Abstract

We consider a stochastic contextual bandit problem where the dimension $d$ of the feature vectors is potentially large, however, only a sparse subset of features of cardinality $s_0 \ll d$ affect the reward function. Essentially all existing algorithms for sparse bandits require a priori knowledge of the value of the sparsity index $s_0$. This knowledge is almost never available in practice, and misspecification of this parameter can lead to severe deterioration in the performance of existing methods. The main contribution of this paper is to propose an algorithm that does not require prior knowledge of the sparsity index $s_0$ and establish tight regret bounds on its performance under mild conditions. We also comprehensively evaluate our proposed algorithm numerically and show that it consistently outperforms existing methods, even when the correct sparsity index is revealed to them but is kept hidden from our algorithm.

Keywords: Contextual Bandit, High-dimensional Statistics, Lasso

1. Introduction

In classical multi-armed bandits (MAB), one of the arms is pulled in each round and a reward corresponding to the chosen arm is revealed to the decision-making agent. The rewards are, typically, independent and identically distributed samples from an arm-specific distribution. The goal of the agent is to devise a strategy for pulling arms that maximizes cumulative rewards, suitably balancing between exploration and exploitation. Linear contextual bandits (Abe and Long, 1999; Auer, 2002; Chu et al., 2011) and generalized linear contextual bandits (Filippi et al., 2010; Li et al., 2017) are more recent important extensions of the basic MAB setting, where each arm $a$ is associated with a known feature vector $x_a \in \mathbb{R}^d$, and the expected payoff of the arm is a (typically, monotone increasing) function of the inner product $x_a^\top \beta^*$ for a fixed and unknown parameter vector $\beta^* \in \mathbb{R}^d$. Unlike the traditional MAB problem, pulling any arm provides some information about the unknown parameter vector, and hence, insight into the average reward of the other arms. These contextual bandit algorithms are applicable in a variety of problem settings, such as recommender systems, assortment selection in online retail, and healthcare analytics (Li et al.,
Oh, Iyengar and Zeevi (2010; Oh and Iyengar, 2019; Tewari and Murphy, 2017), where the contextual information can be used for personalization and generalization.

In most application domains highlighted above, the feature space is high-dimensional \((d \gg 1)\), yet typically only a small subset of the features influence the expected reward. That is, the unknown parameter vector is sparse with only elements corresponding to the relevant features being non-zero, i.e., the sparsity index \(s_0 = \|\beta^*\|_0 \ll d\), where the zero norm \(\|x\|_0\) counts non-zero entries in the vector \(x\). There is an emerging body of literature on contextual bandit problems with sparse linear reward functions (Abbasi-Yadkori et al., 2012; Gilton and Willett, 2017; Bastani and Bayati, 2020; Wang et al., 2018; Kim and Paik, 2019) which propose methods to exploit the sparse structure under various conditions. However, there is a crucial shortcoming in almost all of these approaches: the algorithms require prior knowledge of the sparsity index \(s_0\), information that is almost never available in practice. In the absence of such knowledge, the existing algorithms fail to fully leverage the sparse structure, and their performance does not guarantee the improvements in dimensionality-dependence which can be realized in the sparse problem setting (and can lead to extremely poor performance if \(s_0\) is underspecified). The purpose of this paper is to demonstrate that a relatively simple contextual bandit algorithm that exploits \(\ell_1\)-regularized regression using Lasso (Tibshirani, 1996) in a sparsity-agnostic manner, is provably near-optimal insofar as its regret performance (under suitable regularity). Our contributions are as follows:

(a) We propose the first general\(^1\) sparse bandit algorithm that does not require prior knowledge of the sparsity index \(s_0\).

(b) We establish that the regret bound of our proposed algorithm is \(O(s_0 \sqrt{T \log(dT)})\) for the two-armed case, which affords the most accessible exposition of the key analytical ideas. (Extensions to the general \(K\)-armed case are discussed later.) The regret bound scale in \(s_0\) and \(d\) matches the equivalent terms in the offline Lasso results (see the discussions in Section 5.2).

(c) We comprehensively evaluate our algorithm on numerical experiments and show that it consistently outperforms existing methods, even when these methods are granted prior knowledge of the correct sparsity index (and can greatly outperform them if this information is misspecified).

The salient feature of our algorithm is that it does not rely on forced sampling which was used by almost all previous work, e.g., Bastani and Bayati (2020); Wang et al. (2018); Kim and Paik (2019), to satisfy certain regularity of the empirical Gram matrix. Forced sampling requires prior knowledge of \(s_0\) because such schemes, the key ideas of which go back to Goldenshluger and Zeevi (2013), need to be fine-tuned using the correct sparsity index. (See further discussions in Section 2.2.)

The rest of the paper is organized as follows. In Section 2, we review the related literature and discuss the reason why the previously proposed methods require the knowledge of the sparsity index \(s_0\). In Section 3, we present the problem formulation. Section 4 describes our proposed algorithm. In Section 5, we describe the challenges when the sparsity information

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\(^1\) Carpentier and Munos (2012) do not require to know sparsity, but both their algorithm and analysis are limited to the fixed \(\ell_2\) unit ball arm set. See more discussions in Section 2.
is unknown, and establish an upper bound on the cumulative regret for the two-armed sparse bandits. Section 6 contains the numerical experiments for the two-armed sparse bandits. In Section 7, we extend our analysis and numerical evaluations to the $K$-armed sparse bandits. Section 8 presents discussions and future directions. The complete proofs and additional numerical results are provided in the appendix.

2. Related Work

2.1 Review

Linear bandits and generalized linear bandits have been widely studied (Abe and Long, 1999; Auer, 2002; Dani et al., 2008; Rusmevichientong and Tsitsiklis, 2010; Abbasi-Yadkori et al., 2011; Filippi et al., 2010; Chu et al. 2011; Agrawal and Goyal, 2013; Li et al., 2017; Kveton et al., 2020). However, when ported to the high-dimensional contextual bandit setting, these strategies have difficulty exploiting sparse structure in the unknown parameter vector, and hence may incur regret proportional to the full ambient dimension $d$ rather than the sparse set of features of cardinality $s_0$. To exploit spare structure, Abbasi-Yadkori et al. (2012) propose a framework to construct high probability confidence sets for online linear prediction and establish a regret bound of $\tilde{O}(\sqrt{s_0 dT})$, where $\tilde{O}$ hides logarithmic terms, when the sparsity index $s_0$ is known. Furthermore, their algorithm is not computationally efficient; an implementable version of their framework is not yet known (Section 23.5 in Lattimore and Szepesvári 2019). It is worth noting that the $\sqrt{d}$ dependence in the regret bound is unavoidable unless additional assumptions are imposed; see Theorem 24.3 in Lattimore and Szepesvári (2019). Gilton and Willett (2017) adapt Thompson sampling (Thompson, 1933) to sparse linear bandits; however, they also assume a priori knowledge of a small superset of the support for the parameter.

Bastani and Bayati (2020) address the contextual bandit problem with high-dimensional features using Lasso (Tibshirani, 1996) to estimate the parameter of each arm separately. To ensure compatibility of the empirical Gram matrices, they adapt the forced-sampling technique in Goldenshluger and Zeevi (2013) which is now tuned using the (a priori known) sparsity index, and is implemented for each arm at predefined time points. They establish a regret bound of $O(Ks_0^2[\log d + \log T]^2)$ where $K$ is the number of arms. Note that they invoke several additional assumptions introduced in Goldenshluger and Zeevi (2013), including a margin condition that ensures that the density of the context distribution is bounded near the decision boundary, and arm-optimality which assumes a gap between the optimal and sub-optimal arms exists with some positive probability. In the same problem setting, Wang et al. (2018) propose an algorithm which uses forced-sampling along with the minimax concave penalty (MCP) estimator (Zhang, 2010) and improve the regret bound to $O(Ks_0^2[s_0 + \log d]\log T)$. Note that Bastani and Bayati (2020) and Wang et al. (2018) achieve a poly-logarithmic dependence on $T$ in the regret, exploiting the arm optimality condition which assumes a gap between the optimal and sub-optimal arms exists with some probability. Since we do not assume such “separability” between arms, poly-logarithmic dependence on $T$ is not attainable in our problem setting. Kim and Paik (2019) extend

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2. The regret bounds in both Bastani and Bayati (2020) and Wang et al. (2018) have additional dependence $O(1/p^2)$ where $p_*$ is the arm optimality lower bounding probability. Hence, in the worse case, the regret bounds have additional $O(K^3)$ dependence.
the Lasso bandit (Bastani and Bayati, 2020) to linear bandit settings and propose a different approach to address the non-compatibility of the empirical Gram matrices by using a doubly-robust technique (Bang and Robins, 2005) that originates with the missing data (imputation) literature. They achieve $O(s_0\sqrt{T} \log(dT))$ regret.

All of the aforementioned algorithms require that the learning agent know the sparsity index $s_0$ of the unknown parameter (or a non-trivial upper-bound on sparsity which is strictly less than $d$).\footnote{Besides sparsity, some algorithms require further knowledge, such as arm optimality lower bounding probability (Bastani and Bayati 2020; Wang et al. 2018), which is also not readily available in practice.} That is, only when the algorithm knows $s_0$, it can guarantee the regret bounds mentioned above. Otherwise, the regret bounds would scale polynomially with $d$ instead of $s_0$ or potentially scale linearly with $T$. To our knowledge, the only work in sparse bandits which does not require this prior knowledge of sparsity is the work by Carpentier and Munos (2012) although their algorithm still requires to know the $\ell_2$-norm of the unknown parameter. Their analysis uses a non-standard definition of noise and is restricted to the case where the set of arms is the $\ell_2$ unit ball and fixed over time, a structure they exploit in a significant manner, and which limits the scope of their algorithm.

### 2.2 Why do existing sparse bandit algorithms require prior knowledge of the sparsity index?

The primary reason that a priori knowledge of sparsity index $s_0$ is assumed throughout most of the literature is, roughly speaking, to ensure suitable “size” of the confidence bounds and concentration. For example, Abbasi-Yadkori et al. (2012) require the parameter $s_0$ to explicitly construct a high probability confidence set with its radius proportional to $s_0$ rather than $d$. The recently proposed bandit algorithms of Bastani and Bayati (2020); Kim and Paik (2019) and the variant with MCP estimator in Wang et al. (2018) employ a logic that is similar in spirit (though different in execution). Specifically, the compatibility condition is assumed to hold only for the theoretical Gram matrix, and the empirical Gram matrix may not satisfy such condition (the difficulty in controlling that is due to the non-i.i.d. adapted samples of the feature variables). As a remedy to this issue, Bastani and Bayati (2020) and Wang et al. (2018) utilize the forced-sampling technique of Goldenshluger and Zeevi (2013) to obtain a “sufficient” number of i.i.d. samples and use them to show that the empirical Gram matrices concentrate in the vicinity of the theoretical Gram matrix, and hence, satisfy the compatibility condition after a sufficient amount of forced-sampling. The forced-sampling duration needs to be predefined and scales at least polynomially in the sparsity index $s_0$ to ensure concentration of the Gram matrices. That is, if the algorithm does not know $s_0$, the forced-sampling duration will have to scale polynomially in $d$. Kim and Paik (2019) propose an alternative to forced sampling that builds on doubly-robust techniques used in the missing data literature; however, their algorithm involves random arm selection with a probability that is calibrated using $s_0$, and initial uniform sampling whose duration requires knowledge of $s_0$ and scales polynomially with $s_0$ in order to establish their regret bounds. The sensitivity to the sparsity index specification is also evident in cases where its value is misspecified, which may result in severe deterioration in the performance of the algorithms (see further discussions in Section 5.1).
The key observation in our analysis is that i.i.d. samples, which are the key output of the forced samplings scheme, are, in fact, not required under some mild regularity conditions. We show that the empirical Gram matrix satisfies the required regularity after a sufficient number of rounds, provided the theoretical Gram matrix is also regular; the details of this analysis are in Section 5. Numerical experiments support these findings, and moreover, demonstrate that the performance of our proposed algorithm can be superior to forced-sampling-based schemes that are tuned with foreknowledge of the sparsity index \( s_0 \).

3. Preliminaries

3.1 Notation

For a vector \( x \in \mathbb{R}^d \), we use \( \|x\|_1 \) and \( \|x\|_2 \) to denote its \( \ell_1 \)-norm and \( \ell_2 \) norm respectively, the notation \( \|x\|_0 \) is reserved for the cardinality of the set of non-zero entries of that vector. The minimum and maximum singular values of a matrix \( V \) are written as \( \lambda_{\text{min}}(V) \) and \( \lambda_{\text{max}}(V) \) respectively. For two symmetric matrices \( V \) and \( W \) of the same dimensions, \( V \succ W \) means that \( V - W \) is positive semi-definite. For a positive integer \( n \), we define \( [n] = \{1, \ldots, n\} \). For a real-valued differentiable function \( f \), we use \( \dot{f} \) to denote its first derivative.

3.2 Generalized Linear Contextual Bandits

We consider the stochastic generalized linear bandit problem with \( K \) arms. Let \( T \) be the problem horizon, namely the number of rounds to be played. In each round \( t \in [T] \), the learning agent observes a context consisting of a set of \( K \) feature vectors \( X_t = \{X_{t,i} \in \mathbb{R}^d \mid i \in [K]\} \), where the tuple \( X_t \) is drawn i.i.d. over \( t \in [T] \) from an unknown joint distribution with probability density \( p_X \) with respect to the Lebesgue measure. Note that the feature vectors for different arms are allowed to be correlated. Each feature vector \( X_{t,i} \) is associated with an unknown stochastic reward \( Y_{t,i} \in \mathbb{R} \). The agent then selects one arm, denoted by \( a_t \in [K] \) and observes the reward \( Y_t := Y_{t,a_t} \) corresponding to the chosen arm’s feature \( X_t := X_{t,a_t} \) as a bandit feedback. The policy consists of the sequence of actions \( \pi = \{a_t: t = 1, 2, \ldots\} \) and is non-anticipating, namely each action only depends on past observations and actions.

In this work, we consider the generalized linear model (GLM) in which there is an unknown parameter \( \beta^* \in \mathbb{R}^d \) and a fixed increasing function \( \mu : \mathbb{R} \to \mathbb{R} \) (also known as inverse link function) such that the reward \( Y_{t,i} \) of arm \( i \) is

\[
Y_{t,i} = \mu(X_{t,i}^\top \beta^*) + \epsilon_{t,i}
\]

where each \( \epsilon_{t,i} \) is an independent zero-mean noise. Therefore, \( \mathbb{E}[Y_{t,i} | X_{t,i} = x] = \mu(x^\top \beta^*) \) for all \( i \in [K] \) and \( t \in [T] \). Widely used examples for \( \mu \) are \( s_\mu(z) = z \) which corresponds to the linear model, and \( \mu(z) = 1/(1 + e^{-z}) \) which corresponds to the logistic model. The parameter \( \beta^* \) and the feature vectors \( \{x_{t,i}\} \) are potentially high-dimensional, i.e. \( d \gg 1 \), but \( \beta^* \) is sparse, that is, the number of non-zero elements in \( \beta^* \), \( s_0 = \|\beta^*\|_0 \ll d \). It is important to note that the agent does not know \( s_0 \) or the support of \( \beta^* \).

We assume that there is an increasing sequence of sigma fields \( \{\mathcal{F}_t\} \) such that each \( \epsilon_{t,i} \) is \( \mathcal{F}_t \)-measurable with \( \mathbb{E}[\epsilon_{t,i} | \mathcal{F}_{t-1}] = 0 \). In our problem, \( \mathcal{F}_t \) is the sigma-field generated by
random variables of chosen actions \( \{a_1, ..., a_t\} \), their features \( \{X_1, ..., X_t\} \), and the corresponding rewards \( \{Y_1, ..., Y_t\} \). We assume the noise \( \epsilon_t \) is sub-Gaussian with parameter \( \sigma \), where \( \sigma \) is a positive absolute constant, i.e., \( \mathbb{E}[e^{\alpha \epsilon_t}] \leq e^{\alpha^2 \sigma^2/2} \) for all \( \alpha \in \mathbb{R} \). In practice, for bounded reward \( Y_{t,i} \), the noise \( \epsilon_{t,i} \) is also bounded and hence satisfies the sub-Gaussian assumption with an appropriate \( \sigma \) value.

