Pure Exploration in Multi-armed Bandits with Graph Side Information
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Abstract

We study pure exploration in multi-armed bandits with graph side-information. In particular, we consider the best arm (and near-best arm) identification problem in the fixed confidence setting under the assumption that the arm rewards are smooth with respect to a given arbitrary graph. This captures a range of real world pure-exploration scenarios where one often has information about the similarity of the options or actions under consideration. We propose a novel algorithm GRUB (GRaph based UCB) for this problem and provide a theoretical characterization of its performance that elicits the benefit of the graph-side information. We complement our theory with experimental results that show that capitalizing on available graph side information yields significant improvements over pure exploration methods that are unable to use this information.

1 Introduction

The multi-armed bandit has emerged as an important paradigm for modeling sequential decision making and learning under uncertainty with multiple practical applications such as design policies for sequential experiments [30], combinatorial online learning tasks [6], collaborative learning on social media networks [21, 2], latency reduction in cloud systems [18] and many others [5, 41, 36]. In the traditional multi-armed bandit problem, the goal of the agent is to sequentially choose among a set of actions (or arms) to maximize a desired performance criterion (or reward). This objective demands a delicate tradeoff between exploration (of new arms) and exploitation (of promising arms). An important variation of the reward maximization problem is the identification of arms with the highest (or near-highest) expected reward. This best arm identification [28, 8] problem, which is one of pure exploration, has a wide range of important applications like identifying molecules and drugs to treat infectious diseases like COVID-19, finding relevant users to run targeted ad campaigns, hyperparameter optimization in neural networks and recommendation systems. The broad range of applications of this paradigm is unsurprising given its ability to essentially model any optimization problem of black-box functions on discrete (or discretizable) domains with noisy observations.

While the bandit pure exploration problems harbor considerable promise, there is a significant catch. In modern applications, one is often faced with a tremendously large number of options (sometimes in the millions) that need to be considered rapidly before making a decision. Pulling each bandit arm even once could be intractable. This unfortunately renders traditional best arm identification approaches ineffective both from a statistical and computational viewpoint. Fortunately, in several applications, one often has access to side information, say in terms of how the arms are related to each other. Search and recommendation systems have a graph capturing similarities between items [12, 29, 38]; drugs, molecules and their interactions can be represented on a graph [41]; targeted advertising considers users connected to each other in a social network [13] and hyperparameters for training neural network are often inter-related [40]. One can then hope that leveraging such side information could ease the burden on the agents solving pure exploration
Our Contributions: In this paper, we consider the pure exploration in multi-arm bandits when a graph that captures similarities between the arms is available. We show that leveraging this graph information helps identify the best arm significantly faster than prior approaches. We devise a novel algorithm GRUB that specifically exploits the homophily (strong connections imply similar average rewards) on the graph. We define a novel graph-dependent parameter \( \mathcal{I}(\cdot, \cdot) \) for each arm in the graph. This parameter directly models the influence of the graph on the confidence bounds of the reward distribution for any arm, and plays a central role in the sample complexity bounds we derive. Specifically, in Section 4.1 we show that GRUB can obtain the best arm in

\[
\sum_{i \in B^*} O \left( \frac{1}{\Delta_i^2} \right) + O(|B^*|)
\]

for a multi-armed bandit with \( n \) arms, where \( \Delta_i \) is the gap between the expected rewards of the best arm and arm \( i \), and \( B^* \) is the set of arms that are “close” in terms of rewards to the best arm. The corresponding quantity for standard best arm identification is

\[
\sum_{i=1}^n O \left( \frac{1}{\Delta_i^2} \right),
\]

which can be significantly larger for most real world graphs.

We improve upon our results further, and provide sample complexity bounds for finding a \( \zeta \)-optimal arm in Section 5. We corroborate our results in Section 6 highlighting the benefits of using GRUB on both real world and synthetic datasets. To summarize, our contributions in this paper are as follows:

1. We introduce GRUB, a pure exploration based arm-elimination algorithm that can identify the best arm in a graph-based multi-armed bandit setting in Section 4.

2. We analyze GRUB and provide upper bounds on the number of plays needed to find the best arm, and show that this quantity is significantly smaller than the number of plays needed when no graph information is present. We define the “minimum influence factor” for a graph which plays a central role in our results. (Section 4.1)

3. We extend our results to provide bounds on the number of plays needed to find an approximately \( \zeta \)-optimal best arm in Section 5.

4. We provide extensive empirical evidence in Section 6 highlighting the difference in the number of plays needed to obtain the best arm using GRUB compared to settings where no graph is present. We also motivate the use of novel sampling policies for best arm identification in the presence of graph information.

1.1 Related Work

The recent textbook [22] is an excellent resource for the general problem of multi-armed bandits. The pure exploration variant of the bandit problem is more recent, and has also received considerable attention in the literature [3, 4, 10, 9, 2, 16]. These lines of work treat the bandit arms or actions as independent entities, and thus typically are impractical in scenarios where one has access to a large number of arms.

A recent line of work [25, 22, 13, 39, 11] has proposed the leveraging of structural side-information for the multi-armed bandit problem from the lens of regret minimization. Such topology-based bandit methods work under the assumption that pulling an arm reveals information about other, correlated arms [13, 33], which help in better regret minimization methods. Similarly, spectral bandits [20, 39, 37] assume user features are modelled as signals defined on an underlying graph, and use this to assist in learning.

The above works focus on regret minimization and the pure exploration problem on graphs has received minimal attention. Recently, [20] was the first to attempt at filling the gap in analysis of best arm identification for the spectral bandit setting. They provide an information-theoretic lower bound and a gradient-based algorithm to predict this lower bound to sample the arms. The authors provide performance guarantees for the algorithm, but fall short of providing insights into the explicit impact of graph side information. Our paper explicitly models the graph side information in deriving the sample complexity results.
We derive the mean and confidence bound estimate of arms in Section 3. In Section 4, we propose GRUB for best-arm identification with graph side information. Section 5 provides sample complexity bounds for GRUB. We extend our results to obtain approximately best arms in Section 6. We empirically compare GRUB to standard UCB algorithm in Section 6.

2 Problem Setup and Notation

We consider an $n$-armed bandit problem with the set of arms given by $[n] \triangleq \{1, 2, 3, \ldots, n\}$. Each arm $i \in [n]$ is associated with a $\sigma$-sub-Gaussian distribution $\nu_i$. That is, each $\nu_i$ satisfies the following condition for all $s \in \mathbb{R}$:

$$E_{X \sim \nu_i} [\exp \left( t(X - \mu_i) \right)] \leq \exp \left( \frac{\sigma^2 t^2}{2} \right),$$

where $\mu_i = E_{\nu_i} [X]$ is said to be the (expected or mean) reward associated to arm $i$. We will let $\mathbf{\mu} \in \mathbb{R}^n$ denote the vector of all the arm rewards. A “play” of an arm $i$ is simply an observation of an independent sample from $\nu_i$; this can be thought of as a noisy observation of the corresponding mean $\mu_i$. The goal of the best-arm identification problem is to identify, from such noisy samples, the arm $\mu^* \triangleq \arg \max_{i \in [n]} \mu_i$ that has the maximum expected reward. For each arm $i \in [n]$, we will let $\Delta_i \triangleq \mu_{i^*} - \mu_i$ denote the sub-optimality of the arm.

As discussed in Section 1, our goal is to consider the best-arm identification where one has additional access to information about the similarity of the arms under consideration. In particular, we model this side information as a weighted undirected graph $G = ([n], E_G, A_G)$ where the vertex set is identified with the set of arms, the edge set $E_G \subset \binom{[n]}{2}$, and $A_G \in \mathbb{R}^{n \times n}$ describes the weights of the edges $E$ between the arms; the higher the weight, the more similar the arms. We will let $L_G = D_G - A_G$ denote the combinatorial Laplacian\(^1\) of the graph $G$, where $D_G = \text{diag}(A_G \times 1_n)$ is a diagonal matrix containing the weighted degrees of the vertices. We will suppress the dependence on $G$ when the context is clear. In the sequel we will show that if one has access to this graph, and if the vector of rewards $\mathbf{\mu}$ is smooth with respect to the graph (that is, highly similar arms have highly similar rewards), then one can solve the pure exploration problem extremely efficiently. We will capture the degree of smoothness of $\mathbf{\mu}$ with respect to the graph using the following seminorm\(^2\):

$$\|\mathbf{\mu}\|_G^2 \triangleq \langle \mathbf{\mu}, L_G \mathbf{\mu} \rangle = \sum_{\{i,j\} \in E} A_{ij} (\mu_i - \mu_j)^2. \quad (1)$$

The second equality above can be verified by a straightforward calculation; notice that this expression implies that any $\mathbf{\mu}$ that is such that $\|\mathbf{\mu}\|_G$ is small must vary smoothly across the vertices of $G$. This observation has inspired the use of the Laplacian in several lines of work to enforce smoothness of a vertex-valued function $\mathbf{f} : \mathbb{R} \rightarrow \mathbb{R}^n$. For $\epsilon > 0$, we say that arm (rewards) are $\epsilon$-smooth with respect to a graph $G$ if $\|\mathbf{\mu}\|_G \leq \epsilon$.

For a graph $G$, we will let $k(G)$ denote the number of connected components of $G$ and $\mathcal{C}(G) \subset 2^{[n]}$ denote the set of all connected components; i.e., $k = |\mathcal{C}(G)|$. For a vertex $i \in [n]$, we will let $C_i(G) \in \mathcal{C}(G)$ denote the connected component that contains $i$. With slight abuse of notation, we use $C_i(G)$ to represent both the graph and the set of node.

To solve the best-arm identification problem, an agent needs a sampling policy to sequentially and interactively select the next arm to pull, and a stopping criterion. For any time $t \in \mathbb{N}$, the sampling policy $\pi_t$ is a function that maps $t$ and the history of observations up to time $t - 1$ to an arm in $[n]$. With slight abuse of notation, we will let $\pi_t$ denote the arm chosen by an agent at time $t$, and we will let $\pi_t = \{\pi_s\}_{s \leq t}$ denote the set of all arms chosen up to time $t$; we will typically refer to the latter as the

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1 All our results continue to hold if this is replaced with the normalized, random walk, or generalized Laplacian.

2 $L_G$ is not positive definite, and can be verified to have as many zero eigenvalues as the number of connected components in $G$. 

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3
We will write \( r_{t,\pi_t} \) denote the random reward observed at time \( t \) from arm \( \pi_t \).

Formally, in this paper we tackle the following problems:

**P1:** Given \( n \) arms and an arbitrary graph \( G \) capturing similarity between the arms, can we design a policy \( \pi_T \) that finds the best arm in \( T \) rounds, so that \( T \ll n \).

**P2:** Under the setting in **P1**, can we design a policy \( \pi_T \) so that we can find the set of arms \( B(\zeta) \triangleq \{ i \in [n] : |\mu_i - \mu_{a^*}| \leq \zeta \} \) so that \( T \ll n \).

### 3 Leveraging Graph Side Information

We introduce two key ideas that lie at the heart of the GRUB algorithm. First, at each step, GRUB computes an estimate of the means of all the arms, regularized using the graph Laplacian. This allows the algorithm to infer information about arms it has never sampled.

At any given time step \( T \), the algorithm solves the following Laplacian-regularized least-squares optimization program:

\[
\hat{\mu}_T = \arg \min_{\mu \in \mathbb{R}^n} \left\{ \sum_{t=1}^{T} (r_{t,\pi_t} - \mu_{\pi_t})^2 + \rho \langle \mu, L_G \mu \rangle \right\}
\]

Equation (2) admits a closed form solution of the form

\[
\hat{\mu}_T = V(\pi_T, G)^{-1} \left( \sum_{t=1}^{T} e_{\pi_t} r_{t,\pi_t} \right),
\]

provided the matrix \( V(\pi_T, G) \triangleq \sum_{t=1}^{T} e_{\pi_t} e_{\pi_t}^\top + \rho L_G \) is invertible; \( e_i \) denotes the \( i \)-th standard basis vector for the Euclidean space \( \mathbb{R}^n \). We write \( V_T \) for \( V(\pi_T, G) \) when the context is clear. We refer the reader to Appendix C for a precise characterization of the necessary and sufficient conditions for the invertibility of \( V(\pi_T, G) \). However, note that \( V_T \) can be rewritten as

\[
V(\pi_T, G) = \text{diag}([t_1, t_2, \ldots, t_n]) + \rho L_G,
\]

where \( t_i \) is the number of times arm \( i \) is played under the sampling policy \( \pi_T \). Therefore, it is not hard to see that \( V(\pi_T, G) \) is invertible if and only if the sampling policy yields at least one sample per connected component of \( G \). This is a rather mild condition that we arrange for explicitly in our algorithm, given that we know the graph \( G \). In what follows we will assume that \( V_T \) is invertible.

The second key idea of our algorithm is the utilization of the graph \( G \) in tracking the upper confidence bounds of all the arms simultaneously. Intuitively, any algorithm to identify best arm must be reasonably certain about the sub-optimality of the other arms. This in turn would require the algorithm to track a high-probability upper confidence bound on the means of all the arms. The following lemma, proved in Appendix J, shows precisely how one may construct upper confidence bounds for mean estimates given by (2) and the role played by the graph \( G \).

**Lemma 1.** For any \( \delta > 0 \), the following inequality holds

\[
P \left( |\hat{\mu}_T - \mu_i| \geq 2\sigma \sqrt{|V_T^{-1}|}_{ii} \left( \sqrt{14 \log \left( \frac{2}{\delta} \right)} + \rho \| \mu \|_G \right) \right) \leq \delta,
\]

where \( \hat{\mu}_T^i \) is the \( i \)-th coordinate of the estimate from (2).

This lemma shows that the \( i \)-th diagonal element of \( V_T^{-1} \) critically controls our confidence in our estimate of \( \mu_i \). In order to understand the benefit of the graph side information, consider the following proposition.
Proposition 1. Let $G$ be a connected graph with $n$ nodes. By sampling any node at time $t = 1$ the following holds,

$$\exists \ c > 0 \ s.t. \ [V_t^{-1}]_{jj} < c \ \forall j \in [n]$$

That is, by sampling any arm once, we obtain a finite upper confidence for all the arms. This is in complete contrast with vanilla best arm identification where every arm has to be played at least once before this can be achieved. We refer the reader to Appendix I for a proof.

In what follows, we use the above intuitions to design a novel best arm identification algorithm GRUB that capitalizes effectively on graph side information. We follow this up with a theoretical analysis of the sample complexity of this algorithm by converting these qualitative intuitions into quantitative estimates.

4 GRUB (GRaph based Upper Confidence Bounds)

We introduce our algorithm GRUB for best arm identification when the arms can be cast as nodes on a graph. GRUB uses insights on graph-based mean estimation [2] and upper confidence bound estimation [5] from Section 3 for its elimination policies to search for the optimal arm.

