton cluster for each of the surviving arms in B_m and then clusters those singleton clusters $s_k, s_d \in S_m$ (say) into one, if any arm $i \in s_k$ and $j \in s_d$ is such that $|\hat{r}_i - \hat{r}_j| \leq \epsilon_m$. We cluster based on ϵ_m because we have no prior knowledge of the gaps and we estimate the gap by ϵ_m . Also, we destroy the clusters after every timestep and reconstruct the clusters based on the condition specified. Since, the environment is stochastic, the initial clusters will have very poor purity (arms with ϵ_m -close expected means lying in a single cluster) whereas in the later rounds the purity becomes better which leads to the optimal arm * lying in a single cluster of its own which will eliminate all the other clusters based on the cluster elimination condition. The second difference is that, we limit the cluster size from start by $\ell_m = 2$ and then double it after every round. Since the environment is stochastic, if we do not limit the cluster size, then it will result in huge chains of clusters in the initial rounds because the initial estimates of $\hat{r}_i, \forall i \in A$ will be poor. This condition helps in stopping such large chains of clusters.

One of the main disadvantages of AClusUCB is that it does not come with a regret upper bound proof. We do not believe that its regret upper bound can be proved in the same way as EClusUCB. The reason for this is that $a_{\max_{s_k}}$, the true best arm of a cluster is not fixed in AClusUCB as it deconstructs and then reconstructs the clusters at every timestep. This is

Algorithm 2 AClusUCB

Input: Time horizon T , exploration parameters ρ_a, ρ_s and ψ .

Initialization: Set $m := 0$, $B_0 := A$, $S_0 = S$, $\epsilon_0 := 1$, $M = \lfloor \frac{1}{2} \log_2 \frac{14T}{K} \rfloor$, $n_0 = \left\lceil \frac{2 \log(\psi T \epsilon_0^2)}{\epsilon_0} \right\rceil$, $\ell_0 := 2$ and

$N_0 = Kn_0$.

Pull each arm once

for $t = K + 1, \dots, T$ **do**

Pull arm $i \in \arg \max_{j \in B_m} \left\{ \hat{r}_j + \sqrt{\frac{\rho_s \log(\psi T \epsilon_m^2)}{2z_j}} \right\}$, where z_j is the number of times arm j has been pulled

$t := t + 1$

Call CreateClusters()

Arm Elimination

For each cluster $s_k \in S_m$, delete arm $i \in s_k$ from B_m if

$$\hat{r}_i + \sqrt{\frac{\rho_a \log(\psi T \epsilon_m^2)}{2n_m}} < \max_{j \in s_k} \left\{ \hat{r}_j - \sqrt{\frac{\rho_a \log(\psi T \epsilon_m^2)}{2n_m}} \right\}$$

Cluster Elimination

Delete cluster $s_k \in S_m$ and remove all arms $i \in s_k$ from B_m if

$$\max_{i \in s_k} \left\{ \hat{r}_i + \sqrt{\frac{\rho_s \log(\psi T \epsilon_m^2)}{2n_m}} \right\} < \max_{j \in B_m} \left\{ \hat{r}_j - \sqrt{\frac{\rho_s \log(\psi T \epsilon_m^2)}{2n_m}} \right\}.$$

if $t \geq N_m$ and $m \leq M$ **then**

$$\epsilon_{m+1} := \frac{\epsilon_m}{2}$$

$$\ell_{m+1} := 2\ell_m$$

$$B_{m+1} := B_m$$

$$n_{m+1} := \left\lceil \frac{2 \log(\psi T \epsilon_{m+1}^2)}{\epsilon_{m+1}} \right\rceil$$

$$N_{m+1} := t + |B_{m+1}|n_{m+1}$$

$$m := m + 1$$

Stop if $|B_m| = 1$ and pull $i \in B_m$ till T is reached.

end if

end for

procedure CREATECLUSTERS

Create singleton cluster $\{i\}$ for each arm $i \in B_m$ and call this partition as S_m .

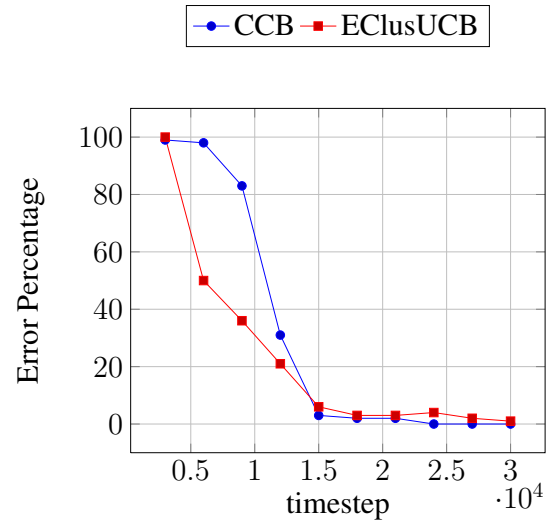
For two cluster $s_k, s_d \in S_m$, join the clusters if any $|\hat{r}_i - \hat{r}_j| \leq \epsilon_m$ and $|s_k| + |s_d| \leq \ell_m$, where $i \in s_k$ and $j \in s_d$

end procedure

not an issue with EClusUCB as it fixes the clusters from beginning and hence $a_{\max_{s_k}}$ for each cluster s_k is fixed from the start.

H. More Experiments

The fifth experiment is conducted to analyze the anytime simple regret guarantee of EClusUCB and CCB. The testbed consists of 300 Gaussian Distributed arms with $r_{i, i \neq *} = 0.6, \forall i \in A$, $r^* = 0.9$ and $\sigma_i^2 = 0.5, \forall i \in A$ (similar to the experiment in Liu & Tsuruoka (2016)). Each algorithm is run independently 100 times for 30000 timesteps and the arm with the maximum $\hat{r}_i, \forall i \in A$ as suggested by the algorithms at every timestep is recorded. The output is considered erroneous if the suggested arm is not the optimal arm. The error percentage over 100 runs is plotted against 30000 timesteps and shown in Figure 3(a). The exploration regulatory factor for CCB is chosen as $d_i = \frac{\sqrt{T}}{z_i}$ (where z_i is the number of times an arm i has been sampled) as this was found to perform the best in Liu & Tsuruoka (2016). Here we see that the



(a) Experiment 5: Error Percentage of EClusUCB and CCB

Figure 3: Cumulative regret and Error Percentage for ClusUCB variants

performance of EClusUCB is slightly poorer than CCB towards the end of the horizon as CCB settles for a lower error percentage than EClusUCB.