The agent’s goal is to maximize the cumulative expected reward \( \mathbb{E}\left[ \sum_{t=1}^{T} \mu(X_{t,a_t}^{\top} \beta^*) \right] \) over \( T \) rounds. Let \( a^*_t = \arg \max_{i \in [K]} \mu(X_{t,i}^{\top} \beta^*) \) denote the optimal arm for each round \( t \). Then, the expected cumulative regret of policy \( \pi = \{a_1, ..., a_T\} \) is defined as

\[
R_\pi(T) := \sum_{t=1}^{T} \mathbb{E}\left[ \mu(X_{t,a^*_t}^{\top} \beta^*) - \mu(X_{t,a_t}^{\top} \beta^*) \right].
\]

Hence, maximizing the expected cumulative rewards of policy \( \pi \) over \( T \) rounds is equivalent to minimizing the cumulative regret \( R_\pi(T) \). Note that all the expectations and probabilities throughout the paper are with respect to feature vectors and noise unless explicitly stated otherwise.

### 3.3 Lasso for Generalized Linear Models

Consider an offline setting where we have samples \( Y_1, ..., Y_n \) and corresponding features \( X_1, ..., X_n \). The log-likelihood function of \( \beta \) under the canonical GLM is

\[
\log \mathcal{L}_n(\beta) := \sum_{j=1}^{n} \left[ \frac{Y_j X_j^{\top} \beta - m(X_j^{\top} \beta)}{g(\eta)} - h(Y_j, \eta) \right].
\]

Here, \( \eta \in \mathbb{R}^+ \) is a known scale parameter, \( m(\cdot) \), \( g(\cdot) \) and \( h(\cdot) \) are normalization functions, and \( m(\cdot) \) is infinitely differentiable with the first derivative

\[
m(x^{\top} \beta^*) = \mathbb{E}[Y|X = x] = \mu(x^{\top} \beta^*).
\]

The Lasso (Tibshirani, 1996) estimate for the GLM can be defined as

\[
\hat{\beta}_n \in \arg \min_{\beta} \left\{ \ell_n(\beta) + \lambda \| \beta \|_1 \right\}
\]

where \( \ell_n(\beta) := -\frac{1}{n} \sum_{j=1}^{n} \left[ Y_j X_j^{\top} \beta - m(X_j^{\top} \beta) \right] \) and \( \lambda \) is a penalty parameter. Lasso is known to be an efficient (offline) tool for estimating the high-dimensional linear regression parameter. The “fast convergence” property of Lasso is guaranteed when the above data are i.i.d. and when the observed covariates are not “highly correlated.” The restricted eigenvalue condition (Bickel et al., 2009; Raskutti et al., 2010), the compatibility condition (Van De Geer and Bühlmann, 2009), and the restricted isometry property (Candes and Tao, 2007) have all been used to ensure that such high correlations are avoided. In sequential learning settings, however, these conditions are often violated because the observations are adapted to the past, and the feature variables of the chosen arms converge to a small region of the feature space as the learning agent updates its arm selection policy.
4. Proposed Algorithm

Our proposed **Sparsity-Agnostic (SA) Lasso Bandit** algorithm for high-dimensional GLM bandits is summarized in Algorithm 1. As the name suggests, our algorithm does not require prior knowledge of the sparsity index $s_0$. It relies on Lasso for parameter estimation, and does not explicitly use exploration strategies or forced-sampling. Instead, in each round, we choose an arm which maximizes the inner product of a feature vector and the Lasso estimate. After observing the reward, we update the regularization parameter $\lambda_t$ and update the Lasso estimate $\hat{\beta}_t$ which minimizes the penalized negative log-likelihood function defined in (1).

**SA Lasso Bandit** requires only one input parameter $\lambda_0$. We show in Section 5 that $\lambda_0 = 2\sigma x_{\text{max}}$ where $x_{\text{max}}$ is a bound the $\ell_2$-norm of the feature vectors $X_{t,i}$. Thus, $\lambda_0$ does not depend on the sparsity index $s_0$ or the underlying parameter $\beta^*$. (Note that, in comparison, Kim and Paik (2019) require three tuning parameters, and Bastani and Bayati (2020) and Wang et al. (2018) require four tuning parameters, most of which are functions of the unknown sparsity index $s_0$.) It is worth noting that tuning parameters, while helping achieve low regret, are challenging to specify in online learning settings. Therefore, our proposed algorithm is practical and easy to implement.

**Algorithm 1** SA Lasso Bandit

1: **Input parameter**: $\lambda_0$
2: for all $t = 1$ to $T$
3: \hspace{1em} Observe $X_{t,i}$ for all $i \in [K]$
4: \hspace{1em} Compute $a_t = \arg \max_{i \in [K]} X_{t,i}^T \hat{\beta}_t$
5: \hspace{1em} Pull arm $a_t$ and observe $Y_t$
6: \hspace{1em} Update $\lambda_t \leftarrow \lambda_0 \sqrt{\frac{4 \log t + 2 \log d}{t}}$
7: \hspace{1em} Update $\hat{\beta}_{t+1} \leftarrow \arg \min_{\beta} \{ \ell_t(\beta) + \lambda_t \| \beta \|_1 \}$
8: end for

**Discussion of the algorithm.** Algorithm 1 may appear to be an **exploration-free** greedy algorithm (e.g., Bastani et al. 2017), but this is not the case. To better see this, recall that upper-confidence bound (UCB) algorithms construct a high-probability confidence ellipsoid around a greedy estimate and choose the parameter value that maximizes the reward. Once the UCB estimate is chosen, the action selection is greedy with respect to the parameter estimate. The UCB algorithms carefully control the size of the confidence ellipsoid to ensure convergence, thus, exploration is loosely equivalent to regularizing the parameter estimate. The algorithm we propose also computes the parameter estimate by **regularizing** the MLE with a sparsifying norm, and then, as in UCB, takes a greedy action with respect to this regularized parameter estimate. We adjust the penalty associated with the sparsifying norm over time at a suitable rate in order to ensure that our estimate is consistent as we collect more samples. (This adjustment and specification do not require knowledge of sparsity $s_0$.) An inadequate choice of this penalty parameter would lead to large regret, which is analogous to poor choice of confidence widths in UCB.

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4. Likewise, in Thompson sampling (Thompson, 1933), the agent chooses the greedy action for the sampled parameter.
5. Regret Analysis

5.1 Regularity Condition

In this section, we establish an upper bound on the expected regret of SA LASSO BANDIT for the two-armed \((K = 2)\) generalized linear bandits. We focus on the two-arm case primarily for clarity and accessibility of key analysis ideas, and later illustrate how this analysis extends to the \(K\)-armed case with \(K \geq 3\) under suitable regularity (see Section 7).

We first provide a few definitions and assumptions used throughout the analysis, starting with assumptions standard in the (generalized) linear bandit literature.

**Assumption 1 (Feature set and parameter)** There exists a positive constant \(x_{\text{max}}\) such that \(\|x\|_2 \leq x_{\text{max}}\) for all \(x \in X_t\) and all \(t\), and a positive constant \(b\) such that \(\|\beta^*\|_2 \leq b\).

**Assumption 2 (Link function)** There exist \(\kappa_0 > 0\) and \(\kappa_1 < \infty\) such that the derivative \(\hat{\mu}(\cdot)\) of the link function satisfies \(\kappa_0 \leq \hat{\mu}(x^\top \beta) \leq \kappa_1\) for all \(x\) and \(\beta\).

Clearly for the linear link function, \(\kappa_0 = \kappa_1 = 1\). For the logistic link function, we have \(\kappa_1 = 1 / 4\).

**Definition 1 (Active set and sparsity index)** The active set \(S_0 := \{j : \beta_j^* \neq 0\}\) is the set of indices \(j\) for which \(\beta_j^*\) is non-zero, and the sparsity index \(s_0 = |S_0|\) denotes the cardinality of the active set \(S_0\).

For the active set \(S_0\), and an arbitrary vector \(\beta \in \mathbb{R}^d\), we can define
\[
\beta_{j,S_0} := \beta_j 1\{j \in S_0\}, \quad \beta_{j,S^c_0} := \beta_j 1\{j \notin S_0\}.
\]

Thus, \(\beta_{S_0} = [\beta_{1,S_0}, ..., \beta_{d,S_0}]^\top\) has zero elements outside the set \(S_0\) and the components of \(\beta_{S^c_0}\) can only be non-zero in the complement of \(S_0\). Let \(C(S_0)\) denote the set of vectors
\[
C(S_0) := \{\beta \in \mathbb{R}^d \mid \|\beta_{S_0}\|_1 \leq 3\|\beta_{S_0}\|_1\}.
\]  \(2\)

Let \(X \in \mathbb{R}^{K \times d}\) denote the design matrix where each row is a feature vector for an arm. (Although we focus on \(K = 2\) case in this section, the definitions and the assumptions introduced here also apply to the case of \(K \geq 3\).) Then, in keeping with the previous literature on sparse estimation and specifically on sparse bandits (Bastani and Bayati, 2020; Wang et al., 2018; Kim and Paik, 2019), we assume that the following compatibility condition is satisfied for the theoretical Gram matrix \(\Sigma := \frac{1}{K} \mathbb{E}[X^\top X]\).

**Assumption 3 (Compatibility condition)** For active set \(S_0\), there exists compatibility constant \(\phi_0^2 > 0\) such that
\[
\phi_0^2 \|\beta_{S_0}\|_2^2 \leq s_0 \beta^\top \Sigma \beta \quad \text{for all } \beta \in C(S_0).
\]

We add to this the following mild assumption that is more specific to our analysis.

**Assumption 4 (Relaxed symmetry)** For a joint distribution \(p_X\), there exists \(\nu < \infty\) such that \(\frac{p_X(-x)}{p_X(x)} \leq \nu\) for all \(x\).
Discussion of the assumptions. Assumptions 1 and 2 are the standard regularity assumptions used in the GLM bandit literature (Filippi et al., 2010; Li et al., 2017; Kveton et al., 2020). It is important to note that unlike the existing GLM bandit algorithms which explicitly use the value of $\kappa_0$, our proposed algorithm does not use $\kappa_0$ or $\kappa_1$ — this information is only needed to establish the regret bound. The compatibility condition in Assumption 3 is analogous to the standard positive-definite assumption on the Gram matrix for the ordinary least squares estimator for linear models but is less restrictive. The compatibility condition ensures that truly active components of the parameter vector are not “too correlated.” As mentioned above, the compatibility condition is a standard assumption in the sparse bandit literature (Bastani and Bayati, 2020; Wang et al., 2018; Kim and Paik, 2019). Assumption 4 states that the joint distribution $p_X$ can be skewed but this skewness is bounded. Obviously, if $p_X$ is symmetrical, we have $\nu = 1$. Assumption 4 is satisfied for a large class of continuous and discrete distributions, e.g., elliptical distributions including Gaussian and truncated Gaussian distributions, multi-dimensional uniform distribution, and Rademacher distribution.

5.2 Regret Bound for SA Lasso Bandit

Theorem 1 (Regret bound for two arms) Suppose $K = 2$ and Assumptions 1-4 hold. Let $\lambda_0 = 2\sigma x_{\max}$. Then the expected cumulative regret of the SA LASSO BANDIT policy $\pi$ over horizon $T \geq 1$ is upper-bounded by

$$R_\pi(T) \leq 4\kappa_1 + \frac{4\kappa_1 x_{\max} b(\log(2d^2) + 1)}{C_0(s_0)^2} + \frac{32\kappa_1 \nu \sigma x_{\max} s_0 \sqrt{T \log(dT)}}{\kappa_0 \phi_0^2}$$

where $C_0(s_0) = \min\left(\frac{1}{12}, \frac{\phi_0^2}{256 s_0 \nu x_{\max}}\right)$.

Discussion of Theorem 1. In terms of key problem primitives, Theorem 1 establishes $O(s_0 \sqrt{T \log(dT)})$ regret without any prior knowledge on $s_0$. The bound shows that the regret of our algorithm grows at most logarithmically in feature dimension $d$. The key takeaway from this theorem is that SA LASSO BANDIT is sparsity-agnostic and is able to achieve “correct” dependence on parameters $d$ and $s_0$. That is, based on the offline Lasso convergence results under the compatibility condition (e.g., Theorem 6.1 in Bühlmann and Van De Geer 2011), we believe that the dependence on $d$ and $s_0$ in Theorem 1 is best possible.5

The regret bound in Theorem 1 is tighter than the previously known bound in the same problem setting (Kim and Paik, 2019) although direct comparison is not immediate, given the difference in assumptions involved — compared to Kim and Paik (2019), we require Assumption 4 whereas they assume the sparsity index $s_0$ is known. Having said that, the numerical experiments in Section 6 support our theoretical claims and provide additional evidence that our proposed algorithm compares very favorably to other existing methods.

5. Since the horizon $T$ does not exist in offline Lasso results, it is not straightforward to see whether $\sqrt{T}$ dependence can be improved comparing only with the offline Lasso results. Clearly, without an additional assumption on the separability of the arms, we know that poly-logarithmic scalability in $T$ is not feasible. We briefly discuss our conjecture in comparison with the lower bound result in the non-sparse linear bandits in Section 5.4 where we discuss the regret bound under the RE condition.
(which are tuned with the knowledge of the correct $s_0$), and moreover, the performance is not sensitive to the assumptions that were imposed primarily for technical tractability purposes. Note that the input parameter $\lambda_0 = 2\sigma x_{\text{max}}$ depends on $\sigma$ and $x_{\text{max}}$ which are parameters required by all parametric bandit methods, and hence our algorithm does not require any additional information.

As mentioned earlier, the previous work on sparse bandits (Bastani and Bayati, 2020; Wang et al., 2018; Kim and Paik, 2019) require the knowledge of the sparsity index $s_0$. In the absence of such knowledge, if sparsity is underspecified, then these algorithms would suffer a regret linear in $T$. On the other hand, if the sparsity is overspecified, the regret of these algorithms may scale with $d$ instead of $s_0$. Our proposed algorithm does not require such prior knowledge, hence there is no risk of under-specification or over-specification, and yet our analysis provides a sharper regret guarantee. Furthermore, our result also suggests that even when the sparsity is known, random sampling to satisfy the compatibility condition, invoked by all existing sparse bandit algorithms to date, can be wasteful since said conditions may be already satisfied even in the absence of such sampling. This finding is also supported by the numerical experiments in Section 6 and Section 7.2. We provide the outline of the proof and the key lemmas in the following section.

5.3 Challenges and Proof Outlines

There are two essential challenges that prevent us from fully benefiting from the fast convergence property of Lasso:

(i) The samples induced by our bandit policy are not i.i.d., therefore the standard Lasso oracle inequality does not hold.

(ii) Empirical Gram matrices do not necessarily satisfy the compatibility condition even under Assumption 3. This is because the selected feature variables for which the rewards are observed do not provide an “even” representation for the entire distribution.

To resolve (i), we provide a Lasso oracle inequality for the GLM with non-i.i.d. adapted samples under the compatibility condition in Lemma 1. For (ii), we aim to provide a remedy without using the knowledge of sparsity or without using i.i.d. samples. Hence, this poses a greater challenge. In Section 5.3.2, we address this issue by showing that the empirical Gram matrix behaves “nicely” even when we choose arms adaptively without deliberate random sampling. In particular, we show that adapted Gram matrices can be controlled by the theoretical Gram matrix and the empirical Gram matrix concentrates properly around the adapted Gram matrix as we collect more samples. Connecting this matrix concentration to the corresponding compatibility constants, we show that the empirical Gram matrix satisfies the compatibility condition with high probability.

5.3.1 Lasso Oracle Inequality for GLM with Non-i.i.d. Data.

We present an oracle inequality for the Lasso estimator for the GLM with non-i.i.d. data. This is a generalization of the standard Lasso oracle inequality (Bühlmann and Van De Geer, 2011; Van de Geer, 2008) that allows adapted sequences of observations. This is also a generalization of Proposition 1 in Bastani and Bayati (2020) to the GLM. This convergence result may be of independent interest.
Lemma 1 (Oracle inequality) Let \( \{X_\tau : \tau \in [t]\} \) be an adapted sequence such that each \( X_\tau \) may depend on \( \{X_s : s < \tau\} \). Suppose the compatibility condition holds for the empirical covariance matrix \( \hat{\Sigma}_t = \frac{1}{t} \sum_{\tau=1}^{t} X_\tau X_\tau^T \) with active set \( S_0 \) and compatibility constant \( \phi_t \).