GRUB accepts as input a graph $G$ on $n$ arms (and its Laplacian $L_G$), a regularization parameter $\rho > 0$, a smoothness parameter $\epsilon > 0$, and an error tolerance parameter $\delta \in (0, 1)$. It is composed of the following major blocks.

Initialization: First, GRUB identifies the clusters in the $G$ using a Cluster-Identification routine. Any algorithm that can efficiently partition a graph can be used here, e.g. METIS [19]. GRUB then samples one arm from each cluster. We prove in Appendix C that sampling one arm per connected component is sufficient to ensure $V_T > 0$, which enables GRUB to estimate $\hat{\mu}_T$ using eq. (5).

Sampling policy: At each round, GRUB obtains a sample from the arm returned by the routine Sampling-Policy, which cyclically samples arms from different clusters while ensuring that no arm is resampled before all arms in consideration have the same number of samples. This is distinct from standard cyclic sampling policies that have been traditionally used for best arm identification [3], but any of them may be modified readily to provide a cluster-aware sampling policy for GRUB to use. In our experiments, we show that replacing cyclic sampling with more statistics- and structure-aware sampling greatly improves performance; a theoretical analysis of these is a promising avenue for future work.

Sub-optimal arm elimination: Let $A$ be the set of all arms in consideration for being optimal. Using the uncertainty bound from [3], GRUB uses the following criteria for sub-optimal arm elimination. Let $t_i$ denote the number of samples of arm $i$ by time $T$. At each iteration, GRUB identifies arm...
\[ a_{\text{max}} \in A \text{ with the highest lower bound on its mean estimate: } a_{\text{max}} = \arg \max_{i \in A} \left[ \hat{\mu}_i - \beta(t_i)\sqrt{[V_t^{-1}]_{ii}} \right], \]

where \( \beta(t) = \left( 2R \sqrt{14 \log \left( \frac{2n(t+1)^2}{\delta} \right)} + \rho \right) \). Following this, GRUB removes arms from the set \( A \) according to the following elimination policy:

\[
A \leftarrow \left\{ a \in A \mid \hat{\mu}_i \geq \beta(t_{a_{\text{max}}})\sqrt{[V_t^{-1}]_{a_{\text{max}}a_{\text{max}}}} + \beta(t_a)\sqrt{[V_t^{-1}]_{aa}} \right\}
\]  

(7)

Next, we derive a high probability sample complexity bound for GRUB to return the best arm.

### 4.1 Sample complexity for GRUB

A key component in our characterization of the performance of GRUB is the minimum influence factor for each arm; this quantity renders the intuition from Proposition 1 more concrete. Recall that for a given graph \( D \), \( C_i(D) \) denotes the connected component that contains \( i \).

**Definition 1.** Let \( D \) be a graph with \( n \) nodes. For each \( j \in [n] \), define minimum influence factor \( \mathcal{I}(j, D) \) as:

\[
\mathcal{I}(j, D) = \min_{i \in C_j(D), i \neq j} \left\{ \frac{1}{|K(i, D)|_{jj}} \right\} \quad \forall j \in [n]
\]

(8)

where, \( K(i, D) \) is the unique matrix such that

\[
1 \mathbf{e}_i^T + \rho K(i, D)L_{D_j} = I, \quad [K(i, D)]_{ik} = 0, \quad [K(i, D)]_{ji} = 0 \quad \forall k \in C_j(D),
\]

(9)

\( 1, \mathbf{e}_i \in \mathbb{R}^{|C_j(D)|} \) are the all 1’s vector and \( i \)-th canonical basis respectively, and \( I \) denotes the identity matrix with dimension \( |C_j(D)| \). For the case of isolated nodes \( i \in D \), we set \( \mathcal{I}(i, D) = 0 \).

We refer the reader to Appendix D for a formal argument about the uniqueness of \( K \), and hence the validity of the definition. As discussed qualitatively in Proposition 1, the confidence width of any arm \( k \) in a graph \( D \) is impacted when any other \( j \in C_k(D) \) is sampled. \( \mathcal{I}(k, D) \) quantifies the least impact sampling some node \( j \in C_k(D) \) has on the confidence width associated with \( j \). Clearly, the structure of the graph must play a key role in the amount of influence the arms have on each other, and the following lemma clarifies this.

**Lemma 2.** Consider the same setting as in Definition 7. For each node \( j \in [n] \), minimum influence factor \( \mathcal{I}(j, D) \) can be bounded as

\[
\frac{1}{|C_j(D)|} \leq \mathcal{I}(j, D) \leq \frac{|C_j(D)|}{2}.
\]

(10)

Furthermore, the upper bound is achieved when \( C_j(D) \) is a completely connected subgraph of \( D \) and the lower bound is achieved when \( C_j(D) \) is a line graph.

Indeed, it makes intuitive sense for the influence factor to be maximized when the graph is highly connected and vice versa. We refer the reader to Appendix D for a complete proof.

As stated in contributions [1] the key insight of our theory is that the vertices in the graph (and more specifically in each connected component) are naturally partitioned into three different sets based on their means and their influence factors: highly competitive, weakly competitive, and non-competitive. The GRUB algorithm treats arms in these sets differently, and our sample complexity result elicits this difference in behavior. We will first define these sets, and then proceed to state our main theorem on the sample complexity.
Definition 2. Fix $\mu \in \mathbb{R}^n$, graph $G$, regularization parameter $\rho$, confidence parameter $\delta$, and smoothness parameter $\epsilon$. We define $\mathcal{H}$ to be the set of highly competitive arms and $\mathcal{N}$ to be the set of non-competitive arms as follows:

$$
\mathcal{H}(G, \mu, \rho, \epsilon, \delta) \triangleq \left\{ j \in [n] \mid \Delta_j \leq \left[ 2\sqrt{\frac{2}{3(j,G)}} \left( 2\sigma \sqrt{14\log \frac{23(j,G)^2|C_j(G)|}{\delta} } + \rho \epsilon \right) \right] \right\},
$$

$$
\mathcal{N}(G, \mu, \rho, \epsilon, \delta) \triangleq \left\{ j \in [n] \mid \Delta_j \geq \left[ 2\sqrt{1 + \frac{2}{3(j,G)}} \left( 2\sigma \sqrt{14\log \frac{2|C_j(G)|}{\delta} } + \rho \epsilon \right) \right] \right\},
$$

and the weakly competitive arms $\mathcal{W} \triangleq \mathbb{R}^n \setminus (\mathcal{H} \cup \mathcal{N})$.

As the name suggests, the arms in $\mathcal{H}$ are very competitive compared to $a^*$ and, as our theorem below will show, require several plays before they can be discarded. Note from the above definition that an arm is more likely to be part of this set if its mean is high (i.e., $\Delta_i$ is low) and its influence factor is high. Similarly, the non-competitive set is composed of arms whose means are not competitive with the best arm.

Armed with these definitions, we are now ready to state our main theorem that characterizes the performance of GRUB.

Theorem 1. Consider $n$-armed bandit problem with mean vector $\mu \in \mathbb{R}^n$. Let $G$ be a given similarity graph on the vertex set $[n]$, and further suppose that $\mu$ is $\epsilon$-smooth. Let $\mathcal{C}$ be the set of connected components of $G$. Define

$$
T \triangleq \sum_{C \in \mathcal{C}} \left[ \sum_{j \in H \cap C} \frac{1}{\Delta_j^2} \left[ 112\sigma^2 \log \left( \frac{112\sigma^2 \sqrt{2n \Delta_j}}{\delta^2 \Delta_j^2} \right) + \frac{\rho \epsilon}{2} \right] - \frac{3(j,G)}{2} \right] + \sum_{C \in \mathcal{C}} \max_{l \in W \cap C} \mathcal{I}(l, G, |W \cap C|) + k(G),
$$

where $k(G) = |\mathcal{C}|$. Then, with probability at least $1 - \delta$, GRUB: (a) terminates in no more than $T$ rounds, and (b) returns the best arm $a^* = \arg \max_i \mu_i$.

We will now make some remarks about the theorem.

Remark 1. The required number of samples for successful elimination of suboptimal arms, and therefore the successful identification of the best arm, can be split into three categories based on the sets defined in Definition 2. All non-competitive arms $\mathcal{N}$ can be eliminated with at most $|\mathcal{C}(G)|$ plays; that is, one play per connected component suffices to eliminate these arms. Each sub-optimal highly competitive arm $j \in \mathcal{H}$ requires $O(1/\Delta_j^2)$ samples, which is comparable to the classical (graph-free) best-arm identification problem. Finally, the moderately competitive arms $\mathcal{M}$ can be eliminated with at most one play, depending on the influence factor. We refer the reader to Appendix L for a more detailed discussion on this. Indeed, the smaller $\mathcal{H}$ is, and the larger the other two sets are, the more the benefit of the graph side information is.

Remark 2. As can be seen from Definition 2, the size of $\mathcal{N}$ grows and $\mathcal{H}$ shrinks as the value of $\mathcal{I}(\cdot, \cdot)$ increases. Hence the best sample complexity is obtained when underlying graph $G$ consists of completely connected clusters.

Proof sketch of Theorem 1. The main criteria required for successful elimination of a suboptimal arm $i$ involves bounding the confidence bound around the mean estimate $\hat{\mu}_i$. Note that the confidence bound depends on $V_T$, which consists of two parts the counting diagonal matrix $\sum_T e_{ni}^T e_{ni}$ and the Laplacian $L_G$. Our proof leverages the fact that the Laplacian matrix $L_G$ has the most effect on information sharing when the counting diagonal matrix has less impact. This happens precisely when the effective number of arm pulls is low. We show that the arms $\mathcal{N}$ and $\mathcal{W}$ can be eliminated by merely sampling arms in the same connected component since GRUB "pools" the data from each connected component.
(characterized by $\mathcal{J}(\cdot, \cdot)$); this leads to the vastly lower sample complexity in the second and last terms in (42). Once the number of effective arm pulls are high enough, the behaviour of $V_T$ is dominated by the counting diagonal matrix $\sum_T e_{x_i}e_{x_i}^T$, and the behavior of GRUB resembles that of vanilla best arm identification methods, leading to the first term in (42).

The complete proof of Theorem 1 can be found in Appendix F. In that section, we also discuss more insights on the behavior of the confidence bound as a function of the number of samples acquired. These results may be of independent interest.

Consider the scenario where our similarity graph $G$ on $[n]$ has two strongly connected components $C_1$ and $C_2$ that are disconnected. For such a graph the nodes will have high influence factors, and therefore, the sample complexity will be significantly smaller than $n$. However, if one adds a single edge that connects these two clusters, one can check that the influence factors as defined in Definition 4 would drop sharply. However, it stands to reason that the algorithm will not perform much worse with this one extra edge. In what follows, we show that this is in-fact true in a rigorous sense. Before we are able to state this result, we will introduce a notion by which two graphs may be considered close.

**Definition 3.** Let graphs $D, H$ consist of $n$ nodes. Then, the graph $H$ is said to be $\gamma$-close to a graph $D$ if the following holds,

$$(1 - \gamma)y^T L_D y \leq y^T L_H y \leq (1 + \gamma)y^T L_D y \quad \forall y \in \mathbb{R}^n/\{0\}$$

This notion is closely related to the notion of spectral approximation of graph [35].

For a given graph $G$, we will let $S(G, \gamma)$ denote the set of all graphs that are $\gamma$-close to $G$. The following theorem shows that GRUB, with a small price, is able to recover the sample complexity that corresponds to the best graph in $S(G, \gamma)$. The following theorem requires slightly modified version of Definition 2, we refer the reader to Definition 5 in Appendix F.

**Theorem 2.** Consider $n$-armed bandit problem with mean vector $\mu \in \mathbb{R}^n$. Let $G$ be the given similarity graph on vertex set $[n]$, and further suppose that $\mu$ is $\epsilon$-smooth. Let $C$ be the set of connected components of $G$. Define,

$$T_\gamma := \min_{H \in S(G, \gamma)} \left\{ \sum_{C \in \mathcal{C}} \left[ \sum_{j \in \mathcal{H} \cap C} \frac{1}{(1 - \gamma) \Delta_j^2} \left[ 112 \sigma^2 \log \left( \frac{112 \sigma^2 \sqrt{2n}^2}{(1 - \gamma) \Delta_j^2} \right) + \frac{\rho \epsilon}{2} \right] - \frac{\mathcal{J}(j, H)}{2} \right] + \sum_{C \in \mathcal{C}} \max_{l \in \mathcal{W} \cap C} \mathcal{J}(l, H), |W \cap C| \right\} + k(H),$$

where $k(G) = |C|$. Then, with probability at least $1 - \delta$, GRUB: (a) terminates in no more than $T$ rounds, and (b) returns the best arm $a^* = \arg \max_i \mu_i$.

## 5 Approximate best arm identification

Given a graph $G$, Theorem 1 shows that the number of samples required for eliminating an arm $j \in \mathcal{H}$, the set of competitive arms, is

$$O \left( \frac{1}{\Delta_j^2} \left( \log \left( \frac{1}{\Delta_j} \right) + \frac{\rho \epsilon}{2} \right) \right) - \frac{\mathcal{J}(j, G)}{2}$$

(15)

Now, consider an arm $j \neq a^*$, but in the same cluster as $a^*$. It can be seen that the fact that the means are $\epsilon$-smooth implies that distinguishing $j$ from $a^*$ would require at least on the order of $\epsilon^{-2}$ samples. That is, the more effective the graph structure is, the harder the best arm identification problem becomes. However, it stands to reason that in such situations, it might be more reasonable to not demand for the absolute best arm, but rather an arm that is nearly optimal. Indeed, in several
modern applications we discuss in Section 1 finding an approximate best arm is tantamount to solving the problem. In such cases, a simple modification of GRUB can be used to quickly eliminate definitely suboptimal arms, and then output an arm that is guaranteed to be nearly optimal. To formalize this, we consider the ζ-best arm identification problem as follows.

**Definition 4.** For a given ζ > 0, arm i is called ζ-best arm if μ_i ≥ μ_{a*} − ζ, where a* = arg max_i μ_i.

The goal of the ζ-best arm identification problem is to return an arm \( \hat{a} \) that is ζ-optimal. We achieve this by a simple modification to GRUB, which we dub ζ-GRUB, which ensures that all the remaining arms i satisfy \( 2\beta(t_i)\sqrt{V_i^{-1}} \leq ζ \). It then outputs the best arm amongst those that are remaining. The following theorem characterizes the sample complexity for ζ-GRUB.

**Theorem 3.** Consider n-armed bandit problem with mean vector \( \mu \in \mathbb{R}^n \). Let G be the given similarity graph on vertex set \([n]\), and further suppose that \( \mu \) is ε-smooth. Let \( C \) be the set of connected components of G. Define,

\[
T_ζ := \sum_{C \in C} \left[ \sum_{j \in H \cap C} \max \left\{ \frac{1}{\Delta_j^2}, \frac{1}{\delta_j^2} \right\} \left[ 112σ^2 \log \left( \frac{112σ^2\sqrt{2n}ε}{δ_j^2} \right) + \frac{ρε}{2} \right] - \mathcal{I}(j, G) \right] + k(G),
\]

where \( k(G) = |C| \). Then, with probability at least \( 1 - δ \), ζ-GRUB: (a) terminates in no more than T rounds, and (b) returns the ζ-best arm.

It should be noted that the sets defined in Definition 2 need to be slightly modified for this theorem to carry through. We refer the reader to Appendix G for more details on this and for the complete proof of the theorem.

### 6 Experiments

Before we proceed to the experiments, we provide alternative sampling policies to the cyclic policy used in GRUB. These policies explicitly use the graph information to pick the next arm to sample. In the following, we assume A is the set of arms currently under consideration by GRUB after time T, and l is the index of the arm to sample at time \( T + 1 \).

**Marginal variance minimization (MVM):** Since picking any arm impacts the confidence widths of all arms in its connected component, we pick the arm with the maximum variance. Specifically, \( l = \arg \max_{i \in A} V_{T+1}^{-1} \).

**Joint variance minimization – nuclear (JVM-N):** This is similar to the concept of V-optimality [17] where in we try to reduce the \( L^2 \) regression loss of the estimator. This policy aims to select the arm that minimizes the confidence interval across all remaining arms in A. Specifically, \( l = \arg \min_{i \in A} ||(V_T + e_i e_i^T)^{-1}|| \).

**Joint variance minimization – operator (JVM-O).** This is similar to Σ-optimality [27, 26]. Specifically, \( l = \arg \min_{i \in A} ||(V_T + e_i e_i^T)^{-1}||_{op} = \arg \max_{i \in A} \frac{||\text{Row}((V_T^{-1})^2)||}{1+||((V_T^-1)_{ii})||} \). The exact derivation of this is provided in Appendix I.

For all our experiments, we use Intel® Core™ i7-10875H CPU @ 2.30GHz × 16 with 32 GB memory for our experiments. We set \( δ = 1, ε = 3, ρ = 1.5, σ = 1.0 \). For every synthetic and real graph G, we generate a mean vector so that \( (\mu, LG\mu) = 20 \). We evaluate GRUB with different sampling strategies form section 6 and compare its performance to standard UCB algorithm on both synthetic and real datasets.

**Synthetic Data:** We consider the setup where G with \( n = 100 \) arms consists of 10 connected components with 10 arms per cluster. We consider 2 cases: G is a Stochastic Block model(SBM) with
Figure 1: (Best seen in color) Performance of GRUB with using various sampling protocols for SBM \((p, q) = (0.9, 5e^{-3})\) [Left] and BA \((m = 2)\) [Right]. The UCB method without graph information is significantly slower compared to the graph-based variants. Note that for these toy datasets, the sampling algorithm used does not alter the results too much.

Figure 2: (Best seen in color) Performance of GRUB using different sampling protocols for Github social graph (left) and LastFM graph (right). With no graph information, UCB requires orders of magnitude more samples compared to policies that use explicitly graph information. The cyclic sampling policy is not as competitive on real world datasets.

parameters \((p, q) = (0.9, 0.0005)\) and \(G\) is a Barabási–Albert (BA) graph with parameter \(m = 2\). Results are provided in Figure 1.

**Real Data:** We use graphs from SNAP [24] for the experiments involving real world graphs. We sub-sample the graphs using Breadth-First Search (to retain connected components) to generate the graphs for our experiments. We use the LastFM [32], subsampled to 229 nodes and Github Social [31] subsampled to 242 nodes.

In all the experiments, it is evident that GRUB with any of the sampling policies outperform UCB algorithm [22], which does not leverage the graph. Further within the various sampling policies, MVM sampling policy seems to outperform other sampling policies (Figure 2). For both Github and LastFM datasets, the MVM policy obtains the best arm in \(\sim 300\) rounds compared to traditional UCB that takes \(\sim 4500\) rounds. A rigorous theoretical characterization of the above sampling policies is an exciting avenue for future research. We refer the reader to Appendix A for a discussion on the results of the paper, potential extensions, and broader impacts.

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Appendix

A Discussion and Broader Impacts

In this work, we consider the problem of best arm identification (and approximate best arm identification) when one has access to similarity information on the arms in the form of a graph. We propose a novel algorithm GRUB for this important family of problems and establish sample complexity guarantees for the same. In particular, our theory explicitly demonstrate that benefit of this side information (in terms of the properties of the graph) in quickly locating the best or approximate best arms. We support these theoretical findings with experimental results in both simulated and real settings.

Limitations and Future Work. We outline several sampling policies inspired by our theory in Section 6; an extension of our theoretical results to account for these improved sampling policies is a natural candidate for further exploration. The algorithm and theory of this paper assume knowledge of (an upper bound) on the smoothness of the reward vector with respect to the graph. While this is where one uses domain expertise, this could be hard to estimate in certain real world problems. A generalization of the algorithmic and theoretical framework proposed here would be adaptive to unknown graph-smoothness is an exciting avenue for future work\(^3\). The sub-Gaussianity assumption on the observation process is another limitation that can be significantly generalized to other tail behaviors in follow up work. Another limitation of this work is that the statistical benefit of the graph-based quadratic penalization comes at a computational cost – each mean estimation step involves the inversion of an \(n \times n\) matrix which has a complexity of \(O(n^2 \log(n))\). However, an exciting recent line of work suggests that this matrix inversion can be made significantly faster when coupled with a spectral sparsification of the graph \(G\)\(^5\) while controlling the statistical impact of such a modification. In the context of this problem, this suggests a compelling avenue for future work that studies the statistics-vs-computation tradeoffs in using graph side information.

Potential Negative Social Impacts. Our methods can be used for various applications such as drug discovery, advertising, and recommendation systems. In scientifically and medically critical applications, the design of the reward function becomes vital as this can have a significant impact on the output of the algorithm. One must take appropriate measures to ensure a fair and transparent outcome for various downstream stakeholders. With respect to applications in recommendation and targeted advertising systems, it is becoming increasingly evident that such systems aid in the creation of highly polarizing filter-bubbles. Especially the techniques proposed in this paper could exacerbate this situation by reinforcing the emerging polarization (which would correspond to more clustered graphs and therefore better recommendation performance) when used in such contexts. It will of course be of significant interest to mitigate such adverse outcomes by well-designed interventions or by considering multiple similarity graphs that capture various dimensions of similarity. This is a compelling avenue for future work.

C Properties of \(V(\pi_T, G)\)

Recall that, given a policy \(\pi_T\) and graph \(G\), the matrix \(V(\pi_T, G)\) is defined as follows

\[
V(\pi_T, G) = \sum_{t=1}^{T} e_{\pi_t} e_{\pi_t}^\top + \rho L_G. 
\]

\(^3\)T. Tony Cai, Ming Yuan “Adaptive covariance matrix estimation through block thresholding,“ The Annals of Statistics, Ann. Statist. 40(4), 2014-2042, (August 2012)

\(^4\)Banerjee, T., Mukherjee, G., & Sun, W. (2020). Adaptive sparse estimation with side information. Journal of the American Statistical Association, 115(532), 2053-2067.

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For any undirected graph $G$, the Laplacian $L_G$ is always positive semidefinite [34] and $\sum_{t=1}^{T} e_{\pi_t} e_{\pi_t}^\top$ is a diagonal matrix with positive integers in the diagonal. Hence, $V(\pi_T, G)$ is positive semidefinite as well. Given that the optimization problem (2) has a quadratic objective, this of course implies (non necessarily strict) convexity. Indeed, if $V(\pi_T, G)$ is strictly positive definite, (2) becomes strictly convex and the solution $\hat{\mu}_T$ is guaranteed to be unique. In what follows, we derive the conditions under which $V(\pi_T, G)$ is positive definite.

**Lemma 3.** Let $k = k(G)$ be the number of connected components of the graph $G$. Then, there exists a policy $\pi_k$ (i.e., one that involves the pull of $k$ arms) such that $V(\pi_k, G) \succ 0$. Moreover, there exists no policy of at most $k - 1$ arm pulls such that the matrix $V$ is strictly positive definite.

**Proof.** We will assume, without loss of generality, that the nodes in the graph $G$ are arranged such that first $n_1$ nodes belong to cluster 1, the next $n_2$ nodes belong to cluster 2 and so on; $\sum_{i=1}^{k} n_i = n$. Accordingly, for any time $T$, the matrix $V(\pi_T, G)$ can be written in a block form as follows

$$V(\pi_T, D) = \text{diag}([V_1(\pi_T, D), V_2(\pi_T, D), \ldots, V_k(G)(\pi_T, D)]),$$

where $V_{n_i}(\pi_T, G)$ is the diagonal sub-block of $V(\pi_T, G)$ with the $n_i$ nodes that constitute cluster $i$. Of course, $V(\pi_T, G)$ is invertible if and only if all of its principal diagonal matrices $\{V_{n_i}(\pi_T, G)\}_{i=1}^{k}$ are invertible. To conclude, we observe that each matrix $V_{n_i}(\pi_T, G)$ corresponds to a connected graph, and from Lemma 3 (in Appendix 3), these matrices become invertible if and only if at least one sample is observed from the corresponding component. \qed

As can be observed in the proof, $\pi_k$ for which $V(\pi_k, G) \succ 0$ is one that samples one node in each disconnected cluster. Therefore, our algorithm GRUB begins by using an off-the-shelf graph partitioning algorithm to first identify the connected components, and then samples at least one node in each cluster. This guarantees that our estimates of $\hat{\mu}_T$ in (2) are well defined.

**D Properties of $I(\cdot, \cdot)$**

One of the distinguishing features of using graph-side information for pure exploration is the ability of arm estimates to be not just improved by sampling the arm itself, but also by sampling any connected arms. We drive this intuition home in the following preliminary result.

**Proposition 2.** Let $G$ be a connected graph with $n$ nodes. By sampling any node at time $t = 1$ the following holds,

$$\exists \ c > 0 \ \ s.t. \ \ [V_1^{-1}]_{jj} < c \ \ \forall j \in [n]$$

(18)

**Proof.** It can be concluded from Lemma 3 that for any connected graph $G$ on $n$ arms, sampling any arm $i \in [n]$ is sufficient to ensure $V_1 \succ 0$. Since $V_1$ is positive definite, $V_1 \succeq \lambda_{\min}(V_1)I$ where $\lambda_{\min}(V_1) > 0$ is the minimum eigenvalue of $V_1$. From the variational definition of the minimum eigenvalue (i.e., the Rayleigh quotient), we have that for every $x \in \mathbb{R}^n$,

$$\langle x, V_1^{-1}x \rangle \leq \frac{\|x\|_2^2}{\lambda_{\min}(V_1)}.$$  

(19)

The desired result follows by setting $x = e_j$ for all $j \in [n]$. \qed

Proposition 2 qualitatively demonstrates that the confidence width of any arm $i$ in a graph $G$ is impacted when any other $j \in C_i(G)$ is sampled. We define the influence factor $\mathcal{I}(i, G)$ in Definition 4 to quantify this influence. As can be noted, the definition of the influence factor $\mathcal{I}(i, G)$ is intrinsically dependent on the matrix $K(\cdot, G)$. Clearly, the structure of the graph must play a key role in the amount of influence the arms have on each other, but in order to be a valid definition, we need $K(\cdot, \cdot)$ used for defining $\mathcal{I}(\cdot, \cdot)$ to be unique. The following lemma ensures this.
Remark: From Definition 1 it can be noted that $K(i, G)$ is a matrix which exploits the local property of the graph (i.e. dependent only on the connected component $C_i$ containing arm $i$). Hence we prove the following result for a connected graph $G$ and the result can be extended to the case of disconnected graphs.

Lemma 4. $K(\cdot, \cdot)$ defined in Definition 1 is unique.

Proof. Let $G$ be a given connected graph. From Definition 1 $K(i, G)$ satisfies

$$1e_i^T + \rho K(i, G)L_G = I$$

Observe that $1e_i^T$ is a rank 1 matrix and Identity matrix $I$ is of rank $n$ with all eigenvalues $1$. It is easy to see that $I - 1e_i^T$ is a rank $n - 1$ matrix. Given $\rho > 0$, we can conclude that

$$K(i, G)L_G \succeq 0 \quad \text{s.t.} \quad \text{rank}(K(i, G)L_G) = n - 1. \quad (20)$$

Now, observe that $L_G \succeq 0$ for all undirected graphs and, since $G$ is connected, $\text{rank}(L_G) = n - 1$. Therefore in order to satisfy eq. (20) we need $K(i, G) \succeq 0$ and $\text{rank}(K(i, G)) \geq n - 1$.

Further, from Definition 1 $K(i, G)$ has a row and column with all 0 and hence $\text{rank}(K(i, G)L_G) = n$ is not possible. Further, the nonzero-subblock of $K(i, G)$ has to be full rank for satisfying $\text{rank}(K(i, G)) = n - 1$. This proves that the matrix $K(i, G)$ is unique.

Note that the influence factor $I(\cdot, \cdot)$ gets directly impacted by adding or removing edges from the graph, which can be observed as follows: Let $G$ and $H$ be two connected graphs with $n$ nodes. Let $E_G, E_H$ denote their edge set respectively such that $E_G \supset E_H$, then from Lemma 17 and Lemma 12 we can prove that,

$$I(i, G) \geq I(i, H) \quad \forall i \in [n] \quad (21)$$

Next we provide bounds for the influence factor $I(\cdot, D)$ to show the sample complexity improvement in Theorem 1. The proof follows from a series of arguments that have been proved in Appendix J.

Lemma 5. Consider the same setting as in Definition 1. For each node $j \in [n]$, minimum influence factor $I(j, D)$ can be bounded as

$$\frac{1}{|C_j(D)|} \leq I(j, D) \leq \frac{|C_j(D)|}{2}. \quad (22)$$

Furthermore, the upper bound is achieved when $C_j(D)$ is a completely connected subgraph of $D$ and the lower bound is achieved when $C_j(D)$ is a line graph.

Proof. We first derive the bound for the case when graph $D$ is continuous. Under the restriction of graph $D$ being connected, $I(\cdot, D)$ attains its maximum when the underlying graph $D$ is completely connected and least when it is line graph (tree graph with longest diameter). Accordingly, the upper and lower bound on $I(\cdot, D)$ can be obtained by looking at Lemma 19 and Lemma 18.

The analysis for the case of connected graphs can be easily extended to the case of disconnected graph by considering the same argument for individual connected clusters.