For \( \delta \in (0, 1) \), define the regularization parameter
\[
\lambda_t := 2\sigma_{x_{\max}} \sqrt{\frac{2[\log(2/\delta) + \log d]}{t}}.
\]

Then with probability at least \( 1 - \delta \), the Lasso estimate \( \hat{\beta}_t \) defined in (1) satisfies
\[
\|\hat{\beta}_t - \beta^*\|_1 \leq \frac{4s_0 \lambda_t}{\kappa_0 \phi_t^2}.
\]

Note that here we assume that the compatibility condition holds for the empirical Gram matrix \( \hat{\Sigma}_t \). In the next section, we show that this holds with high probability. The Lasso oracle inequality holds without further assumptions on the underlying parameter \( \beta^* \) or its support. Therefore, if we show that \( \hat{\Sigma}_t \) satisfies the compatibility condition without the knowledge of \( s_0 \), then the remainder of the result does not require this knowledge as well.

### 5.3.2 Compatibility Condition and Matrix Concentration.

We first define the generic compatibility constant for matrix \( M \) with respect to \( S_0 \).

**Definition 2** The compatibility constant of \( M \) over \( S_0 \) is
\[
\phi^2(M, S_0) := \min_\beta \left\{ \frac{s_0 \beta^T M \beta}{\|\beta_{S_0}\|_1^2} : \|\beta_{S_c}\|_1 \leq 3 \|\beta_{S_0}\|_1 \neq 0 \right\}.
\]

Hence, it suffices to show \( \phi^2(M, S_0) > 0 \) in order to show that matrix \( M \) satisfies the compatibility condition. Although one can define a compatibility constant with respect to any index set, in this section, we will focus on the active index set \( S_0 \) of the parameter \( \beta^* \). Also, note that the constant 3 in the inequality is for ease of exposition and may be replaced by a different value, but then one has to adjust the choice of the regularization parameter accordingly. Now, under Assumption 3, the theoretical Gram matrix \( \Sigma = \frac{1}{K} \mathbb{E}[X^T X] \) satisfies the compatibility condition i.e., \( \phi^2_0 = \phi^2(\Sigma, S_0) > 0 \).

**Definition 3** We define the adapted Gram matrix as \( \Sigma_t := \frac{1}{t} \sum_{\tau=1}^{t} \mathbb{E}[X_{\tau} X_{\tau}^T | \mathcal{F}_{\tau-1}] \) and the empirical Gram matrix as \( \hat{\Sigma}_t := \sum_{\tau=1}^{t} X_{\tau} X_{\tau}^T \).

For each term \( \mathbb{E}[X_{\tau} X_{\tau}^T | \mathcal{F}_{\tau-1}] \) in \( \Sigma_t \), the past observations \( \mathcal{F}_{\tau-1} \) affects how the feature vector \( X_{\tau} \) is chosen. More specifically, our algorithm uses \( \mathcal{F}_{\tau-1} \) to compute \( \hat{\beta}_t \) and then chooses arm \( a_{\tau} \) such that its feature \( x_{a_{\tau}} \) maximizes \( x_{a_{\tau}}^T \hat{\beta}_t \). Therefore, we can rewrite \( \Sigma_t \) as
\[
\Sigma_t = \frac{1}{t} \sum_{\tau=1}^{t} \sum_{i=1}^{2} \mathbb{E}_{X_{\tau}} [X_{\tau,i} X_{\tau,i}^T \mathbbm{1} \{X_{\tau,i} = \arg \max_{X \in \mathcal{X}_\tau} X^T \hat{\beta}_t\} | \hat{\beta}_t].
\]

Since the compatibility condition is satisfied only for the theoretical Gram matrix \( \Sigma \) and we need to show the empirical Gram matrix \( \hat{\Sigma}_t \) satisfies the compatibility condition, the
adapted Gram matrix $\Sigma_t$ serves as a bridge between $\Sigma$ and $\hat{\Sigma}_t$ in our analysis. We first lower-bound the compatibility constant $\phi^2(\Sigma_t, S_0)$ in terms of $\phi^2(\Sigma, S_0)$ so that we can show that $\Sigma_t$ satisfies the compatibility condition as long as $\Sigma$ satisfies the compatibility condition. Then, we show that $\hat{\Sigma}_t$ concentrates around $\Sigma_t$ with high probability and that such matrix concentration guarantees the compatibility condition of $\hat{\Sigma}_t$.

In Lemma 2, we show that the adapted Gram matrix $\Sigma_t$ can be controlled in terms of the theoretical Gram matrix $\Sigma$, which allows us to link the compatibility constant of $\Sigma$ to compatibility constant of $\Sigma_t$. Note that Lemma 2 shows the result for any fixed vector $\beta$; hence, it can be applied to $E[X_T X_T^\top | F_{T-1}]$.

**Lemma 2** For a fixed vector $\beta \in \mathbb{R}^d$, we have

$$\sum_{i=1}^{2} \mathbb{E}_{X_t} \left[ X_{t,i} X_{t,i}^\top 1 \{ X_{t,i} = \arg \max_{X \in \mathcal{X}} X^\top \beta \} \right] \succ \nu^{-1} \Sigma,$$

where $\nu$ the degree of asymmetry of the distribution $p_X$ defined in Assumption 4.s

Therefore, we have $\Sigma_t \succ \nu^{-1} \Sigma$ which implies that $\phi^2(\Sigma_t, S_0) \geq \frac{\phi^2(\Sigma, S_0)}{\nu} > 0$, i.e., $\Sigma_t$ satisfies the compatibility condition. Note that both $\Sigma$ and $\Sigma_t$ can be singular. In Lemma 3, we show that $\hat{\Sigma}_t$ concentrates to $\Sigma_t$ with high probability. This result is crucial in our analysis since it allows the matrix concentration without using i.i.d. samples. The proof of Lemma 3 utilizes a new Bernstein-type inequality for adapted samples (Lemma 8 in the appendix) which may be of independent interest.

**Lemma 3 (Matrix concentration)** For $t \geq \frac{2 \log(2d^2)}{C_0(s_0)^2}$ where $C_0(s_0) = \min \left( \frac{1}{2}, \frac{\phi^2_0}{256s_0\nu \max} \right)$, we have

$$\mathbb{P} \left( \| \Sigma_t - \hat{\Sigma}_t \|_\infty \geq \frac{\phi^2_0}{32s_0\nu} \right) \leq \exp \left( - \frac{tC_0(s_0)^2}{2} \right).$$

Then, we invoke the following corollary to use the matrix concentration results to ensure the compatibility condition for $\hat{\Sigma}_t$.

**Corollary 1 (Corollary 6.8, Bühlmann and Van De Geer (2011))** Suppose that $\Sigma_0$-compatibility condition holds for the index set $S$ with cardinality $s = |S|$, with compatibility constant $\phi^2(\Sigma_0, S)$, and that $\| \Sigma_1 - \Sigma_0 \|_\infty \leq \Delta$, where $32s_0\Delta \leq \phi^2(\Sigma_0, S)$. Then, for the set $S$, the $\Sigma_1$-compatibility condition holds as well, with $\phi^2(\Sigma_1, S) \geq \phi^2(\Sigma_0, S)/2$.

In order to satisfy the hypotheses in Lemma 3 and Corollary 1, we define the initial period $t < T_0 := \frac{2 \log(2d^2)}{C_0(s_0)^2}$ during which the compatibility condition for the empirical Gram matrix is not guaranteed, and the event

$$\mathcal{E}_t := \left\{ \| \Sigma_t - \hat{\Sigma}_t \|_\infty \leq \frac{\phi^2_0}{32s_0\nu} \right\}.$$

Then for all $t \geq [T_0]$ and $\Sigma_t$ for which event $\mathcal{E}_t$ holds, we have

$$\phi^2_t := \phi^2(\Sigma_t, S_0) \geq \frac{\phi^2_0(s_0)}{2} \geq \frac{\phi^2_0}{2\nu} > 0.$$

Hence, the compatibility condition is satisfied for the empirical Gram matrix without using sparsity information.
5.3.3 Proof Sketch of Theorem 1

We combine the results above to analyze the regret bound of SA LASSO BANDIT shown in Theorem 1. First, we divide the time horizon $[T]$ into three groups:

(a) $(t \leq T_0)$. Here the compatibility condition is not guaranteed to hold.

(b) $(t > T_0)$ such that $\mathcal{E}_t$ holds.

(c) $(t > T_0)$ such that $\mathcal{E}_t$ does not hold.

These sets are disjoint, hence we bound the regret contribution from each separately and obtain an upper bound on the overall regret. It is important to note that SA LASSO BANDIT Algorithm does not rely in any way on this partitioning – it is introduced purely for the purpose of analysis. Set (a) is the initial period over which we do not have guarantees for the compatibility condition. Therefore, we cannot apply the Lasso convergence result; hence we can incur $O(s_0^2 \log d)$ regret. Set (b) is where the compatibility condition is satisfied; hence the Lasso oracle inequality in Lemma 1 can apply. In fact, this group can be further divided to two cases: (b-1) when the high-probability Lasso result holds and (b-2) when it does not, where the regret of (b-2) can be bounded by $O(1)$. For (b-1), using the Lasso convergence result and summing the regret over the time horizon gives $O(s_0 \sqrt{T \log(dT)})$ regret, which is the leading factor in the regret bound of Theorem 1. Lastly, (c) contains the failure events of Lemma 3 whose regret is $O(s_0^2)$. The proofs of the lemmas are in Appendix A, followed by the complete proof of Theorem 1 in Appendix B.

5.4 Regret under the Restricted Eigenvalue Condition

In our analysis so far, we have presented the main results under the compatibility condition in order to be consistent with previous results in the sparse bandit literature. In this section, we present the regret bound for SA LASSO BANDIT under the restricted eigenvalue (RE) condition and briefly discuss its implication in terms of potentially matching lower bounds. Similar to the analysis under the compatibility condition, we assume that the RE condition is satisfied only for the theoretical Gram matrix $\Sigma = \frac{1}{K} \mathbb{E}[X^T X]$.

Assumption 5 (RE condition) For active set $S_0$ and $\Sigma$, there exists restricted eigenvalue $\phi_1 > 0$ such that $\phi_1^2 \|\beta\|^2 \leq \beta^T \Sigma \beta$ for all $\beta \in \mathbb{C}(S_0)$ defined in (2).

The RE condition is very similar to the compatibility condition in Assumption 3 but uses the $\ell_2$ norm instead of the $\ell_1$ norm. Based on this condition, we can show the following regret bound.

Theorem 2 (Regret bound under RE condition) Suppose $K = 2$ and Assumptions 1, 2, 4, and 5 hold. Then the expected cumulative regret of the SA LASSO BANDIT policy is $O(\sqrt{s_0 T \log(dT)})$.

Theorem 2 establishes $O(\sqrt{s_0 T \log(dT)})$ regret without any prior knowledge on $s_0$. The regret upper-bound based on the RE condition still enjoys logarithmic dependence on $d$ and furthermore sub-linear dependence on $s_0$. Compared to Theorem 1, the regret bound in Theorem 2 is smaller by $\sqrt{s_0}$ factor, which is again consistent with the offline Lasso results.
under the RE condition (Theorem 7.19 in Wainwright 2019). The difference in the regret bounds in Theorem 1 and Theorem 2 is due to the RE condition being slightly stronger than the compatibility condition.

The RE condition is more directly analogous (as compared to the compatibility condition) to the standard positive-definiteness assumption for covariance matrices in GLM bandits (Li et al., 2017). That is, the RE condition is equivalent to positive-definite covariance when $s_0 = d$, i.e., non-sparse settings. Li et al. (2017) showed $O((\log T)^{3/2} \sqrt{dT \log K})$ regret bound of for GLM bandits, which matches the $\Omega(\sqrt{dT})$ minimax lower bound established (Chu et al., 2011) for linear bandits with finite arms, up to logarithmic factors. Therefore, in sparse settings, we conjecture that $O(\sqrt{s_0 T \log(dT)})$ regret is best possible up to logarithmic factors under the RE condition (and so is $O(s_0 \sqrt{T \log(dT)})$ regret under the compatibility condition). While we present these conjectures, we do not claim our results are minimax. In fact, we discuss in Section 8 that the entire notion of minimax regret is much more delicate in sparse bandits.

6. Numerical Experiments

We conduct numerical experiments to evaluate SA LASSO BANDIT and compare with existing sparse bandit algorithms: DR LASSO BANDIT (Kim and Paik, 2019) and LASSO BANDIT (Bastani and Bayati, 2020) in two-armed contextual bandits. We follow the experimental setup of Kim and Paik (2019) to evaluate algorithms under different levels of correlation between arms. Although we consider $K = 2$ case in this section, the experimental setup introduced here also applies to numerical evaluations for $K \geq 3$ armed case in Section 7.
For each dimension $i \in [d]$, we sample each element of the feature vectors $[X_{t,1}^{(i)}, ..., X_{t,K}^{(i)}]$ from multivariate Gaussian distribution $\mathcal{N}(0_{K}, V)$ where covariance matrix $V$ is defined as $V_{i,i} = 1$ for all diagonal elements $i \in [K]$ and $V_{i,j} = \rho^2$ for all off-diagonal elements $i \neq j \in [K]$. Hence, for $\rho^2 > 0$, feature vectors for each arm are allowed to be correlated. We consider different levels of correlation with $\rho^2 = 0.7$ (strong correlation) in Figure 1 and $\rho^2 = 0.3$ (weak correlation) in Figure 2 as well as $\rho^2 = 0$ (no correlation) in the appendix. In these sets of experiments, we consider feature dimensions $d = 100$ and $d = 200$. For comparison, we use a linear reward with the linear link function $\mu(z) = z$ since both LASSO BANDIT and DR LASSO BANDIT are proposed in linear reward settings. We generate $\beta^*$ with varying sparsity $s_0 = ||\beta^*||_0$. For a given $s_0$, we generate each non-zero element of $\beta^*$ from a uniform distribution in $[0, 1]$. For noise, we sample $\epsilon_t \sim \mathcal{N}(0, 1)$ independently for all rounds. For each case with different experimental configurations, we conduct 20 independent runs, and report the average of the cumulative regret for each of the algorithms. The error bars represent the standard deviations.

DR LASSO BANDIT is proposed for the same problem setting as ours. Therefore, it does not require any modifications for experiments. However, the problem setting of LASSO BANDIT is different from ours: it assumes that the context variable is the same for all arms but each arm has a different parameter. We follow the setup in Kim and Paik (2019), and adapt LASSO BANDIT TO OUR SETTING BY DEFINING a $Kd$-dimensional context vector $X_t = [X_{t,1}^\top, ..., X_{t,K}^\top]^\top \in \mathbb{R}^{Kd}$ and a $Kd$-dimensional parameter $\beta^*_i$ for each arm $i$ where $\beta^* = [\beta^* \mathbf{1} (i = 1), ..., \beta^* \mathbf{1} (i = K)]^\top \in \mathbb{R}^{Kd}$; thus, $X_{t,i}^\top \beta^*_i = X_{t,i}^\top \beta^*$'s. Note that despite the concatenation, the effective dimension of the unknown parameter $\beta^*_i$ remains the same as...
far as estimation is concerned. We defer the other details of the experimental setup and additional results to the appendix.

It is important to note that we report the performances of the benchmarks (DR LASSO BANDIT and LASSO BANDIT) assuming that they have access to correct sparsity index $s_0$; however, this information is hidden from our algorithm. Despite this advantage, the experiment results shown in Figure 1 and Figure 2 demonstrate that SA LASSO BANDIT outperforms the other methods by significant margin consistently across various problem instances. We also verify that the performance of our proposed algorithm is the least sensitive to the details of the problem instances, and scales well with changes in the instance. The regret of our algorithm appears to scale linearly with the sparsity index $s_0$, while its dependence on the feature dimension $d$ appears to be very minimal in most of the instances, which is consistent with our theoretical findings. We also observe that a higher correlation between arms (feature vectors) improves the overall performances of the algorithms. This finding is stronger in the experiments for the $K$-armed case. We discuss this phenomenon in detail in Section 7.

7. Extension to $K$ Arms

Thus far, we have presented our main results in two-armed bandit settings which highlight the main challenges of sparse bandit problems without prior knowledge of sparsity. In this section, we extend our regret analysis to the case of $K \geq 3$ arms. Also, we present additional numerical experiments for $K$-armed bandits.