E Parameter estimation

At any time $T$, GRUB, along with the graph-side information, uses data gathered to estimate the mean $\mu_T$ in order to decide the sampling and elimination protocols. The following lemma gives the estimation routine used for GRUB.
Lemma 6. The closed form expression of $\hat{\mu}_T$ is given by,

$$
\hat{\mu}_T = \left( \sum_{t=1}^{T} e_{\pi_t}e_{\pi_t}^T + \rho L_G \right)^{-1} \left( \sum_{t=1}^{T} e_{\pi_t} r_{\pi_t} \right)
$$

Proof. Using the reward data $\{r_{t,\pi_t}\}_{t=1}^{T}$ gathered up-to time $T$ and the sampling policy $\pi_T$, the mean vector estimate $\hat{\mu}_T$ is computed by solving the following laplacian-regularized least-square optimization schedule:

$$
\hat{\mu}_T = \arg \min_{\mu \in \mathbb{R}^n} \sum_{t=1}^{T} (\mu_{\pi_t} - r_{t,\pi_t})^2 + \rho (\mu, L_G \mu)
$$

where $\rho > 0$ is a tunable penalty parameter. The above optimization problem can be equivalently written in the following quadratic form:

$$
\hat{\mu}_T = \arg \min_{\mu \in \mathbb{R}^n} f(\mu, \pi_T, G) \triangleq \langle \mu, V(\pi_T, G) \mu \rangle - 2 \left( \mu, \left( \sum_{t=1}^{T} e_{\pi_t} r_{t,\pi_t} \right) \right) + \sum_{t=1}^{T} r_{t,\pi_t}^2
$$

where $V(\pi_T, G)$ denotes,

$$
V(\pi_T, G) = \sum_{t=1}^{T} e_{\pi_t}e_{\pi_t}^T + \rho L_G
$$

A major advantage of having the graph penalization function as $\mu^T L_G \mu$ is that $\hat{\mu}_T$ can be computed from (24) as a closed form expression. In order to obtain $\hat{\mu}_T$, we compute vanishing point of $\nabla \mu f(\mu, \pi_T, G)$ as follows,

$$
\nabla \mu f(\mu, \pi_T, G)|_{\mu = \hat{\mu}_T} = 0 \quad \Rightarrow \quad \hat{\mu}_T = V(\pi_T, G)^{-1} \left( \sum_{t=1}^{T} e_{\pi_t} r_{\pi_t} \right)
$$

Hence proved. \qed

Delving further into decision policy of the elimination protocol, GRUB makes use of the variance of the estimate $\hat{\mu}_T$ in order to safely discard arms while keeping the possibility of removing the optimal arm at a minimum.

Lemma 7. Consider a sampling policy $\pi_T$ such that $V_T > 0$. For any $\delta > 0$ the following inequality holds for all $i \in [n]$,

$$
P \left( |\hat{\mu}_T^i - \mu_i| \geq 2\sigma \sqrt{|V_T^{-1}|_{ii}} \left( \sqrt{14 \log \left( \frac{2}{\delta} \right)} + \rho \|\mu\|_G \right) \right) \leq \delta, \quad (28)
$$

Proof. Let the sequence of bounded variance noise and data gathered up-to time $T$ be denoted by $\{\eta_t, r_{t,\pi_t}\}_{t=1}^{T}$. Let $S_T = \sum_{t=1}^{T} \eta_t e_{\pi_t}$ and $N_T = \sum_{t=1}^{T} e_{\pi_t}e_{\pi_t}^T$. Using the closed form expression of $\hat{\mu}_T$ from eq. (24), the difference between the estimate and true value $\hat{\mu}_T^i - \mu_i$ can be obtained as follows:

$$
\hat{\mu}_T^i - \mu_i = \langle e_i, \hat{\mu}_T - \mu \rangle = \langle e_i, V_T^{-1} S_T - \rho V_T^{-1} L_G \mu \rangle
$$

The deviation $\hat{\mu}_T^i - \mu_i$ can be upper-boundeded as follows:

$$
|\langle e_i, \hat{\mu}_T - \mu \rangle| \leq |\langle e_i, V_T^{-1} S_T \rangle| + |\langle e_i, \rho V_T^{-1} L_G \mu \rangle|
$$

Further, in order to obtain the variance of the estimate $\hat{\mu}_T$, we bound the deviation $|\mu_T^i - \mu_i|$ by separately bounding $|\langle e_i, V_T^{-1} S_T \rangle|$ and $|\langle e_i, \rho V_T^{-1} L_G \mu \rangle|$. 

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With regards to the first term \( \langle e_i, V^{-1}_T S_T \rangle \), note that
\[
\langle e_i, V^{-1}_T S_T \rangle = \left \langle e_i, V^{-1}_T \left ( \sum_{t=1}^{T} e_{\pi_t} \eta_t \right ) \right \rangle = \sum_{t=1}^{T} \langle e_i, V^{-1}_T e_{\pi_t} \rangle \eta_t
\]
Using a variant of Azuma’s inequality \([33, 37]\), for any \( \kappa > 0 \) the following inequality holds,
\[
P \left ( \left ( \langle e_i, V^{-1}_T S_T \rangle \right )^2 \leq \kappa^2 \right ) \geq 1 - 2 \exp \left \{ - \frac{\kappa^2}{56 \sigma^2 \sum_{t=1}^{T} \langle (e_i, V^{-1}_T e_{\pi_t}) \rangle^2} \right \}
\]  
(29)

Using the fact that \( V_T \succ \left ( \sum_{t=1}^{T} e_{\pi_t} e_{\pi_t}^T \right ) \), we can further simplify the above bound using the following computation,
\[
\sum_{t=1}^{T} \langle (e_i, V^{-1}_T e_{\pi_t}) \rangle^2 = \left \langle V^{-1}_T e_i, \left ( \sum_{t=1}^{T} e_{\pi_t} e_{\pi_t}^T \right ) V^{-1}_T e_i \right \rangle \leq \langle e_i, V^{-1}_T e_i \rangle = \| V^{-1}_T e_i \|_2^2
\]  
(30)

Substituting \( \delta = 2 \exp \left \{ - \frac{\kappa^2}{56 \sigma^2 \sum_{t=1}^{T} \langle (e_i, V^{-1}_T e_{\pi_t}) \rangle} \right \} \), we can finally conclude,
\[
P \left ( \left ( \langle e_i, V^{-1}_T S_T \rangle \right )^2 \leq 56 \sigma^2 \| V^{-1}_T \|_{ii} \log \left ( \frac{2}{\delta} \right ) | F_{t-1} \right ) \geq 1 - \delta
\]  
(31)

Second term \( \langle e_i, \rho V^{-1}_T L_G \mu \rangle \) can be upperbounded using cauchy-schwartz inequality,
\[
| \langle e_i, \rho V^{-1}_T L_G \mu \rangle | = \rho \langle e_i, V^{-1}_T L_G \mu \rangle
\]
\[
\leq \rho \sqrt{\langle e_i, V^{-1}_T e_i \rangle } \sqrt{ \langle L_G \mu, V^{-1}_T L_G \mu \rangle } 
\]
\[
\leq \rho \sqrt{ \| V^{-1}_T \|_{ii} \| \mu \|_G }
\]  
(32)

Combining the upperbound (32) and (31) we get Lemma 1. Hence proved.  
\[ \square \]

### F GRUB Sample complexity

In order to work out the sampling complexity for GRUB, we differentiate the arms into three categories: highly competitive, weakly competitive and noncompetitive. The judgement of the difficulty level of an arm depends on its suboptimality as well as the structure of the provided graph side information. A modified version of the Definition 2 of highly competitive sets, weakly competitive sets and noncompetitive sets are as follows:

**Definition 5.** Fix \( \mu \in \mathbb{R}^n, \text{ graph } G, \text{ expander parameter } \gamma, \text{ confidence parameter } \delta, \text{ bias parameter } \kappa \text{ and resolution } \omega. \) We define \( \mathcal{H} \) to be the set of highly competitive arms, \( \mathcal{W} \) to be the set of weakly competitive arms and \( \mathcal{N} \) to be the set of non-competitive arms as follows:

\[
\mathcal{H}(G, \mu, \kappa, \delta, \omega, \gamma) \triangleq \left \{ j \in [n] \mid \max \{ \Delta_j, \omega \} \leq 2 \sqrt{\frac{2}{\omega (1-\gamma) \beta(j, G) \delta}} \left ( 2 \sqrt{10 \log \frac{\beta(j, G) [C_j(G)]}{\delta}} + \kappa \right ) \right \},
\]
\[
\mathcal{N}(G, \mu, \kappa, \delta, \omega, \gamma) \triangleq \left \{ j \in [n] \mid \max \{ \Delta_j, \omega \} \geq 2 \sqrt{\frac{1}{1-\gamma} + \frac{2}{\beta(j, G) \delta}} \left ( 2 \sqrt{10 \log \frac{\beta(j, G) [C_j(G)]}{\delta}} + \kappa \right ) \right \},
\]
\[
\mathcal{W} \triangleq [n] \setminus (\mathcal{H} \cup \mathcal{N})
\]  
(33)

When the context is clear, we will use suppress the dependence on the parameters in Definition 5.

Further, we derive an expression for the worst-case sample complexity by analysing the number of samples required to eliminate arms with different difficulty levels, i.e. arms in highly, weakly and non-competitive sets. We first derive the sample complexity results for the case when graph \( G \) is connected and then extend it to disconnected graphs.
Lemma 8. Consider n-armed bandit problem with mean vector $\mu \in \mathbb{R}^n$. Let $G$ be a given connected similarity graph on the vertex set $[n]$, and further suppose that $\mu$ is $\epsilon$-smooth. Define

$$T \triangleq \left[ \sum_{j \in \mathcal{H}} \frac{1}{\Delta_j^2} \left[ 448\sigma^2 \log \left( \frac{224\sigma^2 \sqrt{2n} \delta}{\delta^2 \Delta_j^2} \right) + \frac{\rho \epsilon}{2} \right] - \frac{J(j, G)}{2} \right] + \max_{i \in \mathcal{W}} \left\{ \frac{J(i, G), |\mathcal{W}|}{2} \right\} + 1,$$

Then, with probability at least $1 - \delta$, GRUB: (a) terminates in no more than $T$ rounds, and (b) returns the best arm $a^* = \arg\max_i \mu_i$.

Proof. Without loss of generality, assume that $a^* = 1$. Let $\{t_i\}_{i=1}^n$ denote the number of plays of each arm up to time $T$. Let $P_i$ denote the event that estimate of arm 1 is always better than arm $i$.

$$P_i = \{ \hat{\mu}_1^t \geq \hat{\mu}_i^t \quad \forall \ t > 1 \} \quad (34)$$

As is reflected in the elimination policy (7), at any time $t$, arm 1 can be mistakenly eliminated in GRUB only if $\hat{\mu}_i^t > \hat{\mu}_1^t$. GRUB returns the optimal arm for the set of events $\cap_{i=1}^n P_i$. Accordingly, the total failure probability for GRUB can be upper-bounded as,

$$P(\text{Failure}) \leq P(\bigcup_{i=1}^n (P_i)^C) \leq \sum_{t=1}^T \sum_{i=1}^n P(\hat{\mu}_i^t \geq \hat{\mu}_1^t)$$

Let $\zeta_i \leq \mu_1 - \mu_i \triangleq \Delta_i$, then note that $P(\hat{\mu}_i^t \geq \hat{\mu}_1^t) \leq \left[ P\left( \hat{\mu}_i^t \geq \mu_1^t + \frac{\zeta_i}{2} \right) + P\left( \hat{\mu}_1^t \leq \mu_1^t - \frac{\zeta_i}{2} \right) \right]$. Hence,

$$P(\text{Failure}) \leq \sum_{t=1}^T \sum_{i=1}^n \left[ P\left( \hat{\mu}_i^t \geq \mu_1^t + \frac{\zeta_i}{2} \right) + P\left( \hat{\mu}_1^t \leq \mu_1^t - \frac{\zeta_i}{2} \right) \right] \quad (35)$$

where $\zeta_i \leq \Delta_i$. In order to keep $P(\text{Failure}) \leq \delta$, it is sufficient if the following holds for all $i$,

$$P\left( |\hat{\mu}_i^t - \mu_i^t| \geq \frac{\zeta_i}{2} \right) \leq \frac{\delta}{n(t_i + 1)^2} \quad (36)$$

By using the error bounds from equation (35), the number of plays sufficient to remove suboptimal arm $i \in [n]\backslash\{1\}$ can be obtained by solving $\pi_T$ such that,

$$\sqrt{V(\pi_T, G)^{-1}} \left( 2\sigma \sqrt{14 \log \left( \frac{2n(t_i + 1)^2}{\delta} \right)} + \rho \epsilon \right) \leq \left( \frac{\Delta_i}{2} \right) \quad (37)$$

In the absence of graph information, equation (37) devolves to the same sufficiency condition for number of samples required for suboptimal arm elimination as [8], up to constant factor.

In order to derive the sample complexity, we find explicit expression for the number of samples required to eliminate arms with different difficulty levels. For the rest of the proof, using definition divides highly, weakly and noncompetitive sets as follows:

$$\mathcal{H} := \mathcal{H}(G, \mu, \rho \epsilon, \delta, 0, 0) \quad \mathcal{W} := \mathcal{W}(G, \mu, \rho \epsilon, \delta, 0, 0) \quad \mathcal{N} := \mathcal{N}(G, \mu, \rho \epsilon, \delta, 0, 0)$$

Consider any cyclic sampling policy $\pi_T$ and let any arm $k$ be sampled at time $T = 1$. From Lemma 10 and from the connectedness assumption on graph $G$, we can conclude that $|V(\pi_1, G)^{-1}|_{jj} \leq J(j, G)^{-1} + 1, \forall j \in [n]$. Hence, after one play of the GRUB, all noncompetitive arms $i \in \mathcal{N}$ satisfy the sufficiency criteria for elimination as in eq. (37). Hence all noncompetitive arms $\mathcal{N}$ are eliminated after one play of GRUB.
After a total of $T = \max_{i \in \mathcal{H} \cup \mathcal{W}} [\mathcal{J}(i, G)]$ plays of the algorithm GRUB using cyclic sampling policy, all remaining arms which are played at least once satisfy $[V(\pi_T, G)^{-1}]_{ii} \leq \frac{2}{\sqrt{\delta}}$ (Lemma 16). Hence for all weakly competitive arms $i \in \mathcal{W}$,

$$\sqrt{[V(\pi_T, G)^{-1}]_{ii}} \left(2\sigma \sqrt{14 \log \left(\frac{2n(t_i + 1)^2}{\delta}\right)} + \rho\epsilon\right) \leq \sqrt{[V(\pi_T, G)^{-1}]_{ii}} \left(2\sigma \sqrt{14 \log \left(\frac{2nT^2}{\delta}\right)} + \rho\epsilon\right) \leq \frac{\Delta_i}{2}$$

and hence are eliminated after $\max\{[\max_{i \in \mathcal{W}} \mathcal{J}(i, G)], |\mathcal{W}|\}$ plays of the algorithm.

**Remark:** A curious look at Lemma 16 poses a requirement for the above analysis that $t_i > 0$, the cyclic algorithm might not choose the arms in $\mathcal{W}$. But note here that arms in $\mathcal{N}$ would be eliminated before multiple plays of algorithm and the plays are split between only $\mathcal{W}$ and $\mathcal{H}$. The number of plays required for $\mathcal{H}$ are included in further analysis.

Continuing with sampling policy $\pi_T$ for $T > \max\{[\max_{i \in \mathcal{W}} \mathcal{J}(i, G)], |\mathcal{W}|\}$, it can be seen from Lemma 16 that for all remaining arms $[V(\pi_T, G)^{-1}]_{ii} \leq \frac{1}{t_i + \frac{3(i, G)}{2}}$. Hence the number of sufficient plays of arm $i$ required for successful elimination can be derived by solving the following,

$$\sqrt{\frac{1}{t_i + \frac{3(i, G)}{2}}} \left(2\sigma \sqrt{14 \log \left(\frac{2n(t_i + 1)^2}{\delta}\right)} + \rho\epsilon\right) \leq \left(\frac{\Delta_i}{2}\right)$$

Upperbounding the sufficiency criteria, we arrive at a simplified version to solve:

$$\frac{\log (a_i)}{a_i} \leq \frac{\delta \Delta_i^2}{c_1 c_0}$$

where $c_0 = 16 \times 14 \sigma^2$, $c_1 = 2n e^{\frac{\rho}{16 \times 14 \sigma^2}}$ and $a_i = \sqrt{\frac{\delta}{t_i}} \left(t_i + \frac{3(i, G)}{2}\right)$. The following bound on $a_i$ is sufficient to satisfy eq. (60),

$$a_i \geq 2 \sqrt{\frac{c_1 c_0}{\delta \Delta_i^2}} \log \left(\sqrt{\frac{c_1 c_0}{\delta \Delta_i^2}}\right)$$

Resubstituting $t_i$, we obtain the sufficient number of plays required to eliminate arm $i$ as,

$$t_i \geq \frac{1}{\Delta_i^2} \left[448\sigma^2 \log \left(\frac{224\sigma^2 \sqrt{2n}}{\delta^2 \Delta_i^2}\right) + \frac{\rho\epsilon}{2}\right] - \frac{3(i, G)}{2}$$

For all arms $i \in \mathcal{H}$, let $g_i^*$ denote the sufficient number of samples required to successfully eliminate it, i.e., $g_i^* = \frac{1}{\Delta_i^2} \left[448\sigma^2 \log \left(\frac{224\sigma^2 \sqrt{2n}}{\delta^2 \Delta_i^2}\right) + \frac{\rho\epsilon}{2}\right] - \frac{3(i, G)}{2}$. Let $k_1 = \arg \min_{i \in \mathcal{H}} g_i^*$, then the total number of samples played until the arm $k_1$ is eliminated is $|\mathcal{H}|g_{k_1}^*$. Let $k_2 = \arg \min_{i \in \mathcal{H}/k_1} g_i^*$, then the number of plays until the next arm is eliminated is given by $(|\mathcal{H}|-1)|g_{k_2}^* - g_{k_1}^*|$ and so on.

Summing up all the samples required to converge to the optimal arm is given by, (let $g_{k_0}^* = 0$)

$$\sum_{h=1}^{|\mathcal{H}|} (|\mathcal{H}| - h) |g_{kh}^* - g_{kh-1}^*| = \sum_{h=1}^{|\mathcal{H}|} g_{kh}^* = \sum_{i \in \mathcal{H}} g_i^*$$

Summing the number of plays required by the algorithm over sets of all difficulty regime, we obtain our proof.
We extend Lemma 8 to the case when graph \( G \) has disconnected clusters.

**Theorem 4.** Consider \( n \)-armed bandit problem with mean vector \( \mu \in \mathbb{R}^n \). Let \( G \) be a given similarity graph on the vertex set \([n]\), and further suppose that \( \mu \) is \( \epsilon \)-smooth. Let \( C \) be the set of connected components of \( G \). Define

\[
T \triangleq \sum_{C \in C} \left[ \sum_{j \in H \cap C} \frac{1}{\Delta_j^2} \left[ 448\sigma^2 \log \left( \frac{224\sigma^2 \sqrt{2n\pi}}{\delta^2 \Delta_j^2} \right) + \frac{\rho \epsilon}{2} \right] - \mathfrak{I}(j, G) \right] \\
+ \sum_{C \in C} \max \left\{ \max_{l \in W \cap C} \mathfrak{I}(l, G), |W \cap C| \right\} + k(G),
\]

where \( k(G) = |C| \). Then, with probability at least \( 1 - \delta \), GRUB: (a) terminates in no more than \( T \) rounds, and (b) returns the best arm \( a^* = \arg \max_i \mu_i \).

**Proof.** From Lemma 8, the sample complexity for each connected component \( C \in \mathcal{C} \) can be given as,

\[
T \triangleq \left[ \sum_{j \in H \cap C} \frac{1}{\Delta_j^2} \left[ 448\sigma^2 \log \left( \frac{224\sigma^2 \sqrt{2n\pi}}{\delta^2 \Delta_j^2} \right) + \frac{\rho \epsilon}{2} \right] - \mathfrak{I}(j, G) \right] \\
+ \max \left\{ \max_{l \in W \cap C} \mathfrak{I}(l, G), |W \cap C| \right\} + 1,
\]

where, summing it over all the components \( C \in \mathcal{C} \), we get the required result. Hence proved.

\[ \Box \]

**G \( \zeta \)-GRUB Sample complexity proof**

**Lemma 9.** Consider \( n \)-armed bandit problem with mean vector \( \mu \in \mathbb{R}^n \). Let \( G \) be a given connected similarity graph on the vertex set \([n]\), and further suppose that \( \mu \) is \( \epsilon \)-smooth. Define

\[
T \triangleq \left[ \sum_{j \in H} \frac{1}{\max\{\Delta_j^2, \zeta^2\}} \left[ 448\sigma^2 \log \left( \frac{224\sigma^2 \sqrt{2n\pi}}{\delta^2 \Delta_j^2} \right) + \frac{\rho \epsilon}{2} \right] - \mathfrak{I}(j, G) \right] \\
+ \max \left\{ \max_{l \in W \cap C} \mathfrak{I}(l, G), |W| \right\} + 1,
\]

Then, with probability at least \( 1 - \delta \), GRUB: (a) terminates in no more than \( T \) rounds, and (b) returns the \( \zeta \)-best arm

**Proof.** With out loss of generality, assume that \( a^* = 1 \) and let \( \{t_i\}_{i=1}^n \) denote the number of plays of each arm up to time \( T \).

As can be observed from the elimination policy \( \mathcal{E} \), an arm \( i \) can only be eliminated in GRUB only if \( \hat{\mu}_i > \hat{\mu}_1 \). Let \( P_i \) denote the event that,

\[
P_i = \{ \hat{\mu}_i > \hat{\mu}_1, \forall t > 1 \}
\]

GRUB returns the optimal arm for the set of events \( \bigcup_{i=1}^n P_i \). Accordingly, the total failure probability for GRUB can be upper-bounded as,

\[
P(\text{Failure}) \leq P(\bigcup_{i=1}^n P_i) \leq \sum_{i=1}^n \sum_{t=1}^T P(\hat{\mu}_i > \hat{\mu}_1)
\]
Given that \( \zeta_i \leq \max\{\mu_1 - \mu_i, \zeta\} \), note that \( \mathbb{P}(\hat{\mu}_i^t \geq \mu_i) \leq \mathbb{P}(\hat{\mu}_i^t \geq \mu_i + \frac{\zeta_i}{2}) + \mathbb{P}(\hat{\mu}_i^t \leq \mu_i - \frac{\zeta_i}{2}) \). Hence,

\[
\mathbb{P}({\text{Failure}}) \leq \sum_{t=1}^{T} \sum_{i=1}^{n} \left[ \mathbb{P}(\hat{\mu}_i^t \geq \mu_i + \frac{\zeta_i}{2}) + \mathbb{P}(\hat{\mu}_i^t \leq \mu_i - \frac{\zeta_i}{2}) \right]
\]

(44)

where \( \zeta_i \leq \max\{\Delta_i, \zeta\} \).

In order to keep \( \mathbb{P}({\text{Failure}}) \leq \delta \), it is sufficient if the following holds \( \forall t > 1, i \in [n] \),

\[
\mathbb{P}(\hat{\mu}_i^t - \mu_i \geq \frac{\zeta_i}{2}) \leq \frac{\delta}{n(t_i + 1)^2}
\]

(45)

By using the error bounds from equation [3] the number of plays sufficient to remove suboptimal arm \( i \in [n]/\{1\} \) can be obtained by solving \( \pi_T \) such that,

\[
\sqrt{V(\pi_T, G)^{-1}}_{ii} \left( 2\sigma \sqrt{14 \log \left( \frac{2n(t_i + 1)^2}{\delta} \right)} + \rho \epsilon \right) \leq \frac{\max\{\Delta_i, \zeta\}}{2}
\]

(46)

In the absence of graph information, equation [40] devolves to the same sufficiency condition for number of samples required for suboptimal arm elimination as [3], upto constant factor.

For the rest of the proof, let :

\[
\mathcal{H} := \mathcal{H}(G, \mu, \rho, \delta, \zeta, 0) \quad \mathcal{W} := \mathcal{W}(G, \mu, \rho, \delta, \zeta, 0) \quad \mathcal{N} := \mathcal{N}(G, \mu, \rho, \delta, \zeta, 0)
\]

In order to derive the sample complexity, we find explicit expression for the number of samples required to eliminate arms with different difficulty levels.

Consider any cyclic sampling policy \( \pi_T \) and let any arm \( k \) be sampled at time \( T = 1 \). From Lemma [16] and from the connectedness of graph G, we can conclude that \( [V(\pi_1, G)^{-1}]_{jj} \leq \mathcal{J}(j, G)^{-1} + 1, \forall j \in [n] \). We can thus conclude that for all noncompetitive arms \( i \in \mathcal{N} \) satisfy the sufficiency criteria for elimination as in eq. (37). Hence all noncompetitive arms \( \mathcal{N} \) are eliminated after one play of GRUB.

After a total of \( T = \max_{i \in \mathcal{H} \cup \mathcal{W}} [\mathcal{J}(i, G)] \) plays of the algorithm GRUB using cyclic sampling policy, all remaining arms which are played atleast once satisfy \( [V(\pi_T, G)^{-1}]_{ii} \leq \frac{2\sigma}{\mathcal{J}(i, G)} \) (Lemma [16]). Hence for all weakly competitive arms \( i \in \mathcal{W} \),

\[
\sqrt{[V(\pi_T, G)^{-1}]_{ii}} \left( 2\sigma \sqrt{14 \log \left( \frac{2n(t_i + 1)^2}{\delta} \right)} + \rho \epsilon \right) \leq \sqrt{[V(\pi_T, G)^{-1}]_{ii}} \left( 2\sigma \sqrt{14 \log \left( \frac{2nT^2}{\delta} \right)} + \rho \epsilon \right) \leq \frac{\max\{\Delta_i, \zeta\}}{2}
\]

(47)

and hence are eliminated after \( \max\{\max_{i \in \mathcal{W}} [\mathcal{J}(i, G)], |\mathcal{W}|\} \) plays of the algorithm.

Remark: A curious look at Lemma [16] poses a requirement for the above analysis that \( t_i > 0 \), the cyclic algorithm might not choose the arms in \( \mathcal{W} \). But note here that arms in \( \mathcal{N} \) would be eliminated before multiple plays of algorithm and the plays are split between only \( \mathcal{W} \) and \( \mathcal{H} \). The number of plays required for \( \mathcal{H} \) are included in further analysis.

Continuing with sampling policy \( \pi_T \) for \( T > \max\{\max_{i \in \mathcal{W}} [\mathcal{J}(i, G)], |\mathcal{W}|\} \), it can be seen from Lemma [16] that for all remaining arms \( [V(\pi_T, G)^{-1}]_{ii} \leq \frac{1}{t_i + \frac{2\sigma}{\mathcal{J}(i, G)}} \). Hence the number of sufficient plays of arm \( i \) required for successful elimination can be derived by solving the following,

\[
\sqrt{\frac{1}{t_i + \frac{2\sigma}{\mathcal{J}(i, G)}}} \left( 2\sigma \sqrt{14 \log \left( \frac{2n(t_i + 1)^2}{\delta} \right)} + \rho \epsilon \right) \leq \frac{\max\{\Delta_i, \zeta\}}{2}
\]

(48)
Upperbounding the sufficiency criteria, we arrive at a simplified version of the sufficiency criteria to solve:
\[
\frac{\log (a_i)}{a_i} \leq \sqrt{\frac{\delta}{c_1}} \max \{\Delta_i, \zeta\}^2
\]
where \(c_0 = 16 \times 14 \sigma^2, c_1 = 2ne^{16 \times 14 \sigma^2}\) and \(a_i = \sqrt{\frac{\delta}{c_1}} \left(t_i + \frac{3(i, G)}{2}\right)\). The following bound on \(a_i\) is sufficient to satisfy eq. (60),
\[
a_i \geq 2\sqrt{\frac{c_1}{\delta}} \max \{\Delta_i, \zeta\} \log \left(\sqrt{\frac{c_1}{\delta}} \max \{\Delta_i, \zeta\}^2\right)
\]
Resubstituting \(t_i\), we obtain the sufficient number of plays required to eliminate arm \(i\) as,
\[
t_i \geq \frac{1}{\max \{\Delta_i, \zeta\}^2} \left[448\sigma^2 \log \left(\frac{224\sigma^2 \sqrt{2n}}{\delta \max \{\Delta_i, \zeta\}^2}\right) + \frac{\rho e}{2}\right] - \frac{3(i, G)}{2}
\]
For all arms \(i \in \mathcal{H}\), let \(g^*_i\) denote the sufficient number of samples required to successfully eliminate it, i.e. \(g^*_i = \frac{1}{\max \{\Delta_i, \zeta\}^2} \left[448\sigma^2 \log \left(\frac{224\sigma^2 \sqrt{2n}}{\delta \max \{\Delta_i, \zeta\}^2}\right) + \frac{\rho e}{2}\right] - \frac{3(i, G)}{2}\).
Let \(k_1 = \arg \min_{i \in \mathcal{H}} g^*_i\), then the total number of samples played until the arm \(k_1\) is eliminated is \(|\mathcal{H}|g^*_{k_1}\). Let \(k_2 = \arg \min_{i \in \mathcal{H}/k_1} g^*_i\), then the number of plays until the next arm is eliminated is given by \(|\mathcal{H}| - 1|g^*_{k_2} - g^*_i|\) and so on.
Summing up all the samples required to converge to the optimal arm is given by, (let \(g^*_{k_0} = 0\))
\[
\sum_{h=1}^{\mathcal{H}}(|\mathcal{H}| - h)|g^*_{kh} - g^*_{kh-1}| = \sum_{h=1}^{\mathcal{H}} g^*_{kh} = \sum_{i \in \mathcal{H}} g^*_i
\]
Summing the number of plays required by the algorithm over sets of all difficulty regime, we obtain our proof.