7.1 Regret Analysis for $K$ Arms

Recall that SA LASSO BANDIT is valid for any number of arms; hence, no modifications are required to extend the algorithm to $K \geq 3$ arms. The analysis of SA LASSO BANDIT for the $K$-armed case tackles largely the same challenges described in Section 5.3: the need for a Lasso convergence result for adapted samples and ensuring the compatibility condition without knowing $s_0$ (and without relying on i.i.d. samples). The former challenge is again taken care of by the Lasso convergence result in Lemma 1. However, the latter issue is more subtle in the $K$-armed case than in the two-armed case. In particular, when controlling the adapted Gram matrix $\Sigma_t$ with the theoretical Gram matrix $\Sigma$, the Gram matrix for the unobserved feature vectors could be incomparable with the Gram matrix for the observed feature vectors. For this issue, we introduce an additional regularity condition, which we denote as the “balanced covariance” condition.

**Assumption 6 (Balanced covariance)** Consider a permutation $(i_1, ..., i_K)$ of $(1, ..., K)$. For any integer $k \in \{2, ..., K - 1\}$ and fixed vector $\beta$, there exists $C_X < \infty$ such that

$$E\left[X_{i_k}X_{i_k}^T \mathbb{1}\{X_{i_1}^T \beta < \ldots < X_{i_k}^T \beta\}\right] \preceq C_X E\left[(X_{i_1}X_{i_1}^T + X_{i_K}X_{i_K}^T) \mathbb{1}\{X_{i_1}^T \beta < \ldots < X_{i_K}^T \beta\}\right].$$

This balanced covariance condition implies that there is “sufficient randomness” in the observed features compared to non-observed features. The exact value of $C_X$ depends on the joint distribution of $\mathcal{X}$ including the correlation between arms. In general, the more positive the correlation, the smaller $C_X$ (obviously, with an extreme case of perfectly
correlated arms having a constant $C_X$ independent of any problem parameters). When the arms are independent and identically distributed, Assumption 6 holds with $C_X = O(1)$ for both the multivariate Gaussian distribution and a uniform distribution on a sphere, and for an arbitrary independent distribution for each arm, Assumption 6 holds for $C_X = (K - 1)K_0$ where $K_0 = \lceil (K - 1)/2 \rceil$. It is important to note that even in this pessimistic case, $C_X$ does not exhibit dependence on dimensionality $d$ or the sparsity index $s_0$. These are formalized in Proposition 1 in Appendix D. This balanced covariance condition is somewhat similar to “positive-definiteness” condition for observed contexts in the bandit literature (e.g., Goldenshluger and Zeevi (2013); Bastani et al. (2017)). However, notice that we allow the covariance matrices on both sides of the inequality to be singular. Hence, the positive-definiteness condition for observed context in our setting may not hold even when the balanced covariance condition holds. While this condition admittedly originates from our proof technique, it also provides potential insights on learnability of problem instances. That is, $C_X$ close to infinity implies that the distribution of feature vectors is heavily skewed toward a particular direction. Hence, learning algorithms may require many more samples to learn the unknown parameter, leading to larger regret. It is important to note that our algorithm does not require any prior information on $C_X$. The regret bound for the $K$-armed sparse bandits under Assumption 6 is as follows.

**Theorem 3 (Regret bound for $K$ arms)** Suppose $K \geq 3$ and Assumptions 1-4, and 6 hold. Let $\lambda_0 = 2\sigma_{x_{\max}}$. Then the expected cumulative regret of the SA LASSO BANDIT policy $\pi$ over horizon $T \geq 1$ is upper-bounded by

$$R_{\pi}(T) \leq 4\kappa_1 + \frac{4\kappa_1\sigma_{x_{\max}}b(\log(2d^2) + 1)}{C_1(s_0)^2} + \frac{64\kappa_1\nu C_X \sigma_{x_{\max}} s_0 \sqrt{T \log(dT)}}{\kappa_0 \phi_0^2} \Theta_0.$$ 

where $C_1(s_0) = \min \left(\frac{1}{2}, \frac{\phi_0^2}{256s_0 C_X \sigma_{x_{\max}}} \right)$.

Theorem 3 establishes $O(s_0 \sqrt{T \log(dT)})$ regret without prior knowledge on $s_0$, achieving the same rate as Theorem 1 in terms of the key problem primitives. The proof of Theorem 3 largely follows that of Theorem 1. The main difference is how we control the adapted Gram matrix $\Sigma_t$ with the theoretical Gram matrix $\Sigma$. Under the balanced covariance condition, we can ensure the lower bound of the adapted Gram matrix as a function of the theoretical Gram matrix, which is analogous to the result in Lemma 2. In particular, we can show that for a fixed vector $\beta \in \mathbb{R}^d$,

$$\sum_{i=1}^{K} \mathbb{E}_{\mathcal{X}_i} \left[ X_{t,i} X_{t,i}^\top 1 \{ X_{t,i} = \arg \max_{X \in \mathcal{X}_i} X^\top \beta \} \right] \succeq (2\nu C_X)^{-1} \Sigma.$$ 

The formal result is presented in Lemma 10 in Appendix D along with its proof. Next, we again invoke the matrix concentration result in Lemma 3 to connect the compatibility

6. While it is not our primary goal to derive general tight bounds on $C_X$, we acknowledge that the bound on $C_X$ for an arbitrary distribution for independent arms is very loose, and is the result of conservative analysis driven by lack of information on $p_X$. Numerical evaluation on distributions other than Gaussian and uniform distributions, detailed in Section 7, buttress this point and indicate that the dependence on $K$ is no greater than linear.
constant of empirical Gram matrix $\hat{\Sigma}_t$ to that of $\Sigma_t$, and eventually to the theoretical Gram matrix $\Sigma$. Thus, we ensure the compatibility condition of $\hat{\Sigma}_t$. The additional regret in the $K$-armed case as compared to the two-armed case is essentially a scaling by $C_X$ to ensure the balanced covariance condition.

7.2 Numerical Experiments for $K$ Arms

We now validate the performance of SA Lasso Bandit in $K$-armed sparse bandit settings via additional numerical experiments and provide comparison with the existing sparse bandit algorithms. The setup of the experiments is identical to the setup described in Section 6. We perform evaluations under various instances. In particular, we focus on the performances of algorithms as the number of arms increases. Additionally, to investigate the effect of the balanced covariance condition, we evaluate algorithms on features drawn from a non-Gaussian elliptical distribution, for which we do not have a tight bound of $C_X$ as well as the multi-dimensional uniform distribution.

Figure 3 shows the sample results of the numerical evaluations (averaged over 20 independent runs per problem instance), and the additional results are also presented in the appendix. The experiment results provide the convincing evidence that the performance of our proposed algorithm is superior to the existing sparse bandit methods that we compare with. Again, SA Lasso Bandit outperforms the existing sparse bandit algorithms by significant margins, even though the correct sparsity index $s_0$ is revealed to these algorithms and kept hidden from SA Lasso Bandit. Furthermore, SA Lasso Bandit is much more practical and simple to implement with a minimal number of a hyperparameter.

In the experiments with Gaussian distributions shown in the first and second rows in Figure 3, we again observe that algorithms generally perform better under strong correlation compared to weak correlation instances. This is expected since strongly (positively) correlated arms imply a smaller discrepancy between expected payoffs of the arms. A strong correlation between the arms also implies a smaller $C_X$, hence leading to a lower regret, as briefly discussed earlier when we introduce the balanced covariance condition. Thus, the balanced covariance condition appears to capture the essence of positive correlation between arms. It is important to note that there are two different notions of correlation: correlation between the arms and correlation between the features of an arm. A higher correlation between the features potentially decreases the value of compatibility constant. Thus, the regret may increase with an increase in correlation of the features as far as the compatibility condition is concerned. The plots in the third and fourth rows in Figure 3 show that when the feature vectors are drawn i.i.d. according to the uniform distribution and non-Gaussian elliptical distributions, the performance of existing algorithms (e.g., DR LASSO BANDIT from Kim and Paik (2019)) deteriorates significantly; SA Lasso Bandit still exhibits superior performances. Thus, our proposed algorithm is very robust to the changes in the distribution of the feature vectors.

8. Concluding Remarks

In this paper, we study high-dimensional contextual bandit problem with sparse structure. In particular, we address the fundamental issue that previously known learning algorithms for this problem require a priori knowledge of the sparsity index $s_0$ of the unknown param-
Figure 3: The plots show the $t$-round cumulative regret of SA LASSO BANDIT (Algorithm 1), DR LASSO BANDIT (Kim and Paik, 2019), and LASSO BANDIT (Bastani and Bayati, 2020) with varying number of arms $K \in \{20, 100\}$, feature dimensions $d \in \{100, 200\}$, and different distributions. In the first two rows, features are drawn from a multivariate Gaussian distribution with weak and strong correlation levels. The third row shows evaluations with features drawn from the multi-dimensional uniform distribution. In the fourth row, features are drawn from a non-Gaussian elliptical distribution.

We propose and analyze an algorithm that does not require this information. The proposed algorithm achieves a tight regret upper bound which depends on a logarithmic function of the feature dimension which matches the scaling of the offline Lasso convergence results. The algorithm attains this sharp result without knowing the sparsity of the unknown parameter, overcoming weaknesses of the existing algorithms. We demonstrate that our proposed algorithm significantly outperforms the benchmark, supporting the theoretical claims. We conclude by outlining some of future directions.

**Minimax Regret in Sparse Bandits.** Minimax regret in sparse bandits is more subtle to define than in (non-sparse) linear or GLM bandits. Consider the following setting. Suppose nature is allowed to freely choose $s_0 \in [d]$, it can force the regret for any sparse bandit algorithm to be polynomial in $d$ by choosing $s_0 = d$. On the other hand, if we limit nature to choose $s_0 \in [1, s_{\text{max}}]$, it will choose $s_0 = s_{\text{max}}$, and therefore, sparse bandit algorithms
can assume that the sparsity index $s_0$ is known, and set equal to $s_{\text{max}}$. Thus, it is not clear how to define a minimax criterion in a manner that does not reveal the dominating choice for nature, and therefore, forces learning algorithm to play a strategy which hedges against a range of values of the sparsity index.

**Reinforcement Learning with High-Dimensional Covariates.** Another compelling direction is to extend our analysis and proposed approach to reinforcement learning with high-dimensional context or with high-dimensional function approximation. A main challenge in this direction appears to be the need for an algorithm to be optimistic. To our knowledge, almost all reinforcement learning algorithms with provable efficiency rely on the principle of optimism. But, as we have discussed in this paper, in order to be optimistic in the tightest sense under sparse structure, the knowledge on sparsity is generally needed.

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Appendix A. Proofs of Lemmas for Theorem 1

A.1 Proof of Lemma 1

The proof follows from modifying the proof of the standard Lasso oracle inequality (Bühlmann and Van De Geer, 2011) using martingale theory. Recall from (1) that the negative log-likelihood of the GLM is

$$\ell_t(\beta) = -\frac{1}{t} \sum_{\tau=1}^{t} \left[ Y_\tau X_\tau^\top \beta - m(X_\tau^\top \beta) \right]$$

where $m$ is a normalizing function with its gradient $\dot{m}(X^\top \beta) = \mu(X^\top \beta)$. Now, we denote the expectation of $\ell_t(\beta)$ over $Y$ by $\bar{\ell}_t(\beta)$:

$$\bar{\ell}_t(\beta) := \mathbb{E}_{Y}[\ell_t(\beta)] = -\frac{1}{t} \sum_{\tau=1}^{t} \left[ \mu(X_\tau^\top \beta^*)X_\tau^\top \beta - m(X_\tau^\top \beta) \right].$$

Note that $\nabla_\beta \bar{\ell}_t(\beta) = -\frac{1}{t} \sum_{\tau=1}^{t} \left[ \mu(X_\tau^\top \beta^*) - \mu(X_\tau^\top \beta) \right] X_\tau$. Hence, we have $\nabla_\beta \bar{\ell}_t(\beta^*) = 0_d$ which implies that $\beta^* = \arg \min_\beta \bar{\ell}_t(\beta)$ given the fact that $m$ is convex in the GLM. Hence, for any parameter $\beta \in \mathbb{R}^d$, the excess risk is defined as

$$\mathcal{E}(\beta) := \bar{\ell}_t(\beta) - \bar{\ell}_t(\beta^*).$$

Note that by definition, $\mathcal{E}(\beta) \geq 0$, for all $\beta \in \mathbb{R}^d$ (with $\mathcal{E}(\beta^*) = 0$). The Lasso estimate $\hat{\beta}_t$ for the GLM is given by the minimization of the penalized negative log-likelihood

$$\hat{\beta}_t := \arg \min_\beta \{ \ell_t(\beta) + \lambda_t \| \beta \|_1 \}$$

where $\lambda$ is the penalty parameter whose value needs to be chosen to control the noise of the model. Now, we define the empirical process of the problem as

$$v_t(\beta) := \ell_t(\beta) - \bar{\ell}_t(\beta).$$

Note that the randomness in $\{Y_\tau\}$ still plays a role on $\ell_t(\beta)$ and hence on $v_t(\beta)$. Then by the definition of $\hat{\beta}_t$, we have

$$\ell_t(\hat{\beta}_t) + \lambda_t \| \hat{\beta}_t \|_1 \leq \ell_t(\beta^*) + \lambda_t \| \beta^* \|_1.$$ 

Adding and subtracting terms, we have

$$\ell_t(\hat{\beta}_t) - \bar{\ell}_t(\beta) + \bar{\ell}_t(\beta^*) - \bar{\ell}_t(\beta^*) + \lambda_t \| \hat{\beta}_t \|_1 \leq \ell_t(\beta^*) - \bar{\ell}_t(\beta^*) + \lambda_t \| \beta^* \|_1.$$ 

Rearranging terms gives the following “basic inequality” for the GLM

$$\mathcal{E}(\hat{\beta}_t) + \lambda_t \| \hat{\beta}_t \|_1 \leq -v_t(\hat{\beta}_t) - v_t(\beta^*) + \lambda_t \| \beta^* \|_1. $$

The basic inequality implies that in order to provide an upper-bound for the penalized excess risk, we need to control the deviation of the empirical process $[v_t(\hat{\beta}_t) - v_t(\beta^*)]$ (Bühlmann and Van De Geer, 2011). And we bound this deviation of the empirical process in terms of
the parameter estimation error $||\hat{\beta}_t - \beta^*||_1$. Essentially, $[v_t(\hat{\beta}_t) - v_t(\beta^*)]$ is where the random noise plays a role, and with large enough penalization (suitably large $\lambda$) we can control such randomness in the empirical process. We define the event of the empirical process being controlled by the penalization.

$$\mathcal{T} := \{ |v_t(\hat{\beta}_t) - v_t(\beta^*)| \leq \lambda ||\hat{\beta}_t - \beta^*||_1 \}.$$  (3)

Lemma 4 ensures that we can control this empirical process deviation with high probability. Hence, in the rest of the proof, we restrict ourselves to the case where the empirical process behaves well, i.e., event $\mathcal{T}$ in (3) holds.

**Lemma 4** Assume $X_t$ satisfies $\|X_t\|_2 \leq x_{\text{max}}$ for all $t$. If $\lambda = \sigma x_{\text{max}} \sqrt{\frac{2 \log(2/\delta) + \log d}{t}}$, then with probability at least $1 - \delta$ we have

$$|v_t(\hat{\beta}_t) - v_t(\beta^*)| \leq \lambda ||\hat{\beta}_t - \beta^*||_1.$$  

On event $\mathcal{T}$, for $\lambda_t \geq 2\lambda$, we have

$$2\mathcal{E}(\hat{\beta}_t) + 2\lambda_t ||\hat{\beta}_t||_1 \leq \lambda_t ||\hat{\beta}_t - \beta^*||_1 + 2\lambda_t ||\beta^*||_1.$$  (4)

Let $\hat{\beta} := \hat{\beta}_t$ for brevity. Using the active set $S_0$, we can define the following:

$$\beta_{j,S_0} := \beta_j 1\{j \in S_0\} \quad \beta_{j,S_0^c} := \beta_j 1\{j \notin S_0\}$$

so that $\beta_{S_0} = [\beta_{1,S_0}, ..., \beta_{d,S_0}]^T$ has zero elements outside the set $S_0$ and the elements of $\beta_{S_0^c}$ can only be non-zero in the complement of $S_0$. We can then lower-bound $||\hat{\beta}||_1$ using the triangle inequality,

$$||\hat{\beta}||_1 = ||\hat{\beta}_{S_0}||_1 + ||\hat{\beta}_{S_0^c}||_1 \geq ||\beta_{S_0}||_1 - ||\beta_{\hat{S}_0} - \beta_{\hat{S}_0}^*||_1 + ||\hat{\beta}_{S_0^c}||_1.$$  

Also, we can rewrite

$$||\hat{\beta} - \beta^*||_1 = ||\hat{\beta}_{S_0} - \beta_{S_0}^*||_1 + ||\hat{\beta}_{S_0^c} - \beta_{S_0^c}^*||_1 = ||\hat{\beta}_{S_0} - \beta_{S_0}^*||_1 + ||\hat{\beta}_{S_0^c}||_1.$$  

Then we continue from (4)

$$2\mathcal{E}(\hat{\beta}) + 2\lambda_t ||\beta_{S_0}^*||_1 - 2\lambda_t ||\hat{\beta}_{S_0} - \beta_{S_0}^*||_1 + 2\lambda_t ||\hat{\beta}_{S_0^c}||_1 \leq \lambda_t ||\hat{\beta}_{S_0} - \beta_{S_0}^*||_1 + \lambda_t ||\hat{\beta}_{S_0}||_1 + 2\lambda_t ||\beta_{S_0}^*||_1$$

$$= \lambda_t ||\hat{\beta}_{S_0} - \beta_{S_0}^*||_1 + \lambda_t ||\hat{\beta}_{S_0}||_1 + 2\lambda_t ||\beta_{S_0}^*||_1.$$  

Therefore, we have

$$0 \leq 2\mathcal{E}(\hat{\beta}) \leq 3\lambda_t ||\hat{\beta}_{S_0} - \beta_{S_0}^*||_1 - \lambda_t ||\hat{\beta}_{S_0}|_1$$

$$= \lambda_t \left( 3||\hat{\beta}_{S_0} - \beta_{S_0}^*||_1 - ||\hat{\beta}_{S_0} - \beta_{S_0}^*||_1 \right)$$  (5)
Then the compatibility condition can be applied to the vector $\hat{\beta} - \beta^*$ which gives

$$\|\hat{\beta}_{S_0} - \beta_{S_0}^*\|_2^2 \leq s_0(\hat{\beta} - \beta^*)^\top \hat{\Sigma}(\hat{\beta} - \beta^*)/\phi_t^2. \quad (6)$$

From (5), we have

$$2\mathcal{E}(\hat{\beta}) + \lambda_t \|\hat{\beta}_{S_0}\|_1 \leq 3\lambda_t \|\hat{\beta}_{S_0} - \beta_{S_0}^*\|_1.$$

Therefore, we have

$$2\mathcal{E}(\hat{\beta}) + \lambda_t \|\hat{\beta} - \beta^*\|_1 = 2\mathcal{E}(\hat{\beta}) + \lambda_t \|\hat{\beta}_{S_0}\|_1 + \lambda_t \|\hat{\beta}_{S_0} - \beta_{S_0}^*\|_1$$
$$\leq 3\lambda_t \|\hat{\beta}_{S_0} - \beta_{S_0}^*\|_1 + \lambda_t \|\hat{\beta}_{S_0} - \beta_{S_0}^*\|_1$$
$$= 4\lambda_t \|\hat{\beta}_{S_0} - \beta_{S_0}^*\|_1$$
$$\leq 4\lambda_t \sqrt{s_0(\hat{\beta} - \beta^*)^\top \hat{\Sigma}(\hat{\beta} - \beta^*)/\phi_t}$$
$$\leq \kappa_0(\hat{\beta} - \beta^*)^\top \hat{\Sigma}(\hat{\beta} - \beta^*) + \frac{4\lambda_t^2 s_0}{\kappa_0 \phi_t^2}$$
$$\leq 2\mathcal{E}(\hat{\beta}) + \frac{4\lambda_t^2 s_0}{\kappa_0 \phi_t^2}$$

where the second inequality is from applying the compatibility condition (6) and the third inequality is by using $4uv \leq u^2 + 4v^2$ with $u = \sqrt{\kappa_0(\hat{\beta} - \beta^*)^\top \hat{\Sigma}(\hat{\beta} - \beta^*)}$ and $v = \frac{\lambda_t \sqrt{s_0}}{\phi_t \sqrt{\kappa_0}}$. The last inequality is from Lemma 5. Hence, rearranging gives

$$\|\hat{\beta} - \beta^*\|_1 \leq \frac{4 s_0 \lambda_t}{\kappa_0 \phi_t^2}.$$

This completes the proof. \[\square\]

### A.2 Proof of Lemma 4

**Proof** By the definitions of the negative log-likelihood $\ell_t(\beta)$ and its expectation $\bar{\ell}_t(\beta)$, we can rewrite the empirical process $v_t(\beta)$ as

$$v_t(\beta) = \ell_t(\beta) - \bar{\ell}_t(\beta)$$
$$= -\frac{1}{t} \sum_{\tau=1}^t [Y_\tau X_\tau^\top \beta - m(X_\tau^\top \beta)] + \frac{1}{t} \sum_{\tau=1}^t [\mu(X_\tau^\top \beta^*)X_\tau^\top \beta - m(X_\tau^\top \beta)]$$
$$= -\frac{1}{t} \sum_{\tau=1}^t [Y_\tau X_\tau^\top \beta - \mu(X_\tau^\top \beta^*)X_\tau^\top \beta]$$
$$= -\frac{1}{t} \sum_{\tau=1}^t \epsilon_\tau X_\tau^\top \beta$$
where the last equality uses the definition of $\epsilon_{\tau}$. Then, the empirical process deviation is

$$v_t(\hat{\beta}_t) - v_t(\beta^*) = -\frac{1}{t} \sum_{\tau=1}^{t} \epsilon_{\tau}X_{\tau}^\top(\hat{\beta}_t - \beta^*).$$

Applying Hölder’s inequality, we have

$$|v_t(\hat{\beta}_t) - v_t(\beta^*)| \leq \frac{1}{t} \left\| \sum_{\tau=1}^{t} \epsilon_{\tau}X_{\tau} \right\|_{\infty} \|\hat{\beta}_t - \beta^*\|_1.$$

Then controlling the empirical process reduces to controlling $\frac{1}{t} \left\| \sum_{\tau=1}^{t} \epsilon_{\tau}X_{\tau} \right\|_{\infty}$. Then, using the union bound, it follows that

$$\mathbb{P}\left( \frac{1}{t} \left\| \sum_{\tau=1}^{t} \epsilon_{\tau}X_{\tau} \right\|_{\infty} \leq \lambda \right) = 1 - \mathbb{P}\left( \frac{1}{t} \left\| \sum_{\tau=1}^{t} \epsilon_{\tau}X_{\tau} \right\|_{\infty} > \lambda \right) \geq 1 - \sum_{j=1}^{d} \mathbb{P}\left( \frac{1}{t} \left\| \sum_{\tau=1}^{t} \epsilon_{\tau}X_{\tau}^{(j)} \right\| > \lambda \right)$$

where $X_{\tau}^{(j)}$ is the $j$-th element of $X_{\tau}$. For each $j \in [d]$, and $\tau \in [t]$, we let $Z_{\tau}^{(j)} := \epsilon_{\tau}X_{\tau}^{(j)}$. Let $\mathcal{F}_{t-1}$ denote the sigma sigma-field that contains all observed information prior to taking an action in round $t$, i.e., $\mathcal{F}_{t-1}$ is generated by random variables of previously chosen actions $\{a_1, ..., a_{t-1}\}$, their features $\{X_1, ..., X_{t-1}\}$, the corresponding rewards $\{Y_1, ..., Y_{t-1}\}$ and the set of feature vectors $X_t = \{X_{t,1}, ..., X_{t,K}\}$ in round $t$.

Then, each $\{Z_{\tau}^{(j)}\}_{\tau=1}^{t}$ for $j \in [d]$ is a martingale difference sequence adapted to the filtration $\mathcal{F}_1 \subset ... \subset \mathcal{F}_t$ since $\mathbb{E}[\epsilon_{\tau}X_{\tau}^{(j)}|\mathcal{F}_{\tau-1}] = X_{\tau}^{(j)}\mathbb{E}[\epsilon_{\tau}|\mathcal{F}_{\tau-1}] = 0$ for each $j$. Note that each $X_{\tau}^{(j)}$ is a bounded random variable with $|X_{\tau}^{(j)}| \leq \|X_{\tau}\|_{\infty} \leq \|X_{\tau}\|_2 \leq x_{\max}$. Then from the fact that $\epsilon_{\tau}$ is $\sigma^2$-sub-Gaussian, it follows that $Z_{\tau}^{(j)}$ is also $\sigma^2$-sub-Gaussian. That is,

$$\mathbb{E}\left[ \exp(\alpha Z_{\tau}^{(j)}) | \mathcal{F}_{\tau-1} \right] = \mathbb{E}\left[ \exp\left( \alpha X_{\tau}^{(j)} \right) \epsilon_{\tau} | \mathcal{F}_{\tau-1} \right] \leq \mathbb{E}\left[ \exp(\alpha x_{\max} \epsilon_{\tau}) | \mathcal{F}_{\tau-1} \right] \leq \exp\left( \frac{\alpha^2 x_{\max}^2 \sigma^2}{2} \right)$$

for any $\alpha \in \mathbb{R}$. Then, using the concentration result in Lemma 14, we have

$$\mathbb{P}\left( \frac{1}{t} \sum_{\tau=1}^{t} \epsilon_{\tau}X_{\tau}^{(j)} > t\lambda \right) \leq 2 \exp\left( -\frac{t^2 \lambda^2}{2t\sigma^2 x_{\max}^2} \right) \leq 2 \exp\left( -\frac{t \lambda^2}{2\sigma^2 x_{\max}^2} \right).$$

So, with $\lambda = \sigma x_{\max} \sqrt{\frac{2\log(2/\delta) + \log d}{t}}$, we have

$$\mathbb{P}\left( \frac{1}{t} \left\| \sum_{\tau=1}^{t} \epsilon_{\tau}X_{\tau} \right\|_{\infty} \leq \lambda \right) \geq 1 - 2d \exp\left( \frac{\log \delta}{2} - \log d \right) = 1 - \delta.$$
Lemma 5 The excess risk is lower-bounded by

\[ E(\hat{\beta}_t) \geq \frac{\kappa_0}{2} (\hat{\beta}_t - \beta^*)^T \hat{\Sigma} (\hat{\beta}_t - \beta^*). \]

Proof By the definition of the excess risk \( E(\beta) \), we have

\[
E(\beta) = \bar{\ell}_t(\beta) - \bar{\ell}_t(\beta^*)
= -\frac{1}{t} \sum_{\tau=1}^t \left[ \mu(X_{\tau}^T \beta^*)X_{\tau}^T \beta - m(X_{\tau}^T \beta) \right] + \frac{1}{t} \sum_{\tau=1}^t \left[ \mu(X_{\tau}^T \beta^*)X_{\tau}^T \beta^* - m(X_{\tau}^T \beta^*) \right].
\]

Since \( \dot{\mu}(\cdot) = \mu(\cdot) \), we have \( \nabla_\beta \bar{\ell}_t(\beta^*) = 0_d \). Hence, the gradient of the excess risk \( \nabla_\beta E(\beta) \) and the Hessian are given as

\[
\nabla_\beta E(\beta) = -\frac{1}{t} \sum_{\tau=1}^t \left[ \mu(X_{\tau}^T \beta^*)X_{\tau}^T - \mu(X_{\tau}^T \beta)X_{\tau} \right],
\]

\[
H_E(\beta) := \nabla^2_\beta E(\beta) = \frac{1}{t} \sum_{\tau=1}^t \mu(X_{\tau}^T \beta)X_{\tau}X_{\tau}^T.
\]

Using the Taylor expansion, with \( \bar{\beta} = c\beta^* + (1-c)\hat{\beta} \) for some \( c \in (0,1) \)

\[
E(\hat{\beta}_t) = E(\beta^*) + \nabla_\beta E(\beta^*)^T (\hat{\beta}_t - \beta^*) + \frac{1}{2} (\hat{\beta}_t - \beta^*)^T H_E(\beta)(\hat{\beta}_t - \beta^*).
\]  

Note that by the definition of \( \beta^* \), we have \( E(\beta^*) = 0 \) and \( \nabla_\beta E(\beta^*) = \nabla_\beta \ell(\beta^*) = 0_d \). Hence, combining with the definition of the Hessian, we have

\[
E(\hat{\beta}_t) = \frac{1}{2} (\hat{\beta}_t - \beta^*)^T \left[ \frac{1}{t} \sum_{\tau=1}^t \mu(X_{\tau}^T \beta)X_{\tau}X_{\tau}^T \right] (\hat{\beta}_t - \beta^*)
\geq \frac{\kappa_0}{2} (\hat{\beta}_t - \beta^*)^T \hat{\Sigma} (\hat{\beta}_t - \beta^*)
\]

where the last inequality is from Assumption 2 and \( \hat{\Sigma} = \frac{1}{t} \sum_{\tau=1}^t X_{\tau}X_{\tau}^T \). \qed

A.3 Proof of Lemma 2

Proof Consider \( \mathcal{X} = \{X_1, X_2\} \). Let the joint density function of \( x_1, x_2 \) as \( p_\mathcal{X}(x_1, x_2) \). Then we have

\[
E[X^T X] = \int (x_1 x_1^T + x_2 x_2^T )p_\mathcal{X}(x_1, x_2)dx_1, x_2
= \int x_1 x_1^T \left[ 1 \left\{ (x_1 - x_2)^T \beta \geq 0 \right\} + 1 \left\{ (x_1 - x_2)^T \beta \leq 0 \right\} \right] p_\mathcal{X}(x_1, x_2)dx_1, x_2
+ \int x_2 x_2^T \left[ 1 \left\{ (x_1 - x_2)^T \beta \geq 0 \right\} + 1 \left\{ (x_1 - x_2)^T \beta \leq 0 \right\} \right] p_\mathcal{X}(x_1, x_2)dx_1, x_2
\]
Let’s first look at the first integral.

\[
\int x_1 x_1^T \left[ \mathbb{1} \left\{ (x_1 - x_2)^\top \beta \geq 0 \right\} + \mathbb{1} \left\{ (x_1 - x_2)^\top \beta \leq 0 \right\} \right] p_X(x_1, x_2) dx_1, x_2
\]

\[
= \int x_1 x_1^T \left[ \mathbb{1} \left\{ (x_1 - x_2)^\top \beta \geq 0 \right\} p_X(x_1, x_2) + \mathbb{1} \left\{ -(x_1 - x_2)^\top \beta \geq 0 \right\} p_X(x_1, x_2) \right] dx_1, x_2
\]

\[
\leq \int x_1 x_1^T \mathbb{1} \left\{ (x_1 - x_2)^\top \beta \geq 0 \right\} p_X(x_1, x_2) dx_1, x_2
\]

\[
+ \nu \int x_1 x_1^T \mathbb{1} \left\{ -(x_1 - x_2)^\top \beta \geq 0 \right\} p_X(-x_1, -x_2) dx_1, x_2
\]

\[
= \int x_1 x_1^T \mathbb{1} \left\{ (x_1 - x_2)^\top \beta \geq 0 \right\} p_X(x_1, x_2) dx_1, x_2
\]

\[
+ \nu \int x_1 x_1^T \mathbb{1} \left\{ (x_1 - x_2)^\top \beta \geq 0 \right\} p_X(x_1, x_2) dx_1, x_2
\]

\[
= (1 + \nu) \int x_1 x_1^T \mathbb{1} \left\{ (x_1 - x_2)^\top \beta \geq 0 \right\} p_X(x_1, x_2) dx_1, x_2
\]

\[
= (1 + \nu) \mathbb{E} \left[ X_1 X_1^\top \mathbb{1} \{ X_1 = \arg \max_{X \in \mathcal{X}} X^\top \beta \} \right]
\]

where the inequality follows from Assumption 4. Likewise, we can show for the second integral that

\[
\int x_2 x_2^T \left[ \mathbb{1} \left\{ (x_1 - x_2)^\top \beta \geq 0 \right\} + \mathbb{1} \left\{ (x_1 - x_2)^\top \beta \leq 0 \right\} \right] p_X(x_1, x_2) dx_1, x_2
\]

\[
= (1 + \nu) \mathbb{E} \left[ X_2 X_2^\top \mathbb{1} \{ X_2 = \arg \max_{X \in \mathcal{X}} X^\top \beta \} \right].
\]

Hence,

\[
\mathbb{E} [X^\top X] = (1 + \nu) \left( \mathbb{E} \left[ X_1 X_1^\top \mathbb{1} \{ X_1 = \arg \max_{X \in \mathcal{X}} X^\top \beta \} \right] + \mathbb{E} \left[ X_2 X_2^\top \mathbb{1} \{ X_2 = \arg \max_{X \in \mathcal{X}} X^\top \beta \} \right] \right).
\]

Therefore, with the fact that \( \nu \geq 1 \), we have

\[
\sum_{i=1}^2 \mathbb{E} \left[ X_i X_i^\top \mathbb{1} \{ X_i = \arg \max_{X \in \mathcal{X}} X^\top \beta \} \right] \geq \frac{2}{1 + \nu} \cdot \frac{1}{2} \mathbb{E} [X^\top X] \geq \nu^{-1} \Sigma.
\]

\[\text{A.4 Bernstein-type Inequality for Adapted Samples}\]

In this section, we derive a Bernstein-type inequality for adapted samples which is shown in Lemma 8. We first define the following function of a random variable \( X_t \) which is used throughout this section.

\[\text{28}\]
Definition 4 For all \( i, j \) with \( 1 \leq i \leq j \leq d \), we define \( \gamma_{ij}^t(X_t) \) to be a real-value function which takes random variable \( X_t \in \mathbb{R}^d \) as input:

\[
\gamma_{ij}^t(X_t) := \frac{1}{2 \tau_{\max}^2} \left( X_t^{(i)} X_t^{(j)} - \mathbb{E}[X_t^{(i)} X_t^{(j)} \mid \mathcal{F}_{t-1}] \right)
\]  

(8)

where \( X_t^{(i)} \) is the \( i \)-th element of \( X_t \).