We extend Lemma [9] to the case when graph \(G\) has disconnected clusters.

**Remark:** Please note that the constants reported in the main paper had a typographical error (and the actual constants are as reported in Theorem [9]); this does not affect the nature of our results.

**Theorem 5.** Consider \(n\)-armed bandit problem with mean vector \(\mu \in \mathbb{R}^n\). Let \(G\) be the given similarity graph on vertex set \([n]\), and further suppose that \(\mu\) is \(\epsilon\)-smooth. Let \(\mathcal{C}\) be the set of connected components of \(G\). Define
\[
T_\zeta := \sum_{C \in \mathcal{C}} \left[\sum_{j \in \mathcal{H} \cap C} \frac{1}{\max \{\Delta_j^*, \zeta^2\}} \left[448\sigma^2 \log \left(\frac{224\sigma^2 \sqrt{2n}}{\delta \Delta_j^*}\right) + \frac{\rho e}{2}\right] - \frac{\mathcal{J}(j, G)}{2}\right] + \sum_{C \in \mathcal{C}} \max_{l \in W \cap C} \mathcal{J}(l, G), |W \cap C| + k(G)
\]
where \(k(G) = |\mathcal{C}|\), Then, with probability at least \(1 - \delta\), \(\zeta\)-GRUB: (a) terminates in no more than \(T\) rounds, and (b) returns the \(\zeta\)-best arm.

**Proof.** From Lemma [9] the sample complexity for each connected component \(C \in \mathcal{C}\) can be given as,
\[
\left[\sum_{j \in \mathcal{H} \cap C} \frac{1}{\max \{\Delta_j^*, \zeta^2\}} \left[448\sigma^2 \log \left(\frac{224\sigma^2 \sqrt{2n}}{\delta \Delta_j^*}\right) + \frac{\rho e}{2}\right] - \frac{\mathcal{J}(j, G)}{2}\right] + \sum_{C \in \mathcal{C}} \max_{l \in W \cap C} \mathcal{J}(l, G), |W \cap C| + 1
\]
Then, with probability at least $1 - \delta$, the best arm $a^*$ can be observed from the elimination policy (7), an arm $i$ can only be eliminated in GRUB only if $\hat{\mu}_i > \hat{\mu}_1$. Let $P_i$ denote the event that,

$$P_i = \{\hat{\mu}_i \geq \hat{\mu}_1 \ \forall \ t > 1\}$$

GRUB returns the optimal arm for the set of events $\bigcup_{i=1}^{n} P_i$. Accordingly, the total failure probability for GRUB can be upper-bounded as,

$$\mathbb{P}(\text{Failure}) \leq \mathbb{P}\left(\bigcup_{i=1}^{n} (P_i)^C\right) \leq \sum_{t=1}^{T} \sum_{i=1}^{n} \mathbb{P}\left(\hat{\mu}_i \geq \hat{\mu}_1\right)$$

Given that $\zeta_i \leq \mu_1 - \mu_i$, note that $\mathbb{P}\left(\hat{\mu}_i \geq \hat{\mu}_1\right) \leq \mathbb{P}\left(\hat{\mu}_i \geq \mu_1 + \frac{\zeta_i}{2}\right) + \mathbb{P}\left(\hat{\mu}_1 \leq \mu_1 - \frac{\zeta_i}{2}\right)$. Hence,

$$\mathbb{P}(\text{Failure}) \leq \sum_{t=1}^{T} \sum_{i=1}^{n} \left[\mathbb{P}\left(\hat{\mu}_i \geq \mu_1 + \frac{\zeta_i}{2}\right) + \mathbb{P}\left(\hat{\mu}_1 \leq \mu_1 - \frac{\zeta_i}{2}\right)\right]$$

(54)

where $\zeta_i \leq \Delta_i$.

In order to keep $\mathbb{P}(\text{Failure}) \leq \delta$, it is sufficient if the following holds $\forall t > 1, i \in [n]$,

$$\mathbb{P}\left(|\hat{\mu}_i - \mu_i| \geq \frac{\zeta_i}{2}\right) \leq \frac{\delta}{n(t_i + 1)^2}$$

(55)

By using the error bounds from equation (5) the number of plays sufficient to remove suboptimal arm $i \in [n]/\{1\}$ can be obtained by solving $\pi_T$ such that,

$$\sqrt{[V(\pi_T,G)^{-1}]}_{ii} \left(2\sigma \sqrt{14 \log \left(\frac{2n(t_i + 1)^2}{\delta}\right)} + \rho \epsilon\right) \leq \left(\frac{\Delta_i}{2}\right)$$

(56)

In the absence of graph information, equation (56) devolves to the same sufficiency condition for number of samples required for suboptimal arm elimination as [8], upto constant factor.

By using the Definition of $\gamma$-close, the bound on diagonal elements of $V(\pi_T,H)^{-1}$ can be given using Lemma 10

$$[V(\pi_T,H)]^{-1}_{ii} \leq \frac{1}{(1 - \gamma)}[V(\pi_T,G)]^{-1}_{ii}$$

(57)
Further in the proof, in order to find the sample complexity for the case of finding optimal arm, we analyse bounds for \([V(\pi_T, G)]_{ii}^{-1}\) and link to graph \([V(\pi_T, H)]_{ii}^{-1}\) using the above statement.

For the rest of the proof, let:
\[
H := H(G, \mu, \rho \epsilon, \delta, 0, \gamma) \quad W := W(G, \mu, \rho \epsilon, \delta, 0, \gamma) \quad N := N(G, \mu, \rho \epsilon, \delta, 0, \gamma)
\]

In order to derive the sample complexity, we find explicit expression for the number of samples required to eliminate arms with different difficulty levels.

Consider any cyclic sampling policy \(\pi_T\) and let any arm \(k\) be sampled at time \(T = 1\). From Lemma[16] and from the connectedness of graph \(G\), we can conclude that \([V(\pi_1, H)]_{jj}^{-1} \leq \mathcal{J}(j, H)^{-1} + 1\), \(\forall j \in [n]\). We can thus conclude that for all noncompetitive arms \(i \in N\) satisfy the sufficiency criteria for elimination as in eq. (37). Hence all noncompetitive arms \(N\) are eliminated after one play of GRUB.

After a total of \(T = \max_{i \in H \cup W} [\mathcal{J}(i, H)]\) plays of the algorithm GRUB using cyclic sampling policy, all remaining arms which are played at least once satisfy \([V(\pi_T, H)]_{ii}^{-1} \leq \frac{2}{\mathcal{J}(i, H)}\) (Lemma [16]). Hence for all weakly competitive arms \(i \in W\),
\[
\sqrt{[V(\pi_T, H)]_{ii}^{-1}} \leq \sqrt{[V(\pi_T, H)]_{ii}^{-1}} \left(2\sigma \sqrt{14 \log \left(\frac{4n(t_i + 1)^2}{\delta} + \rho \epsilon\right)} \leq \frac{\sqrt{1 - \gamma \Delta_i}}{2} \right)
\]
and hence are eliminated after \(\max\{\max_{i \in W}[\mathcal{J}(i, H)], |W|\}\) plays of the algorithm.

**Remark:** A curious look at Lemma [16] poses a requirement for the above analysis that \(t_i > 0\), the cyclic algorithm might not choose the arms in \(W\). But note here that arms in \(N\) would be eliminated before multiple plays of algorithm and the plays are split between only \(W\) and \(H\). The number of plays required for \(H\) are included in further analysis.

Continuing with sampling policy \(\pi_T\) for \(T > \max\{\max_{i \in W}[\mathcal{J}(i, H)], |W|\}\), it can be seen from Lemma[16] that for all remaining arms \([V(\pi_T, H)]_{ii}^{-1} \leq \frac{1}{t_i + \frac{2\rho \epsilon}{\Delta_i}}\). Hence the number of sufficient plays of arm \(i\) required for successful elimination can be derived by solving the following,
\[
\sqrt{t_i + \frac{2\rho \epsilon}{\Delta_i}} \left(2\sigma \sqrt{14 \log \left(\frac{4n(t_i + 1)^2}{\delta} + \rho \epsilon\right)} \leq \left(\frac{\sqrt{1 - \gamma \Delta_i}}{2}\right)\right)
\]
Upperbounding the sufficiency criteria, we arrive at a simplified version of the sufficiency criteria to solve:
\[
\frac{\log (a_i)}{a_i} \leq \sqrt{\frac{\delta}{c_1}} (1 - \gamma) \Delta_i^2 \frac{c_0}{c_1}.
\]
where \(c_0 = 16 \times 14 \sigma^2\), \(c_1 = 2n \epsilon e^{16 \times 14 \sigma^2}\) and \(a_i = \sqrt{\frac{\Delta_i}{\delta}} \left(t_i + \frac{3(i, H)}{2}\right)\). The following bound on \(a_i\) is sufficient to satisfy eq. (60),
\[
a_i \geq 2 \sqrt{\frac{c_1}{\delta} \frac{c_0}{(1 - \gamma) \Delta_i^2} \log \left(\sqrt{\frac{c_1}{\delta} \frac{c_0}{(1 - \gamma) \Delta_i^2}}\right)}
\]
Resubstituting \(t_i\), we obtain the sufficient number of plays required to eliminate arm \(i\) as,
\[
t_i \geq \frac{1}{(1 - \gamma) \Delta_i^2} \left[448 \sigma^2 \log \left(\frac{224 \sigma^2 \sqrt{2n}}{\delta^2 (1 - \gamma) \Delta_i^2} + \frac{\rho \epsilon}{2}\right) - \frac{3(i, H)}{2}\right]
\]
For all arms $i \in \mathcal{H}$, let $g_i^*$ denote the sufficient number of samples required to successfully eliminate it, i.e. $g_i^* = \frac{1}{(1-\gamma)\Delta_i} \left[ 448\sigma^2 \log \left( \frac{224\sigma^2 \sqrt{2n}}{(1-\gamma)\delta^2\Delta_i^2} \right) + \frac{\rho\epsilon}{2} - \frac{3\sigma(j,H)}{2} \right].$

Let $k_1 = \arg \min_{i \in \mathcal{H}} g_i^*$, then the total number of samples played until the arm $k_1$ is eliminated is $|\mathcal{H}|g_{k_1}^*$. Let $k_2 = \arg \min_{i \in \mathcal{H}/k_1} g_i^*$, then the number of plays until the next arm is eliminated is given by $(|\mathcal{H}|-1)g_{k_2}^* - g_{k_1}^*$ and so on.

Summing up all the samples required to converge to the optimal arm is given by, (let $g_{k_0}^* = 0$)

$$\sum_{h=1}^{\lceil |\mathcal{H}| \rceil} (|\mathcal{H}| - h)g_{kh}^* - g_{kh-1}^* = \sum_{h=1}^{\lceil |\mathcal{H}| \rceil} g_{kh}^* = \sum_{i \in \mathcal{H}} g_i^*$$  \hspace{1cm} (60)

Summing the number of plays required by the algorithm over sets of all difficulty regime, we obtain our proof.

$$\square$$

We extend Lemma 10 to the case when graph $G$ has disconnected clusters.

**Theorem 6.** Consider $n$-armed bandit problem with mean vector $\mu \in \mathbb{R}^n$. Let $G$ be the given similarity graph on vertex set $[n]$, and further suppose that $\mu$ is $\epsilon$-smooth. Let $C$ be the set of connected components of $G$. Define

$$T_\gamma := \min_{H \in \mathcal{S}(G,\gamma)} \left\{ \sum_{C \in \mathcal{C}} \left[ \sum_{j \in \mathcal{H} \cap C} \frac{1}{(1-\gamma)\Delta_j} \left[ 448\sigma^2 \log \left( \frac{224\sigma^2 \sqrt{2n}}{(1-\gamma)\delta^2\Delta_j^2} \right) + \frac{\rho\epsilon}{2} - \frac{3\sigma(j,G)}{2} \right] \right] + \sum_{C \in \mathcal{C}} \max_{i \in \mathcal{W} \cap C} \mathcal{J}(l,G), |\mathcal{W} \cap C| + k(H) \right\},$$  \hspace{1cm} (61)

where $k(G) = |\mathcal{C}|$. Then, with probability at least $1 - \delta$, GRUB: (a) terminates in no more than $T$ rounds, and (b) returns the best arm $a^* = \arg \max_i \mu_i$.

**Proof.** From Lemma 10 summing it over all the components $C \in \mathcal{C}$, we get the following sample complexity,

$$\sum_{C \in \mathcal{C}} \left[ \sum_{j \in \mathcal{H} \cap C} \frac{1}{(1-\gamma)\Delta_j} \left[ 448\sigma^2 \log \left( \frac{224\sigma^2 \sqrt{2n}}{(1-\gamma)\delta^2\Delta_j^2} \right) + \frac{\rho\epsilon}{2} - \frac{3\sigma(j,G)}{2} \right] \right] + \sum_{C \in \mathcal{C}} \max_{i \in \mathcal{W} \cap C} \mathcal{J}(l,G), |\mathcal{W} \cap C| + k(H),$$  \hspace{1cm} (62)

We prove the non-monotonic nature of $\mathcal{J}(\cdot, G)$ w.r.t. graph $G$ in Lemma 20.

Thus the sample complexity stated eq. (62) can be further reduced by taking the minimum over all $\gamma$-close graphs $\mathcal{S}(G,\gamma)$. Thus the final sample complexity form becomes,

$$T_\gamma := \min_{H \in \mathcal{S}(G,\gamma)} \left\{ \sum_{C \in \mathcal{C}} \left[ \sum_{j \in \mathcal{H} \cap C} \frac{1}{(1-\gamma)\Delta_j} \left[ 448\sigma^2 \log \left( \frac{224\sigma^2 \sqrt{2n}}{(1-\gamma)\delta^2\Delta_j^2} \right) + \frac{\rho\epsilon}{2} - \frac{3\sigma(j,H)}{2} \right] \right] + \sum_{C \in \mathcal{C}} \max_{i \in \mathcal{W} \cap C} \mathcal{J}(l,H), |\mathcal{W} \cap C| + k(H) \right\},$$  \hspace{1cm} (63)

where,

$$\mathcal{H} := \mathcal{H}(H,\mu,\rho\epsilon,\delta,0,\gamma) \quad \mathcal{W} := \mathcal{W}(H,\mu,\rho\epsilon,\delta,0,\gamma) \quad \mathcal{N} := \mathcal{N}(H,\mu,\rho\epsilon,\delta,0,\gamma)$$

Hence proved. $\square$
I Sampling policies

The main objective of sampling policies is to decrease the value of $[V_T^{-1}]_{ii}$ for every arm $i$ as fast as possible. The notion of decrease leads to different sampling policies for GRUB. The algorithm chooses the arm which maximizes this notion of decreases.

The objective of the sampling policy Joint variance minimization – operator (JVM-O) is equivalent to:

$$\max_{k \in A} \sum_{j \in [n]} |(V_T^{-1})_{k,j} - |(V_T + e_k e_k^T)^{-1}_{k,j}|$$

(64)

Using Sherman-morrison rank 1 update we split the summation into different cases:

- For $j = k$,
  $$|\langle e_k V_T^{-1} e_k \rangle| - |\langle e_k (V_T + e_k e_k^T)^{-1} e_k \rangle| = \frac{\|e_k\|^2_{V_T^{-1}}}{1 + \|e_k\|^2_{V_T^{-1}}}$$
  (65)

- For all connected-nodes of $j \in N_k$,
  $$|\langle e_k V_T^{-1} e_j \rangle| - |\langle e_k (V_T + e_k e_k^T)^{-1} e_j \rangle| = \frac{\langle e_j, e_k \rangle^2_{V_T^{-1}}}{1 + \|e_k\|^2_{V_T^{-1}}}$$
  (66)

- For all other non-connected $j \notin N_k, i \neq k$,
  $$|\langle e_k V_T^{-1} e_i \rangle| - |\langle e_k (V_T + e_k e_k^T)^{-1} e_i \rangle| = 0$$
  (67)

Hence the sampling policy decides on the arm to sample based on the following optimization problem,

$$\sum_{j \in [n]} |(V_T^{-1})_{k,j} - |(V_T + e_k e_k^T)^{-1}_{k,j}| = \frac{\|e_k\|^2_{V_T^{-1}} + \sum_{j \in N_k} \langle e_j, e_k \rangle^2_{V_T^{-1}}}{1 + \|e_k\|^2_{V_T^{-1}}} = \frac{\|\text{Row}_k(V_T^{-1})\|^2_2}{1 + [(V_T^{-1})_{kk}]}$$

Hence we try to find the arm $k$ within the remaining arms in consideration which maximizes $\frac{\|\text{Row}_k(V_T^{-1})\|^2_2}{1 + [(V_T^{-1})_{kk}]}$.

J Supporting Results

This appendix is devoted to providing supporting results for many of the theorems and lemmas in the paper. We first state some notations used throughout this appendix section. Let $\{t_i\}_{i=1}^n$ denote the number of plays of each arm until time $T$. Given a matrix $X \in \mathbb{R}^{n \times n}$, let $\{\lambda_i(X)\}_{i=1}^n$ indicate the eigenvalues of matrix $X$ in an increasing order. Given a graph $D$, we define a class of sampling policies $\mathcal{U}(T, D)$ as follows,

**Definition 6.** Let $\mathcal{U}(T, D)$ denote the set of sampling policies, 

$$\mathcal{U}(T, D) = \{\pi_T | \exists l \in D \text{ s.t. } \pi_t = l \ \forall t \leq T\}$$

Let $N(\pi_T) = \sum_{t=1}^T e_{\pi_t} e_{\pi_t}^T$ be the diagonal counting matrix. Note that $N(\pi_T)$ can be written as $N(\{t_i\}_{i=1}^n)$ since the diagonal counting matrix only depends on the number of plays of each arm, rather than the each sampling sequence $\pi_T$. Hence we can rewrite $V(\pi_T, G)$ as $V(\pi_T, G) = V(\{t_i\}_{i=1}^n, G) = \cdots$
Given a graph $D$, let $\{D_i\}_{i=1}^{k(G)}$ indicate the connected components of $D$, from [17] note that

$$V(\bm{\pi}_T, D) = \text{diag}([V_1(\bm{\pi}_T, D), V_2(\bm{\pi}_T, D_2), \ldots, V_{k(G)}(\bm{\pi}_T, D)])$$

where $V_i(\bm{\pi}_T, D)$ corresponds to the subblock relating to all the nodes in sub-component $D_i$. Since $V(\bm{\pi}_T, G)$ obeys a block diagonal structure, we prove the all the result for connected graph $G$ and they can be easily extended to the case when graph $G$ is disconnected.

The following lemma establishes the invertibility of $V(\bm{\pi}_T, G)$ for a connected graph and $T > 1$.

**Lemma 11.** For a connected graph $G$, $V(\bm{\pi}_1, G)$ is invertible, but $V(\bm{\pi}_0, G)$ is not invertible.

**Proof.** Since the graph $G$ is connected, $\lambda_1(L_G) = 0$ and $\lambda_2(L_G) > 0$. The eigenvector corresponding to $\lambda_1(L_G)$ is $1$, the all $1$ vector. At time $T = 0$, $V(\bm{\pi}_T, G) = L_G$ and hence $V(\bm{\pi}_T, G)$ is positive semi-definite matrix with one zero eigenvalues.

Let arm $i$ be pulled, i.e. $\pi_1 = i$. At $T = 1$, let arm $\pi_1 = i$ be pulled, then the corresponding counting matrix is a positive semi definite matrix of rank one with the eigen value $\lambda_n(N) = 1$ for the eigenvector $e_i$.

Observe that $e_i^T 1 > 0$. Also, $N_T$ and $L_G$ are positive semi-definite matrices with ranks $1$ and $n - 1$ respectively. The subspace without information (corresponding to the direction of zero eigenvalue) for matrix $L_G$ is now provided by $N(\pi_1)$ and hence $\lambda_{\min}(V(\pi_1, G)) > 0$ making it invertible.

We next establish some properties of the influence function $\mathfrak{I}$, which we will use in Appendix [D].

**Lemma 12.** Let $D$ be an arbitrary graph with $n$ nodes and let $\{t_i\}_{i=1}^n$ be the number of times all arms are sampled till time $T$. For each node $j \in [n]$, the following are equivalent:

$$\frac{1}{\mathfrak{I}(j, D)} = \max_{\sum_{i \in D_j, i \neq j} t_i = T} \{[K(i, D)]_{jj}\}$$

$$= \max_{k \in D_j, \sum_{i \in D_j, i \neq j} t_i = T} \{[V_j(\{t_i\}_{i \in D_j}, D)^{-1}]_{jj} - [V_j(\{t_i\}_{i \in D_j}, D)^{-1}]_{kk}\}$$

$$= \max_{\sum_{i \in D_j, i \neq j} t_i = T} \left\{[V_j(\{t_i\}_{i \in D_j}, D)^{-1}]_{jj} - \min_{k \in D_j} [V_j(\{t_i\}_{i \in D_j}, D)^{-1}]_{kk}\right\}$$

$$= \max_{\sum_{i \in D_j, i \neq j} t_i = T} \left\{[V_j(\{t_i\}_{i \in D_j}, D)^{-1}]_{jj} - \frac{1}{T}\right\} \quad (68)$$

where $K(i, D)$ be defined as in Definition [7]

**Proof.** Let $f(\cdot, \cdot)$ denote the following:

$$f(i, D) = \frac{1}{\mathfrak{I}(j, D)}$$

Then by Definition [4] it can be easily seen that,

$$f(i, D) = \max_{\sum_{i \in D_j, i \neq j} t_i = T} \{[K(i, D)]_{jj}\}$$

We prove the rest by showing equivalence between $(A), (B), (C)$ and $(D)$.

- $(A) \Leftrightarrow (D)$ : A simple extension of Lemma [14] to the case of disconnected clustered graph $D$, $\forall \bm{\pi}_T \in \mathcal{U}(T, D_j)$ we obtain,

$$V_j(\bm{\pi}_T, D)^{-1} = \frac{1}{T}\mathbb{1}\mathbb{1}^T + K(\pi_1, D)$$
where $K(\pi_1, D)$ is as defined in Definition 11. Thus, we have the equivalence by explicitly writing the diagonal element of eq (69),

$$[V_j(\pi_T, D)^{-1}]_{jj} - \frac{1}{T} = [K(\pi_1, D)]_{jj}$$

(70)

Hence we have the equivalence as,

$$f(i, D) = \max_{\sum_{i \in D_j, i \neq j}^T, t_i = T} \left\{ [V_j(\{t_i\}_{i\in D_j}, D)^{-1}]_{jj} - \frac{1}{T} \right\}$$

(71)

• $(C) \iff (D)$: Let $\{t_i^*(j)\}_{i \in D_j}$ denote the following:

$$\{t_i^*(j)\}_{i \in D_j} \in \arg \max_{\sum_{i \in D_j, i \neq j}^T, t_i = T} \left\{ [V_j(\{t_i\}_{i\in D_j}, D)]_{jj}^{-1} - \frac{1}{T} \right\}$$

(72)

From Lemma 13, the optimal $\{t_i^*(j)\}_{i \in D_j}$ occurs in $\mathcal{U}(j, T)$, i.e. $\exists \{t_i^*(j)\}_{i \in D_j}$ such that $t_i^*(j) = T$ and $t_k^*(j) = 0 \ \forall k \neq l$ for some $l \in D_j$. Further by Lemma 15

$$\min_{k \in D_j} [V_j(\{t_i\}_{i\in D_j}, D)^{-1}]_{kk} = \frac{1}{T}$$

(73)

Hence $\{t_i^*(j)\}_{i \in D_j}$ is also a solution for the following problem:

$$\{t_i^*(j)\}_{i \in D_j} \in \arg \max_{\sum_{i \in D_j, i \neq j}^T, t_i = T} \left\{ [V_j(\{t_i\}_{i\in D_j}, D)]_{jj}^{-1} - \min_{k \in D_j} [V_j(\{t_i\}_{i\in D_j}, D)^{-1}]_{kk} \right\}$$

(74)

Hence we can conclude that,

$$f(i, D) = \max_{\sum_{i \in D_j, i \neq j}^T, t_i = T} \left\{ [V_j(\{t_i\}_{i\in D_j}, D)]_{jj}^{-1} - \min_{k \in D_j} [V_j(\{t_i\}_{i\in D_j}, D)^{-1}]_{kk} \right\}$$

(75)

• $(B) \iff (C)$: Note that $\max_{k \in D_j, \sum_{i \in D_j, i \neq j}^T, t_i = T} [V_j(\{t_i\}_{i\in D_j}, D)^{-1}]_{jj}$ does not depend on arm node index $k \in D_j$. Hence, the equivalence follows.

Hence proved. \qed

**Lemma 13.** Let $D$ be a given graph with $n$ nodes. For every node $j \in D$, let $\{t_i^*(j)\}_{i \in D_j}$ denote the following:

$$\{t_i^*(j)\}_{i \in D_j} \in \arg \max_{\sum_{i \in D_j, i \neq j}^T, t_i = T} \left\{ [V_j(\{t_i\}_{i\in D_j}, D)]_{jj}^{-1} - \frac{1}{T} \right\}$$

(76)

Then $\exists \{t_i^*(j)\}_{i \in D_j}, l \in D_j$ such that $t_i^*(j) = T$ and $t_k^*(j) = 0 \ \forall k \neq l$.

**Proof.** To simplify our proof, let graph $D$ be connected. The proof for the case of disconnected components is an extension of the connected graph case, by analysing each individual connected component together.

If graph $D$ is connected then $D_l = D$. For the rest of the proof we sometimes denote $V(\pi_T, D)$ as $V(\{t_i\}_{i=1}^n, D)$ to make it more context relevant.

Let $g : \mathbb{R}^n \to \mathbb{R}^{n \times n}$ be a partial function of $V(\pi_T, D)$ as follows:

$$g(\{t_i\}_{i=1}^n) = V(\{t_i\}_{i=1}^n, D)$$

(77)
For all $i \in [n]$, let $t_i = \alpha_i T$ such that $\sum_{i=1}^{n} \alpha_i = 1$. Then we can say that,
\[
g(\{t_i\}_{i=1}^{n}) = g(\{\alpha_i T\}_{i=1}^{n}) = \sum_{i=1}^{n} \alpha_i g(\{0, 0, \ldots t_i = T, \ldots 0\})
\]  
(78)
Hence the function $g(\cdot)$ is linear. Another way of stating it is $V(\pi T, G)$ is a linear function of $\{V(\{i\}_i=1, G)\}_{i=1}^{n}$ and hence $V(\pi T, G)^{-1}$ satisfies,
\[
g(\{t_i\}_{i=1}^{n})^{-1} \leq \sum_{i=1}^{n} \alpha_i g(\{0, 0, \ldots t_i = T, \ldots 0\})^{-1}
\]  
(79)
Hence $g(\cdot)^{-1}$ is a convex function. Since we have the restriction as $\sum_{i=1}^{n} t_i = T$. We can say that,
\[
\arg\max_{\sum_{i=1}^{n} t_i = T} \left\{ [V(\{t_i\}_{i=1}^{n}, D)]^{-1}_{jj} - \frac{1}{\sum_{i=1}^{n} t_i} \right\} = \arg\max_{\sum_{i=1}^{n} t_i = T} \left\{ [V(\{t_i\}_{i=1}^{n}, D)]^{-1}_{jj} \right\}
\]  
(80)
\[
= \arg\max_{\sum_{i=1}^{n} t_i = T} \langle e_j, [V(\{t_i\}_{i=1}^{n}, D)]^{-1} e_j \rangle
\]  
(81)
Since $g(\cdot)^{-1}$ is convex, for a convex function the maximization over a simplex happens at one of the vertices. Hence the max happens when $t_i = T$ and $t_k = 0 \ \forall k \neq i$.
Hence proved. \[\square\]

**Lemma 14.** Let $G$ be a given connected graph of $n$ nodes and $t_i$ be the number of samples of each arm $i$. Then $\forall \pi T \in \mathcal{U}(T),$  
\[
V(\pi T, G)^{-1} = \frac{1}{T} \mathbb{1} \mathbb{1}^T + K(\pi_1, G)
\]  
(81)
where, $\mathbb{1} \in \mathbb{R}^n$ is a vector or all ones and $K(\pi_1, G) \in \mathbb{R}^{n \times n}$ is the matrix defined in Definition 1.