It is easy to see that \( \mathbb{E}[\gamma_{ij}^t(X_t) \mid \mathcal{F}_{t-1}] = 0 \) and \( \mathbb{E}[|\gamma_{ij}^t(X_t)|^m \mid \mathcal{F}_{t-1}] \leq 1 \) for all integer \( m \geq 2 \). While we introduce this specific function \( \gamma_{ij}^t(X_t) \) in order to connect to the matrix concentration \( \| \Sigma - \tilde{\Sigma} \|_\infty \), Lemma 7 and Lemma 8 can be applied to any function \( \gamma_{ij}^t(X_t) \) that satisfies the zero mean and the bounded \( m \)-th moment conditions.

Lemma 6 (Bühlmann and Van De Geer (2011), Lemma 14.1) Let \( Z_t \in \mathbb{R} \) be a random variable with \( \mathbb{E}[Z_t \mid \mathcal{F}_{t-1}] = 0 \). Then it holds that

\[
\log \mathbb{E}[e^{Z_t} \mid \mathcal{F}_{t-1}] \leq \mathbb{E}[|Z_t| \mid \mathcal{F}_{t-1}] - 1 - \mathbb{E}[|Z| \mid \mathcal{F}_{t-1}].
\]

Proof The proof follows directly from the proof of Lemma 14.1 in Bühlmann and Van De Geer (2011), applying their result to a conditional expectation. For any \( c > 0 \),

\[
\exp(Z_t - c) - 1 \leq \frac{\exp(Z_t)}{1 + c} - 1 = \frac{e^{Z_t} - 1 - Z_t + Z_t - c}{1 + c} \leq \frac{e^{|Z_t|} - 1 - |Z_t| + Z_t - c}{1 + c}.
\]

Let \( c = \mathbb{E}[|Z_t| \mid \mathcal{F}_{t-1}] - 1 - \mathbb{E}[|Z| \mid \mathcal{F}_{t-1}] \). Hence, since \( \mathbb{E}[Z_t \mid \mathcal{F}_{t-1}] = 0 \),

\[
\mathbb{E}[\exp(Z_t - c) \mid \mathcal{F}_{t-1}] - 1 \leq \frac{\mathbb{E}[e^{|Z_t|} \mid \mathcal{F}_{t-1}] - 1 - \mathbb{E}[|Z_t| \mid \mathcal{F}_{t-1}] - c}{1 + c} = 0.
\]

Lemma 7 Suppose \( \mathbb{E}[\gamma_{ij}^t(X_t) \mid \mathcal{F}_{t-1}] = 0 \) and \( \mathbb{E}[|\gamma_{ij}^t(X_t)|^m \mid \mathcal{F}_{t-1}] \leq m! \) for all integer \( m \geq 2 \), all \( t \geq 1 \) and all \( 1 \leq i \leq j \leq d \). Then, for \( L > 1 \) we have

\[
\mathbb{E} \left[ \exp \left( \frac{1}{L} \sum_{t=1}^\tau \gamma_{ij}^t(X_t) \right) \right] \leq \exp \left( \frac{\tau}{L(L - 1)} \right).
\]

Proof

\[
\mathbb{E} \left[ \exp \left( \frac{1}{L} \sum_{t=1}^\tau \gamma_{ij}^t(X_t) \right) \right] = \mathbb{E} \left[ \mathbb{E} \left[ \exp \left( \sum_{t=1}^\tau \gamma_{ij}^t(X_t) \mid \mathcal{F}_{t-1} \right) \mid \mathcal{F}_{t-1} \right] \mathbb{E} \left[ \exp \left( \frac{\gamma_{ij}^{t-1}(X_{t-1})}{L} \right) \mid \mathcal{F}_{t-1} \right] \right]
\]

\[
\leq e^{\mathbb{E} \left[ \sum_{t=1}^{\tau-1} \gamma_{ij}^t(X_t) \mid \mathcal{F}_{t-1} \right]} \mathbb{E} \left[ \exp \left( \frac{1}{L} \sum_{t=1}^{\tau-1} \gamma_{ij}^t(X_t) \right) \right]
\]

\[
\leq e^{\mathbb{E} \left[ \sum_{t=1}^{\tau-1} \gamma_{ij}^t(X_t) \mid \mathcal{F}_{t-1} \right]} \mathbb{E} \left[ \exp \left( \frac{1}{L} \sum_{t=1}^{\tau-1} \gamma_{ij}^t(X_t) \right) \right]
\]
where the inequality is from Lemma 6 and noting that

\[
\log \mathbb{E} \left[ \exp \left( \frac{\gamma_{ij}^T (X_T)}{L} \right) \mid F_{T-1} \right] \leq \mathbb{E} \left[ e^{\frac{|\gamma_{ij}^T (X_T)|}{\tau}} - 1 \frac{|\gamma_{ij}^T (X_T)|}{L} \mid F_{T-1} \right]
\]

\[
= \mathbb{E} \left[ \sum_{m=2}^{\infty} \frac{|\gamma_{ij}^T (X_T)|^m}{L^m m!} \mid F_{T-1} \right]
\]

\[
= \sum_{m=2}^{\infty} \mathbb{E} \left[ \frac{|\gamma_{ij}^T (X_T)|^m}{L^m m!} \mid F_{T-1} \right]
\]

\[
\leq \frac{1}{L(L-1)}.
\]

Then, repeatedly applying this to the rest of the sum \( \frac{1}{L} \sum_{t=1}^{T-1} \gamma_{ij}^T (X_t) \), we have

\[
\mathbb{E} \left[ \exp \left( \frac{1}{L} \sum_{t=1}^{T} \gamma_{ij}^T (X_t) \right) \right] \leq \exp \left( \frac{\tau}{L(L-1)} \right).
\]

**Lemma 8 (Bernstein-type inequality for adapted samples)** Suppose \( \mathbb{E}[\gamma_{ij}^T (X_t) \mid F_{t-1}] = 0 \) and \( \mathbb{E}[|\gamma_{ij}^T (X_t)|^m \mid F_{t-1}] \leq m! \) for all integer \( m \geq 2 \), all \( t \geq 1 \) and all \( 1 \leq i \leq j \leq d \).

Then for all \( w > 0 \), we have

\[
P \left( \max_{1 \leq i \leq j \leq d} \left| \frac{1}{\tau} \sum_{t=1}^{\tau} \gamma_{ij}^T (X_t) \right| \geq w + \sqrt{2w} + \sqrt{\frac{4 \log(2d^2)}{\tau} + \frac{2 \log(2d^2)}{\tau}} \right) \leq \exp \left( -\frac{\tau w}{2} \right).
\]

**Proof** Using the Chernoff bound and Lemma 7, for any \( L > 1 \) we have

\[
P \left( \sum_{t=1}^{\tau} \gamma_{ij}^T (X_t) \geq a \right) = P \left( \exp \left( \frac{1}{L} \sum_{t=1}^{\tau} \gamma_{ij}^T (X_t) \right) \geq \exp \left( \frac{a}{L} \right) \right)
\]

\[
= \mathbb{E} \left[ \exp \left( \frac{1}{L} \sum_{t=1}^{\tau} \gamma_{ij}^T (X_t) \right) \mid \mathcal{F}_{T-1} \right]
\]

\[
\leq \frac{\mathbb{E} \left[ \exp \left( \frac{1}{L} \sum_{t=1}^{\tau} \gamma_{ij}^T (X_t) \right) \right]}{\exp \left( \frac{a}{L} \right)}
\]

\[
\leq \exp \left( -\frac{a}{L} \right) \exp \left( \frac{\tau}{L(L-1)} \right)
\]

\[
= \exp \left( -\frac{a}{L} + \frac{\tau}{L(L-1)} \right).
\]
Here, \( L = \frac{\tau + a + \sqrt{\tau^2 + \tau a}}{a} \) minimizes the right hand side above for \( L > 1 \). Therefore,

\[
\mathbb{P} \left( \sum_{t=1}^{\tau} \gamma_{ij}^t (X_t) \geq a \right) \leq \exp \left\{ - \frac{a^2}{\tau + a + \sqrt{\tau^2 + \tau a}} + \frac{\tau a^2}{(\tau + a + \sqrt{\tau^2 + \tau a})(\tau + \sqrt{\tau^2 + \tau a})} \right\}
\]

\[
= \exp \left\{ - \left( \frac{\sqrt{1 + a/\tau}}{1 + \sqrt{1 + a/\tau}} \right) \frac{a^2}{\tau + a + \sqrt{\tau^2 + \tau a}} \right\}
\]

\[
\leq \exp \left\{ - \frac{a^2}{2 \left( \tau + a + \sqrt{\tau^2 + \tau a} \right)} \right\}
\]

Choosing \( a = \tau \left( w + \sqrt{2w} \right) \) gives

\[
\mathbb{P} \left( \frac{1}{\tau} \sum_{t=1}^{\tau} \gamma_{ij}^t (X_t) \geq w + \sqrt{2w} \right) \leq \exp \left( - \frac{\tau w}{2} \right).
\]

Then for the maximal inequality, we first apply the union bound to (9).

\[
\mathbb{P} \left( \max_{1 \leq i \leq j \leq d} \left| \frac{1}{\tau} \sum_{t=1}^{\tau} \gamma_{ij}^t (X_t) \right| \geq w + \sqrt{2w} \right) \leq \sum_{1 \leq i \leq j \leq d} 2\mathbb{P} \left( \frac{1}{\tau} \sum_{t=1}^{\tau} \gamma_{ij}^t (X_t) \geq w + \sqrt{2w} \right)
\]

\[
\leq 2d^2 \exp \left( - \frac{\tau w}{2} \right)
\]

\[
= \exp \left( - \frac{\tau w}{2} + \log(2d^2) \right).
\]

Then,

\[
\mathbb{P} \left( \max_{1 \leq i \leq j \leq d} \left| \frac{1}{\tau} \sum_{t=1}^{\tau} \gamma_{ij}^t (X_t) \right| \geq w + \sqrt{2w} + \sqrt{\frac{4\log(2d^2)}{\tau}} + \frac{2\log(2d^2)}{\tau} \right)
\]

\[
\leq \mathbb{P} \left( \max_{1 \leq i \leq j \leq d} \left| \frac{1}{\tau} \sum_{t=1}^{\tau} \gamma_{ij}^t (X_t) \right| \geq \left( w + \frac{2\log(2d^2)}{\tau} \right) + \sqrt{2 \left( w + \frac{2\log(2d^2)}{\tau} \right)} \right)
\]

\[
= \mathbb{P} \left( \max_{1 \leq i \leq j \leq d} \left| \frac{1}{\tau} \sum_{t=1}^{\tau} \gamma_{ij}^t (X_t) \right| \geq w' + \sqrt{2w'} \right)
\]

\[
\leq \exp \left( - \frac{\tau w'}{2} + \log(2d^2) \right)
\]

\[
= \exp \left( - \frac{\tau w}{2} \right)
\]

where \( w' = w + \frac{2\log(2d^2)}{\tau} \).
A.5 Proof of Lemma 3

Proof Notice the difference between the unconditional theoretical Gram matrix $\Sigma$ and its adapted version $\mathbb{E}[X_tX_t^\top | \mathcal{F}_{t-1}]$ which is a conditional covariance matrix conditioned on the history $\mathcal{F}_{t-1}$. Recall that from Algorithm 1, in each round $t$ we choose $X_t$ given the history $\mathcal{F}_{t-1}$. More precisely, we compute $\beta_t$ based on $\mathcal{F}_{t-1}$ and choose $X_t$ which maximizes the product $X_t^\top \hat{\beta}_t$, i.e., $\arg \max_{X_t} X_t^\top \hat{\beta}_t$ where $X_t = \{X_{t,1}, X_{t,2}\}$. Hence, we can write $\mathbb{E}[X_tX_t^\top | \mathcal{F}_{t-1}]$ as the following:

$$
\mathbb{E}[X_tX_t^\top | \mathcal{F}_{t-1}] = \sum_{i=1}^2 \mathbb{E}_{X_t} \left[ X_{t,i}X_{t,i}^\top \{X_{ti} = \arg \max_{X_t} X_t^\top \hat{\beta}_t \mid \hat{\beta}_t \} \right].
$$

From Lemma 2, it follows that

$$
\mathbb{E}[X_tX_t^\top | \mathcal{F}_{t-1}] \succeq \nu^{-1} \Sigma.
$$

Now, taking an average over $t$ gives,

$$
\Sigma_T = \frac{1}{T} \sum_{t=1}^T \mathbb{E}[X_tX_t^\top | \mathcal{F}_{t-1}] \succeq \nu^{-1} \Sigma.
$$

Then, we define $\bar{\beta}$ corresponding to compatibility constant $\phi^2(\Sigma_T, S_0)$, that is,

$$
\bar{\beta} := \arg \min_{\beta} \left\{ \beta^\top \Sigma_T \beta : \|\beta S_0\|_1 \leq 3\|\beta S_0\|_1 \neq 0 \right\}.
$$

Therefore, it follows that

$$
\frac{\bar{\beta}^\top \Sigma_T \bar{\beta}}{\|\beta S_0\|_1^2} \geq \frac{\bar{\beta}^\top \Sigma \bar{\beta}}{\|\beta S_0\|_1^2} \geq \frac{\phi^2_0}{\nu} \tag{10}
$$

where the second inequality is by the compatibility condition on $\Sigma$. Thus, $\Sigma_T$ satisfies the compatibility condition with compatibility constant $\phi^2(\Sigma_T, S_0) = \phi^2_0/\nu$.

Now, noting that $\frac{1}{2x_{\max}^2} \|\Sigma_T - \hat{\Sigma}_T\|_\infty = \max_{1 \leq i, j \leq d} \frac{1}{\tau} \sum_{t=1}^T \gamma_{ij}^t(X_t)$ for $\gamma_{ij}^t(\cdot)$ defined in (8), we can use a Bernstein-type inequality for adapted samples in Lemma 8 to get

$$
P \left( \frac{\|\Sigma_T - \hat{\Sigma}_T\|_\infty}{2x_{\max}^2} \geq w + \sqrt{2w} + \sqrt{\frac{4\log(2d^2)}{\tau} + \frac{2\log(2d^2)}{\tau}} \right) \leq \exp \left( -\frac{\tau w}{2} \right).
$$

For $\tau \geq \frac{2\log(2d^2)}{\tau C_0(s_0)^2}$ where $C_0(s_0) = \min \left( \frac{1}{2}, \frac{\phi^2_0}{2560\nu x_{\max}^2} \right)$, letting $w = C_0(s_0)^2$ gives

$$
w + \sqrt{2w} + \sqrt{\frac{4\log(2d^2)}{\tau} + \frac{2\log(2d^2)}{\tau}} \leq 2 \left( C_0(s_0)^2 + \sqrt{2C_0(s_0)} \right) \leq 4C_0(s_0) \leq \frac{\phi^2_0}{64\nu x_{\max}^2} = \frac{\phi^2(\Sigma_T, S_0)}{64\nu x_{\max}^2}.
$$

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Hence,
\[
\mathbb{P}\left(\frac{\|\Sigma - \hat{\Sigma}\|_\infty}{2x_{\max}^2} \geq \frac{\phi^2(\Sigma, S_0)}{64s_0^2x_{\max}^2}\right) \leq \mathbb{P}\left(\frac{\|\Sigma - \hat{\Sigma}\|_\infty}{2x_{\max}^2} \geq w + \sqrt{2w} + \sqrt{\frac{4\log(2d^2)}{\tau}} + \frac{2\log(2d^2)}{\tau}\right)
\]
\[
\leq \exp\left(-\frac{\tau w}{2}\right)
\]
\[
= \exp\left(-\frac{\tau C_0(s_0)^2}{2}\right).
\]

Corollary 2 For \(t \geq \frac{2\log(2d^2)}{C_0(s_0)^2}\) where \(C_0(s_0) = \min\left(\frac{1}{2}, \frac{\phi_0^2}{256s_0^2x_{\max}^2}\right)\), the empirical Gram matrix \(\hat{\Sigma}_t\) satisfies the compatibility condition with compatibility constant \(\phi_t \geq \frac{\phi_0^2}{2\nu} > 0\) with probability at least \(1 - \exp\left\{-tC_0(s_0)^2/2\right\}\).

Proof We can use Corollary 1 (Bühlmann and Van De Geer (2011), Corollary 6.8) to show that the empirical Gram matrix \(\hat{\Sigma}_t\) satisfies the compatibility condition as long as \(\Sigma\) satisfies the compatibility condition. From (10), we know \(\Sigma\) satisfies the compatibility condition with compatibility constant \(\phi_0^2\nu > 0\). Then, combining Lemma 3 and Corollary 1, it follows that given \(\|\Sigma - \hat{\Sigma}\|_\infty \leq \frac{\phi_0^2}{32s_0\nu}\) for \(t \geq [T_0]\), we have
\[
\phi_t^2(\hat{\Sigma}_t, S_0) \geq \frac{\phi_0^2(\Sigma, S_0)^2}{2} \geq \frac{\phi_0^2}{2\nu} > 0.
\]
That is, \(\hat{\Sigma}_t\) satisfies the compatibility condition with compatibility constant which is at least \(\frac{\phi_0^2}{2\nu} > 0\).

Appendix B. Proof of Theorem 1

Proof First, let \(T_0 := \frac{2\log(2d^2)}{C_0(s_0)^2}\) where \(C_0(s_0) = \min\left(\frac{1}{2}, \frac{\phi_0^2}{256s_0^2x_{\max}^2}\right)\). Also, we define the high probability event \(\mathcal{E}_t:\)
\[
\mathcal{E}_t := \left\{\|\Sigma - \hat{\Sigma}\|_\infty \geq \frac{\phi_0^2}{32s_0\nu}\right\}
\]
Hence, on this event \(\mathcal{E}_t\), if \(t \geq T_0\), then from Corollary 2 we have \(\phi_t^2 \geq \frac{\phi_0^2}{2\nu}\), i.e., the compatibility condition holds in round \(t\). Slightly overloading the subscript for brevity, let \(X_t := X_{t,a_t}\) be a feature of the arm chosen in round \(t\) and \(X_{a_t}^* := X_{t,a_t}^*\) be the feature of the optimal arm in round \(t\). First, we look at the (non-expected) immediate regret \(\mathcal{R}(t) = \mathbb{E}[\text{Reg}(t)]\) in round \(t\). Notice that by Assumptions 1 and 2 and by the mean value theorem, \(\text{Reg}(t)\) is bounded by
\[
\text{Reg}(t) \leq \kappa_1 \left(\|X_{a_t}^T\beta - X_t^T\beta\|_2^2\right) \leq \kappa_1 \|X_{a_t}^* - X_t\|_2 \|\beta^*\|_2 \leq 2\kappa_1 x_{\max} b
\]
Then we can decompose the immediate regret as follows.

\[
\text{Reg}(t) = \text{Reg}(t) \mathbb{1}(t \leq T_0) + \text{Reg}(t) \mathbb{1}(t > T_0, \mathcal{E}_t) + \text{Reg}(t) \mathbb{1}(t > T_0, \mathcal{E}^c_t)
\]

\[
\leq 2\kappa_1 x_{\max} b \mathbb{1}(t \leq T_0) + \text{Reg}(t) \mathbb{1}(t > T_0, \mathcal{E}_t) + 2\kappa_1 x_{\max} b \mathbb{1}(t > T_0, \mathcal{E}^c_t)
\]

\[
= 2\kappa_1 x_{\max} b \mathbb{1}(t \leq T_0) + \text{Reg}(t) \mathbb{1} \left( \mu(X^T_t \hat{\beta}_t) \geq \mu(X^T_{a_t^*} \hat{\beta}_t), t > T_0, \mathcal{E}_t \right)
\]

\[
+ 2\kappa_1 x_{\max} b \mathbb{1}(t > T_0, \mathcal{E}^c_t)
\]

where the last equality follows from the optimality of \(X_t\) with respect to parameter \(\hat{\beta}_t\), i.e., \(X_t = \arg \max_{X \in \mathcal{X}} \mu(X^T \hat{\beta}_t)\). For the second term, we have

\[
P \left( \mu(X^T_t \hat{\beta}_t) \geq \mu(X^T_{a_t^*} \hat{\beta}_t) + \text{Reg}(t) \geq \text{Reg}(t) \right)
\]

\[
= P \left( \mu(X^T_t \hat{\beta}_t) - \mu(X^T_{a_t^*} \hat{\beta}_t) \geq \text{Reg}(t) \right)
\]

\[
\leq P \left( |\mu(X^T_t \hat{\beta}_t) - \mu(X^T_{a_t^*} \hat{\beta}_t)| + |\mu(X^T_{a_t^*} \hat{\beta}_t) - \mu(X^T_{a_t^*} \hat{\beta}^*)| \geq \text{Reg}(t) \right)
\]

\[
\leq P \left( \kappa_1 \|\hat{\beta}_t - \hat{\beta}^*\|_1 \|X_t\|_\infty + \kappa_1 \|\hat{\beta}_t - \hat{\beta}^*\|_1 \|X_{a_t^*}\|_\infty \geq \text{Reg}(t) \right)
\]

\[
\leq P \left( 2\kappa_1 \|\hat{\beta}_t - \hat{\beta}^*\|_1 \geq \text{Reg}(t) \right)
\]

where the last inequality is from the fact that each \(X_{t,i}\) is bounded. For an arbitrary constant \(g_t > 0\), we continue with expected regret \(R(t) = \mathbb{E}[\text{Reg}(t)]\) for \(t > T_0\).

\[
R(t) \leq \mathbb{E} \left[ \text{Reg}(t) \mathbb{1} \left( 2\kappa_1 \|\hat{\beta}_t - \hat{\beta}^*\|_1 \geq \text{Reg}(t), \mathcal{E}_t \right) \right] + 2\kappa_1 x_{\max} b \mathbb{P}(\mathcal{E}^c_t)
\]

\[
= \mathbb{E} \left[ \text{Reg}(t) \mathbb{1} \left( 2\kappa_1 \|\hat{\beta}_t - \hat{\beta}^*\|_1 \geq \text{Reg}(t), \text{Reg}(t) \leq \kappa_1 g_t, \mathcal{E}_t \right) \right]
\]

\[
+ \mathbb{E} \left[ \text{Reg}(t) \mathbb{1} \left( 2\kappa_1 \|\hat{\beta}_t - \hat{\beta}^*\|_1 \geq \text{Reg}(t), \text{Reg}(t) > \kappa_1 g_t, \mathcal{E}_t \right) \right] + 2\kappa_1 x_{\max} b \mathbb{P}(\mathcal{E}^c_t)
\]

\[
\leq \kappa_1 g_t + \kappa_1 \mathbb{P} \left( 2\|\hat{\beta}_t - \hat{\beta}^*\|_1 \geq g_t, \mathcal{E}_t \right) + 2\kappa_1 x_{\max} b \mathbb{P}(\mathcal{E}^c_t)
\]

Summing over all rounds after the initial \(T_0\) rounds, we have

\[
\sum_{t=[T_0]}^{T} R(t) \leq \kappa_1 \sum_{t=[T_0]}^{T} g_t + \kappa_1 \sum_{t=[T_0]}^{T} \mathbb{P} \left( 2\|\hat{\beta}_t - \hat{\beta}^*\|_1 \geq g_t, \mathcal{E}_t \right) + 2\kappa_1 x_{\max} b \sum_{t=[T_0]}^{T} \mathbb{P}(\mathcal{E}^c_t) . \tag{11}
\]

We first bound the term \(b) in (11). We choose \(g_t := \frac{2\mu \lambda}{\kappa_0 \phi^2} = \frac{4\sigma x_{\max} s_n}{\kappa_0 \phi^2} \sqrt{\frac{1 + 2 \log d}{t}}\). Then using Lemma 1, we have

\[
\mathbb{P} \left( 2\|\hat{\beta}_t - \hat{\beta}^*\|_1 \geq g_t, \mathcal{E}_t \right) \leq \frac{2}{t^2}
\]

for all \(t > T_0\). Therefore, it follows that

\[
\sum_{t=[T_0]}^{T} \mathbb{P} \left( 2\|\hat{\beta}_t - \hat{\beta}^*\|_1 \geq g_t, \mathcal{E}_t \right) \leq \sum_{t=[T_0]}^{T} \frac{2}{t^2} \leq \sum_{t=1}^{\infty} \frac{2}{t^2} \leq \frac{\pi^2}{3} < 4.
\]
For the term (a) in (11), we have $\phi_t^2 \geq \frac{\phi_0^2}{20}$ provided that event $\mathcal{E}_t$ holds. Hence, we have

$$\sum_{t=[T_0]}^{T} g_t = \sum_{t=[T_0]}^{T} \frac{4\sigma x_{\max} s_0}{\kappa_0 \phi_t^2} \sqrt{\frac{4 \log t + 2 \log d}{t}}$$

where the last inequality is from the fact that $\sum_{t=1}^{T} \frac{1}{\sqrt{t}} \leq \int_{t=0}^{T} \frac{1}{\sqrt{t}} = 2\sqrt{T}$.

Finally, for the term (c) in (11), we have from Lemma 3:

$$\sum_{t=[T_0]}^{T} \mathbb{P}(\mathcal{E}_t) \leq \sum_{t=[T_0]}^{T} \mathbb{P}\left(\|\Sigma_t - \hat{\Sigma}_t\|_{\infty} \geq \frac{\phi_0^2}{32 s_0 \nu}\right)$$

where

$$\sum_{t=1}^{T} \exp\left(-\frac{tC_0(s_0)^2}{2}\right) \leq \sum_{t=1}^{\infty} \exp\left(-\frac{tC_0(s_0)^2}{2}\right) \leq \frac{2}{C_0(s_0)^2}.$$ 




Appendix C. Proof of Theorem 2

The proof follows similar arguments as the proof of Theorem 1. The key difference is that the RE condition involves $\ell_2$ norm and therefore the analysis requires the Lasso oracle inequality of the GLM in $\ell_2$ norm, which we provide as an extension of Lemma 1.

**Corollary 3** Assume that the RE condition holds for $\hat{\Sigma}_t$ with active set $S_0$ and restricted eigenvalue $\phi_t$. For some $\delta \in (0, 1)$, let the regularization parameter $\lambda_t$ be

$$\lambda_t := 2\sigma x_{\max} \sqrt{\frac{2[\log(2/\delta) + \log d]}{t}}.$$
Then with probability at least $1 - \delta$, we have
\[
\|\hat{\beta}_t - \beta^*\|_2 \leq \frac{3\sqrt{s_0} \lambda_t}{\kappa_0 \phi_t^2}.
\]

**Proof** Continuing from (5) in Lemma 1, the RE condition can be applied to the vector $\hat{\beta} - \beta^*$ which gives
\[
\|\hat{\beta} - \beta^*\|_2^2 \leq \frac{(\hat{\beta} - \beta^*)^\top \hat{\Sigma}_t (\hat{\beta} - \beta^*)}{\phi_t^2}.
\]

(12)

Again from (5), we can use the margin condition in Lemma 5
\[
3\lambda_t \|\hat{\beta}_{S_0} - \beta^*_{S_0}\|_1 \geq 2\mathbb{E}(\hat{\beta}_n)
\geq \kappa_0 (\hat{\beta} - \beta^*)^\top \hat{\Sigma}_t (\hat{\beta} - \beta^*)
\geq \kappa_0 \phi_t^2 \|\hat{\beta} - \beta^*\|_2^2
\]

where the last inequality is from (12) applying the RE condition. Then, it follows that
\[
\kappa_0 \phi_t^2 \|\hat{\beta} - \beta^*\|_2^2 \leq 3\lambda_t \|\hat{\beta}_{S_0} - \beta^*_{S_0}\|_1
\leq 3\lambda_t \sqrt{s_0} \|\hat{\beta}_{S_0} - \beta^*_{S_0}\|_2
\leq 3\lambda_t \sqrt{s_0} \|\hat{\beta} - \beta^*\|_2.
\]

Hence, dividing the both sides by $\|\hat{\beta} - \beta^*\|_2$ and rearranging gives
\[
\|\hat{\beta} - \beta^*\|_2 \leq \frac{3\sqrt{s_0} \lambda_t}{\kappa_0 \phi_t^2}.
\]

This complete the proof. \(\blacksquare\)

C.1 Ensuring the RE Condition for the Empirical Gram Matrix

To distinguish from the compatibility constant, we introduce the definition of a generic restricted eigenvalue of matrix $M$ over active set $S_0$.

**Definition 5** The restricted eigenvalue of $M$ over $S_0$ is
\[
\phi_{RE}(M, S_0) := \min_{\beta} \left\{ \frac{\beta^\top M \beta}{\|\beta\|_2^2} : \|\beta_{S_0}\|_1 \leq 3\|\hat{\beta}_{S_0}\|_1 \neq 0 \right\}.
\]

Note that Assumption 5 only provides the RE condition for the theoretical Gram matrix $\Sigma$. Then, we follow the same arguments as in the analysis under the compatibility condition to show that $\phi_{RE}(\Sigma_t, S_0) \geq \phi_{RE}(\Sigma, S_0) > 0$, i.e., $\Sigma_t$ satisfies the RE condition.

Then using Lemma 3, we can show that $\hat{\Sigma}_t$ concentrates to $\Sigma_t$ with high probability. The following lemma (similar to Corollary 1) ensures the RE condition of $\hat{\Sigma}_t$ conditioned on the matrix concentration of the empirical Gram matrix $\hat{\Sigma}_t$. 

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Lemma 9  Suppose that the RE condition holds for $\Sigma_0$ and the index set $S$ with cardinality $s = |S|$, with restricted eigenvalue $\phi^2_{RE}(\Sigma_0, S) > 0$, and that $\|\Sigma_1 - \Sigma_0\|_\infty \leq \Delta$, where $32s\Delta \leq \phi^2_{RE}(\Sigma_0, S)$. Then, for the set $S$, the RE condition holds as well for $\Sigma_1$, with $\phi^2_{RE}(\Sigma_1, S) \geq \phi^2_{RE}(\Sigma_0, S)/2$.