**Proof.** Let $I$ be an identity matrix of dimension $n \times n$. We prove the result by showing that, $\forall \pi T \in \mathcal{U}(T), V(\pi T, G)^{-1} V(\pi T, G) = I,$
\[
V(\pi T, G)^{-1} V(\pi T, G) = \left( \frac{1}{T} \mathbb{1} \mathbb{1}^T + K(\pi_1, G) \right) \left( \sum_{i=1}^{T} e_{\pi_i} e_{\pi_i}^T + \rho L_G \right)
\]  
(82)
\[
= \left( \frac{1}{T} \mathbb{1} \mathbb{1}^T + K(\pi_1, G) \right) (T e_{\pi_1} e_{\pi_1}^T + \rho L_G)
\]  
(83)
\[
= \mathbb{1} e_{\pi_1}^T + TK(\pi_1, G)e_{\pi_1}e_{\pi_1}^T + \rho K(\pi_1, G)L_G
\]  
(84)
From Definition 1, $K(\pi_1, G)e_{\pi_1}e_{\pi_1}^T = 0$ and $\mathbb{1} e_{\pi_1}^T + \rho K(\pi_1, G)L_G = I$ implying that $V(\pi T, G)^{-1} V(\pi T, G) = I$.
Hence proved. \[\square\]

**Lemma 15.** Let $G$ be any connected graph and $\pi T \in \mathcal{U}(T, G)$. Then,
\[
\min_{j \in [n]} \{ [V(\pi T, G)^{-1}]_{jj} \} = \frac{1}{T}
\]  
(83)
**Proof.** From Definition 1, $K(\pi_1, G)$ satisfies
\[
K(\pi_1, G)L_G = \frac{1}{\rho} (I - \mathbb{1} e_{\pi_1}^T)
\]  
(84)
Observe that $1e_i^T$ is a rank 1 matrix with eigenvalue 1 and eigenvector $e_i$ and Identity matrix $I$ is of rank $n$ with all eigenvalues 1 and eigenvectors $\{e_i\}_{i=1}^n$. Hence $(I - 1e_i^T)$ is a rank $n-1$ matrix with rest nonzero eigenvalues as 1. Since the graph $G$ is connected, $\lambda_1(L_G) = 0$ and $\lambda_2(L_G) > 0$. The eigenvector corresponding to $\lambda_1(L_G)$ is $1$, the all 1 vector. 

Given $\rho > 0$, we can conclude,

$$K(\pi_1, G)L_G \geq 0 \quad \text{s.t.} \quad \text{rank}(K(\pi_1, G)L_G) = n - 1$$

(84)

Hence, in order to satisfy eq. (84), $K(\pi_1, G) \geq 0$ and $\text{rank}(K(\pi_1, G)) \geq n - 1$. By lower bounds on Rayleigh quotient we can conclude,

$$\langle e_j, (K(\pi_1, G)e_j) \rangle = |K(\pi_1, G)|_{jj} \geq 0 \quad \forall j \in [n]$$

(85)

From Lemma 14 $|K(\pi_1, G)|_{jj} = |V(\pi_T, G)^{-1}|_{jj} - \frac{1}{T}$ implying that $|V(\pi_T, G)^{-1}|_{jj} \geq \frac{1}{T}$. From Definition 1 it can be seen that $|K(\pi_1, G)|_{11} = 0$ and hence $|V(\pi_T, G)^{-1}|_{11} = \frac{T}{T}$ which concludes the proof.

**Lemma 16.** Given a connected graph $G$, the following bound holds for all the diagonal entries of $[V(\pi_T, G)^{-1}]_{ii}$ for $i \in [n]$:

$$[V(\pi_T, G)^{-1}]_{ii}^{-1} \leq 1 \cdot t_i = 0 \left( \frac{1}{3(i, G)} + \frac{1}{T} \right) + 1 \cdot t_i > 0 \max \left\{ \frac{1}{t_i + \frac{3(i, G)}{2}}, \frac{1}{t_i + \frac{T}{2}} \right\}$$

(86)

Proof. From Definition 1 of $\mathcal{J}(\cdot, G)$ and Lemma 12 Breaking the lemma statement into cases:

- **Unsampled Arms**: From Lemma 12

  $$\frac{1}{\mathcal{J}(j, G)} = \max_{t_i \in \mathcal{J}_j, \pi_1 \neq j} \left\{ \frac{1}{|V_j\{t_i \in \mathcal{G}_j, G\}^{-1}|_{jj} - \frac{1}{T}} \right\} \quad \forall j \in [n]$$

  (87)

  Thus for any unsampled arm $j$,

  $$[V(\pi_T, G)]_{jj}^{-1} \leq \left( \frac{1}{\mathcal{J}(j, G)} + \frac{1}{T} \right)$$

  (88)

- **Sampled Arms**: Since the matrix $V(\pi_T, G)$ depends only on the final sampling distribution $\{t_i\}_{i=1}^n$ rather than the sampling path $\pi_T$. Consider a sampling path such that $\pi_t \neq j$ for $t \leq T - t_j$ and $\pi_t = j$ for $T - t_j \leq t \leq T$.

  Assuming such a sampling path $\pi_T$, after $\pi_T - t_j$ samples,

  $$[V(\pi_T - t_j, G)^{-1}]_{jj} \leq \frac{1}{T} + \frac{1}{\mathcal{J}(j, G)}$$

  (89)

  Then by the Sherman-Morrison rank 1 update identity,

  $$\frac{1}{[V(\pi_T, G)^{-1}]_{jj}} = \frac{1}{[V(\pi_T - t_j, G)^{-1}]_{jj}} + t_j$$

  $$[V(\pi_T, G)^{-1}]_{jj} = \frac{1}{t_j + \frac{1}{[V(\pi_T - t_j, G)^{-1}]_{jj}}}$$

  $$\leq \frac{1}{t_j + \frac{1}{(3Gj_{jj} + T)}}$$

  Hence we have the bound on $[V(\pi_T, G)^{-1}]_{jj}$ as follows:

  $$[V(\pi_T, G)^{-1}]_{jj} \leq \max \left\{ \frac{1}{t_j + \frac{3(i, G)}{2}}, \frac{1}{t_j + \frac{T}{2}} \right\}$$

(90)

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Hager, W. (1989). Updating the Inverse of a Matrix. SIAM Rev., 31, 221-239.
Hence proved.

Lemma 17. Let \( G = ([n], E_G, A) \) and \( H = ([n], E_H, A) \) are two graphs with \( n \) nodes such that \( E_G \supset E_H \). Then, assuming invertibility, \( [V(G, T)^{-1}] \preceq [V(H, T)^{-1}] \).

Proof. Given graphs \( G = ([n], E_G) \) and \( H = ([n], E_H) \) satisfy \( E_G \supset E_H \).

The quadratic form of Laplacian for the graph \( G, H \) is given by,

\[
xL_Gx = \sum_{(i,j) \in E_G} (x_i - x_j)^2 \\
xL_Hx = \sum_{(i,j) \in E_H} (x_i - x_j)^2
\]

Since \( E_G \supset E_H \),

\[
xL_Gx \geq xL_Hx \quad \forall \ x \in \mathbb{R}^n \\
\Rightarrow L_G \succeq L_H
\]

Further, provided a sampling policy \( \pi_T \), we can say that,

\[
V(\pi_T, G) \succeq V(\pi_T, H)
\]

For the number of samples \( T \) sufficient to ensure invertibility of \( V(\pi_T, H) \), we have

\[
V(\pi_T, G)^{-1} \preceq V(\pi_T, H)^{-1}
\]

Hence proved.

Lemma 18. Let \( D \) be a graph with \( n \) nodes and \( k \) disconnected components. If each of the connected components \( \{C_i(D)\}_{i=1}^k \) is a complete graph then \( \forall \ j \in [n], \)

\[
\mathcal{J}(j, D) = \frac{|C(j, D)|}{2}
\]

Proof. Let \( D \) be a complete graph \( (k = 1), \pi_T \in \mathcal{U}(T) \) and \( \rho = 1. \) Then,

\[
V(\pi_T, G)^{-1} = \frac{1}{T} 1 1^T + K
\]

where \( 1 \in \mathbb{R}^n \) is a vector or all ones and \( K \in \mathbb{R}^{n \times n} \) is a matrix given by,

\[
K_{\pi_1 \pi_1} = 0, \quad K_{jj} = \frac{2}{n} \quad \forall j \in [n]/\{\pi_1\} \\
K_{k\pi_1} = 0, \quad K_{\pi_1 j} = 0, \quad K_{jk} = \frac{1}{n} \quad \forall j, k \in [n]/\{\pi_1\}, \ j \neq k
\]

The form of \( V(\pi_T, G)^{-1} \) in eq.\((92)\) can be verified by \( V(\pi_T, G)^{-1}V(\pi_T, G) = I. \)

The final statement of the lemma can be obtained by considering this analysis to just the nodes within a connected component of a disconnected graph \( G \) and Lemma \(\Box\)

Lemma 19. Let \( D \) be a graph with \( n \) nodes and \( k \) disconnected components. If each of the connected components \( \{C_i(D)\}_{i=1}^k \) is a line graph then \( \forall \ j \in [n], \)

\[
\mathcal{J}(j, D) > \frac{1}{|C(j, D)|}
\]
Proof. Let $D$ be a complete graph ($k = 1$), $\pi_T \in \mathcal{U}(T)$ and $\rho = 1$. Then,
\[ V(\pi_T, G)^{-1} = \frac{1}{2} \mathbb{1} \mathbb{1}^T + K \]  
where $\mathbb{1} \in \mathbb{R}^n$ is a vector or all ones and $K \in \mathbb{R}^{n \times n}$ is a matrix given by,
\[ K_{\pi_1 \pi_1} = 0, \quad K_{jj} = d(\pi_1, j) \quad \forall j \in [n]/\{\pi_1\} \]
\[ K_{\pi_1 j} = 0, \quad K_{jk} = \min\{d(\pi_1, j), d(\pi_1, k)\} \quad \forall j, k \in [n]/\{\pi_1\}, \ j \neq k \]
The form of $V(\pi_T, G)^{-1}$ in eq.(94) can be verified by $V(\pi_T, G)^{-1} V(\pi_T, G) = I$.

The final statement of the lemma can be obtained by considering this analysis to just the nodes within a connected component of a disconnected graph $G$ and Lemma 12.

Lemma 20. Let $A = ([n], E)$ be any graph and let $e \in E$ be an edge of graph $A$. Let $B = ([n], E - \{e\})$ be a subgraph of $A$ with one edge removed. Then the following holds for all non-isolated nodes $i$ in $B$:

- If $|\mathcal{C}(A)| = |\mathcal{C}(B)|$,
  \[ J(i, A) \geq J(i, B) \]
- If $|\mathcal{C}(A)| < |\mathcal{C}(B)|$,
  \[ J(i, A) \leq J(i, B) \]

Proof. From Lemma 12 for any graph $D$, $J(\cdot, \cdot)$ satisfies,
\[ \frac{1}{J(i, D)} = \frac{1}{\max_{k \in D_j, \sum_{t \in D_j} T_t} \{ [V_j(\{t_i\}_{i \in D_j}, D)^{-1}]_{jj} - [V_j(\{t_i\}_{i \in D_j}, D)^{-1}]_{kk} \}} \forall j \in [n] \]  

Case I : $|\mathcal{K}(A)| = |\mathcal{K}(B)|$

The edge set of $B$ is smaller than edge set of $A$. Hence, from Lemma $J(i, A) \geq J(i, B)$ For the case when $|\mathcal{K}(A)| < |\mathcal{K}(B)|$, then $|B| \leq |A|$. Hence since the max is over a smaller set of options, we can conclude that $J(i, A) \leq J(i, B)$.

Hence proved.

K Code Availability

The full code used for conducting experiments can be found at the following Github repository.

L Improvement Analysis

We compare the number of time steps required to eliminate arm $j$ when graph side information is provided and when it is missing ($L_G = 0$). Note that the sample complexity in Theorem 11 with $L_G = 0$ is, in order, same as sample complexity of UCB algorithm 8 22.

We compare the improvement in sample complexity by the following quantity:
\[ \mathfrak{R} = \frac{T_{\text{no graph}}}{T_{\text{graph}}} \]  

We compute this improvement factor ratio $\mathfrak{R}$ when the arm $j$ is highly competitive, weakly competitive or noncompetitive.
1. **Noncompetitive arms**: As noted in Theorem 1, the number of samples required to eliminate all arms in clusters \(N\) is \(k(G)\). In the absence of graphs, the number of minimum plays required would be \(|N|\) (one per arm). Hence there is at least a \(\frac{|N|}{k(G)}\) improvement factor for the case of noncompetitive arms.

2. **Weakly competitive arms**: The improvement factor for weakly competitive arms heavily depends on the underlying graph of the individual clusters. With the help of graphs, the number of samples required for eliminating weakly competitive arms is

\[
\max \left\{ \max_{l \in W \cap C} \mathcal{I}(l, G), |W \cap C| \right\}
\]

The number of samples required for eliminating the same number of arms without graphs is,

\[
T_{\text{no graph}} = \sum_{W} \frac{1}{\Delta_j^2} \left[ 448R^2 \log \left( \frac{224R^2 \sqrt{2n^2}}{\delta^2 \Delta_j^2} \right) \right] = O \left( \sum_{W} \frac{1}{\Delta_j^2} \log \left( \frac{224R^2 \sqrt{2n^2}}{\delta^2 \Delta_j^2} \right) \right)
\]

(97)

Using the definition of weakly competitive arms \(W\), the ratio \((j)\) can be written as,

\[
\mathfrak{R} = \sum_{W} \frac{1}{\Delta_j^2} \left[ 448R^2 \log \left( \frac{224R^2 \sqrt{2n^2}}{\delta^2 \Delta_j^2} \right) \right] \leq O \left( \sum_{W} \frac{\mathcal{I}(j, D)}{2} \log \left( \frac{\mathcal{I}(j, D)}{\delta} \right) \right)
\]

As can be seen the improvement is a direct consequence of the minimum influence factor \(\mathcal{I}(j, D)\). The highest this ratio \((j)\) can go is,

\[
1 \leq \mathfrak{R} \leq O \left( \frac{k}{4} \log \left( \frac{k}{\delta} \right) \right)
\]

(98)

which is in the case of completely connected clusters.

3. **Highly competitive arms**: The ratio of samples required for arm \(j \in m\) with and without graph can be given by,

\[
\mathfrak{R} = \frac{1}{\Delta_j^2} \left[ 448R^2 \log \left( \frac{224R^2 \sqrt{2n^2}}{\delta^2 \Delta_j^2} \right) \right] \left( \frac{1}{\Delta_j^2} \left[ 448R^2 \log \left( \frac{224R^2 \sqrt{2n^2}}{\delta^2 \Delta_j^2} \right) + \rho \epsilon \right] + \mathcal{I}(j, G) \right)
\]

\[
\approx 1 + O \left( \mathcal{I}(j, G) - \frac{\rho \epsilon}{\Delta_j^2} \right)
\]

(99)

A net positive impact can be guaranteed with,

\[
\mathcal{I}(j, G) - \frac{\rho \epsilon}{\Delta_j^2} > 0
\]

(100)

The ratio \((j) > 1\) if \(\rho \epsilon < \mathcal{I}(j, G)\Delta_j^2\).

This bound shows an interesting trade-off, between the accuracy on the graph information and the graph parameter \(\mathcal{I}(j, D)\) which relies on the density of the graph. In summary, the factor improvement is \(O(k)\) for easy arms and \(> 1\) for highly competitive arms and the set of medium arms has an improvement factor in between \(O(k)\) and \(> 1\), highly dependent on the \(\mathcal{I}(\cdot, \cdot)\).