Proof  The proof is an adaptation of Lemma 6.17 in Bühlmann and Van De Geer (2011) to the RE condition.

$$\left| \beta^\top \Sigma_1 \beta - \beta^\top \Sigma_0 \beta \right| = \left| \beta^\top (\Sigma_1 - \Sigma_0) \beta \right| \leq \|\Sigma_1 - \Sigma_0\|_\infty \|\beta\|_1^2 \leq \Delta \|\beta\|_1^2$$

For $\beta$ such that $\|\beta_S\| \leq 3\|\beta_S\|$, we have the RE condition satisfied for $\Sigma_0$. Hence, we have

$$\|\beta\|_1 \leq 4\|\beta_S\|_1 \leq 4\sqrt{s}\|\beta_S\|_2 \leq 4\sqrt{s}\|\beta\|_2 \leq \frac{4\sqrt{s}\|\beta\|^2}{\phi_{RE}(\Sigma_0, S)}.$$ 

Therefore, it follows that

$$\left| \beta^\top \Sigma_1 \beta - \beta^\top \Sigma_0 \beta \right| \leq \frac{16s\Delta \beta^\top \Sigma_0 \beta}{\phi^2_{RE}(\Sigma_0, S)}.$$ 

Since $\beta^\top \Sigma_0 \beta > 0$, dividing the both sides by $\beta^\top \Sigma_0 \beta$ gives

$$\left| \beta^\top \Sigma_1 \beta \right| \leq \frac{16s\Delta}{\phi^2_{RE}(\Sigma_0, S)}.$$

Now, since $32s\Delta \leq \phi^2_{RE}(\Sigma_0, S)$, it follows that

$$\frac{1}{2} \cdot \frac{\beta^\top \Sigma_0 \beta}{\|\beta\|_2^2} \leq \frac{\beta^\top \Sigma_1 \beta}{\|\beta\|_2^2} \leq \frac{3}{2} \cdot \frac{\beta^\top \Sigma_0 \beta}{\|\beta\|_2^2}.$$ 

Hence,

$$\phi^2_{RE}(\Sigma_1, S) \geq \frac{\phi^2_{RE}(\Sigma_0, S)}{2}.$$ 

C.2 Proof of Theorem 2

Proof  The proof of Theorem 2 follows the similar arguments as the proof of Theorem 1. The only difference is that we use $\ell_2$ error bound $\|\hat{\beta}_t - \beta^*\|_2$ instead of $\|\hat{\beta}_t - \beta^*\|_1$. First, note that

$$\mathbb{P} \left( \mu(X_t^\top \hat{\beta}_t) \geq \mu(X_{a_t}^\top \hat{\beta}_t) \right) \leq \mathbb{P} \left( \left| \mu(X_{a_t}^\top \hat{\beta}_t) - \mu(X_t^\top \hat{\beta}_t) \right| + \left| \mu(X_{a_t}^\top \hat{\beta}_t) - \mu(X_t^\top \beta^*) \right| \geq \text{Reg}(t) \right)$$

$$\leq \mathbb{P} \left( k_1 \|\hat{\beta}_t - \beta^*\|_2 \|X_t\|_2 + k_1 \|\hat{\beta}_t - \beta^*\|_2 \|X^*_t\|_2 \geq \text{Reg}(t) \right)$$

$$\leq \mathbb{P} \left( 2k_1 \|\hat{\beta}_t - \beta^*\|_2 \geq \text{Reg}(t) \right).$$
For an arbitrary constant $g_t > 0$, we continue with expected regret $\mathbb{E}[\text{Reg}(t)]$ for $t > T_0$.

$$R(t) \leq \kappa_1 g_t + \kappa_1 \mathbb{E} \left( 2 \| \hat{\beta}_t - \beta^* \|_2 \geq g_t, \mathcal{E}_t \right) + 2\kappa_1 x_{\max} b \mathbb{P}(\mathcal{E}_t^c).$$

Hence, the cumulative regret is bounded by

$$\sum_{t=1}^{T} R(t) \leq 2\kappa_1 x_{\max} b T_0 + \kappa_1 \sum_{t=[T_0]}^{T} g_t + \kappa_1 \sum_{t=[T_0]}^{T} \mathbb{P} \left( 2 \| \hat{\beta}_t - \beta^* \|_2 \geq g_t, \mathcal{E}_t \right) + 2\kappa_1 x_{\max} b \sum_{t=[T_0]}^{T} \mathbb{P}(\mathcal{E}_t^c).$$

Let $g_t := \frac{3\sqrt{s_0} \kappa_t}{2\kappa_0 \phi_1^2} = \frac{6\sigma x_{\max}}{\kappa_0 \phi_1^2} \sqrt{s_0 (4 \log t + 2 \log d)} t$. From Lemma 1, we have

$$\mathbb{P} \left( 2 \| \hat{\beta}_t - \beta^* \|_2 \geq g_t, \mathcal{E}_t \right) \leq \frac{2}{t^2}$$

for all $t$. Therefore, it follows that

$$\sum_{t=[T_0]}^{T} \mathbb{P} \left( 2 \| \hat{\beta}_t - \beta^* \|_2 \geq g_t, \mathcal{E}_t \right) \leq \sum_{t=1}^{T} \mathbb{P} \left( 2 \| \hat{\beta}_t - \beta^* \|_2 \geq g_t, \mathcal{E}_t \right) \leq \frac{\pi^2}{3} < 4.$$

For $t \geq T_0$, we have $\phi_1^2 \geq \frac{\phi_t^2}{\nu}$ provided that event $\mathcal{E}_t$ holds. Hence, we have

$$\sum_{t=[T_0]}^{T} g_t = \sum_{t=[T_0]}^{T} \frac{6\sigma x_{\max}}{\kappa_0 \phi_1^2} \sqrt{s_0 (4 \log t + 2 \log d)} t \leq \sum_{t=[T_0]}^{T} \frac{12 \nu \sigma x_{\max}}{\kappa_0 \phi_1^2} \sqrt{s_0 (4 \log t + 2 \log d)} t \leq \frac{12 \nu \sigma x_{\max} \sqrt{s_0 (4 \log T + 2 \log d)}}{\kappa_0 \phi_1^2} \sum_{t=1}^{T} \frac{1}{\sqrt{t}} \leq \frac{24 \nu \sigma x_{\max} \sqrt{s_0 (4 \log T + 2 \log d)}}{\kappa_0 \phi_1^2} \sqrt{T}$$

where the last inequality is from the fact that $\sum_{t=1}^{T} \frac{1}{\sqrt{t}} \leq \int_{t=0}^{T} \frac{1}{\sqrt{t}} = 2\sqrt{T}$. Combining all the results with the bounds on $T_0$ and $\sum_{t=[T_0]}^{T} \mathbb{P}(\mathcal{E}_t^c)$ from the proof of Theorem 1, the expected regret under the RE condition is bounded by

$$\mathcal{R}^\pi(T) \leq 4\kappa_1 + \frac{4\kappa_1 x_{\max} b (\log(2d^2) + 1)}{C_2(\phi_1, s_0)^2} + \frac{48\kappa_1 \nu \sigma x_{\max} \sqrt{s_0 T \log(dT)}}{\kappa_0 \phi_1^2}$$

where $C_2(\phi_1, s_0) = \min \left( \frac{1}{2}, \frac{\phi_t^2}{256 s_0 \nu x_{\max}} \right)$.
Appendix D. Regret Analysis for K-Armed Case

D.1 Proof Outline of Theorem 3

As discussed in Section 7, the analysis for the K-armed bandit mostly follows the proof of the two-armed bandit analysis in Section 5. Assuming the compatibility condition of the empirical Gram matrix $\hat{\Sigma}_t$, the Lasso oracle inequality for adapted samples in Lemma 1 can be directly applied. Hence, what we have left is ensuring the compatibility condition of $\hat{\Sigma}_t$. As before, for each $E[X_\tau X_\tau^\top | F_\tau]$ in $\Sigma_t$, the history $F_\tau$ affects how feature vector $X_\tau$ is chosen. Similar to the two-armed bandit case, we rewrite $\Sigma_t$ as

$$\Sigma_t = \frac{1}{t} \sum_{\tau=1}^t \sum_{i=1}^K \mathbb{E}_{X_\tau} [X_{\tau,i} X_{\tau,i}^\top 1 \{X_{\tau,i} = \arg\max_{X \in \mathcal{X}} X^\top \hat{\beta}_\tau\} | \hat{\beta}_\tau].$$

Recall that the compatibility condition is only assumed for the theoretical Gram matrix $\Sigma$ (Assumption 3). Again, the adapted Gram matrix $\hat{\Sigma}_t$ is used to bridge $\Sigma$ and $\hat{\Sigma}_t$ to ensure the compatibility of $\hat{\Sigma}_t$. The key difference between the two-armed bandit analysis and the K-armed bandit analysis lies in how $\Sigma_t$ is controlled by $\Sigma$. In particular, under the balanced covariance condition in Assumption 6, we show the following lemma which is a generalization of Lemma 2.

**Lemma 10** Suppose Assumption 6 holds. For a fixed vector $\beta \in \mathbb{R}^d$, we have

$$\sum_{i=1}^K \mathbb{E}_{X_\tau} [X_{\tau,i} X_{\tau,i}^\top 1 \{X_{\tau,i} = \arg\max_{X \in \mathcal{X}} X^\top \beta\}] \succ (2\nu C_X)^{-1} \Sigma.$$

With this result, we can lower-bound the compatibility constant $\phi^2(\Sigma_t, S_0)$ of the adapted Gram matrix in terms of the compatibility constant $\phi^2(\Sigma, S_0)$ for the theoretical Gram matrix. That is, we have $\Sigma_t \succ (2\nu C_X)^{-1} \Sigma$ which implies that

$$\phi^2(\Sigma_t, S_0) \geq \frac{\phi^2(\Sigma, S_0)}{2\nu C_X} > 0.$$

Hence, $\Sigma_t$ satisfies the compatibility condition. Then, we can show that $\hat{\Sigma}_t$ concentrates to $\Sigma_t$ with high probability which directly follows from applying Lemma 2, which is formally stated as follows.

**Corollary 4** For $t \geq \frac{2\log(2d^2)}{C_1(s_0)^2}$ where $C_1(s_0) = \min\left(\frac{1}{2}, \frac{\phi_0^2}{2s_0 \nu C_X x_{\text{max}}} \right)$, we have

$$\mathbb{P}\left(\|\Sigma_t - \hat{\Sigma}_t\|_\infty \geq \frac{\phi_0^2}{32 s_0 \nu C_X}\right) \leq \exp\left\{-\frac{tC_1(s_0)^2}{2}\right\}.$$

Now, we can invoke Corollary 1 to connect this matrix concentration result to guaranteeing the compatibility condition of $\hat{\Sigma}_t$. Therefore, $\hat{\Sigma}_t$ satisfies the compatibility condition with compatibility constant $\phi_2^2 = \frac{\phi_0^2}{4\nu C_X} > 0$. The rest of the proof of Theorem 3 directly follows the proof of Theorem 1 using this compatibility constant.
D.2 Proof of Lemma 10

**Proof** Since the distribution of $X_t = \{X_{t,1}, \ldots, X_{t,K}\}$ is time-invariant, we suppress the subscript on $t$ and write $X = \{X_1, \ldots, X_K\}$. Let joint distribution of $X$ as $p_X(x_1, \ldots, x_K) = p_X(x)$ where we let $x = (x_1, \ldots, x_K)$. All expectations in this proof is taken with respect to the tuple $X$. Then the theoretical Gram matrix is defined as

$$
E[X^\top X] = E \left[ \sum_{i=1}^{K} X_i X_i^\top \right] = \int (x_1 x_1^\top + \ldots + x_K x_K^\top) p_X(x) dx
$$

Let’s first focus on $\int x_1 x_1^\top p_X(x) dx$.

$$
\int x_1 x_1^\top p_X(x) dx = \int x_1 x_1^\top 1 \{ x_1 = \arg \max_{x_i \in X} x_i^\top \beta \} p_X(x) dx \\
+ \int x_1 x_1^\top 1 \{ x_1 = \arg \min_{x_i \in X} x_i^\top \beta \} p_X(x) dx \\
+ \int x_1 x_1^\top 1 \{ x_1 \neq \arg \max_{x_i \in X} x_i^\top \beta, x_1 \neq \arg \min_{x_i \in X} x_i^\top \beta \} p_X(x) dx.
$$

We define three disjoint sets of possible orderings for $\{1, \ldots, K\}$ as follows.

**Definition 6** We define the following sets of permutations of $(1, \ldots, K)$.

$$
\mathcal{I}_1^\max := \{ \text{indices } (i_1, \ldots, i_K) \text{ such that } i_K = 1 \}
$$

$$
\mathcal{I}_1^\min := \{ \text{indices } (i_1, \ldots, i_K) \text{ such that } i_1 = 1 \}
$$

$$
\mathcal{I}_1^\mid := \{ \text{indices } (i_1, \ldots, i_K) \text{ such that } i_1 \neq 1 \text{ and } i_K \neq 1 \}.
$$

Then, for $\int x_1 x_1^\top 1 \{ x_1 = \arg \min_{x_i \in X} x_i^\top \beta \} p_X(x) dx$, we can write

$$
\int x_1 x_1^\top 1 \{ x_1 = \arg \min_{x_i \in X} x_i^\top \beta \} p_X(x) dx = \sum_{(i_1, \ldots, i_K) \in \mathcal{I}_1^\min} \int x_1 x_1^\top 1 \{ x_{i_1}^\top \beta \leq \ldots \leq x_{i_K}^\top \beta \} p_X(x) dx
$$

Then for any $(i_1, \ldots, i_K) \in \mathcal{I}_1^\min$,

$$
\int x_1 x_1^\top 1 \{ x_{i_1}^\top \beta \leq \ldots \leq x_{i_K}^\top \beta \} p_X(x) dx = \int x_1 x_1^\top 1 \{ -x_{i_1}^\top \beta \geq \ldots \geq -x_{i_K}^\top \beta \} p_X(x) dx
$$

$$
\leq \nu \int x_1 x_1^\top 1 \{ -x_{i_1}^\top \beta \geq \ldots \geq -x_{i_K}^\top \beta \} p_X(-x) dx
$$

$$
= \nu \int x_1 x_1^\top 1 \{ x_{i_1}^\top \beta \geq \ldots \geq x_{i_K}^\top \beta \} p_X(x) dx
$$

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where the inequality is again from Assumption 4. Since the elements in $\mathcal{I}^\text{min}$ can be considered as reversed orderings of elements in $\mathcal{I}^\text{max}$ (and obviously $|\mathcal{I}^\text{min}| = |\mathcal{I}^\text{max}|$),

\[
\mathbb{E} \left[ X_1X_1^T \mathbb{1} \{ X_1 = \arg \min_{X \in \mathcal{X}} X^T \beta \} \right] = \int x_1x_1^T \mathbb{1} \{ x_1 = \arg \min_{x_i \in \mathcal{X}} x_i^T \beta \} p_X(x) dx \\
= \sum_{(i_1, \ldots, i_K) \in \mathcal{I}^\text{min}} \int x_1x_1^T \mathbb{1} \{ x_{i_1}^T \beta \leq \ldots \leq x_{i_K}^T \beta \} p_X(x) dx \\
\leq \sum_{(i_1, \ldots, i_K) \in \mathcal{I}^\text{min}} \nu \int x_1x_1^T \mathbb{1} \{ x_{i_1}^T \beta \geq \ldots \geq x_{i_K}^T \beta \} p_X(x) dx \\
= \nu \int x_1x_1^T \mathbb{1} \{ x_1 = \arg \max_{x_i \in \mathcal{X}} x_i^T \beta \} p_X(x) dx \\
= \nu \mathbb{E} \left[ X_1X_1^T \mathbb{1} \{ X_1 = \arg \max_{X \in \mathcal{X}} X^T \beta \} \right].
\]

Also, using the definitions of $\mathcal{I}^\text{min}$, $\mathcal{I}^\text{mid}$ and $\mathcal{I}^\text{max}$, we can rewrite $\mathbb{E} \left[ X_1X_1^T \right]$.

\[
\mathbb{E} \left[ X_1X_1^T \right] = \mathbb{E} \left[ X_1X_1^T \mathbb{1} \{ X_1 = \arg \min_{X \in \mathcal{X}} X^T \beta \} \right] + \mathbb{E} \left[ X_1X_1^T \mathbb{1} \{ X_1 = \arg \max_{X \in \mathcal{X}} X^T \beta \} \right] \\
+ \mathbb{E} \left[ X_1X_1^T \mathbb{1} \{ X_1 \neq \arg \min_{X \in \mathcal{X}} X^T \beta, X_1 \neq \arg \max_{X \in \mathcal{X}} X^T \beta \} \right] \\
= \sum_{(i_1, \ldots, i_K) \in \mathcal{I}^\text{min}} \mathbb{E} \left[ X_1X_1^T \mathbb{1} \{ X_{i_1}^T \beta < \ldots < X_{i_K}^T \beta \} \right] \\
+ \sum_{(i_1, \ldots, i_K) \in \mathcal{I}^\text{max}} \mathbb{E} \left[ X_1X_1^T \mathbb{1} \{ X_{i_1}^T \beta < \ldots < X_{i_K}^T \beta \} \right] \\
+ \sum_{(i_1, \ldots, i_K) \in \mathcal{I}^\text{mid}} \mathbb{E} \left[ X_{i_1}X_{i_1}^T \mathbb{1} \{ X_{i_1}^T \beta < \ldots < X_{i_K}^T \beta \} \right] \\
+ \sum_{(i_1, \ldots, i_K) \in \mathcal{I}^\text{mid}} \mathbb{E} \left[ X_{i_K}X_{i_K}^T \mathbb{1} \{ X_{i_1}^T \beta < \ldots < X_{i_K}^T \beta \} \right] \\
+ \sum_{(i_1, \ldots, i_K) \in \mathcal{I}^\text{mid}} \mathbb{E} \left[ X_1X_1^T \mathbb{1} \{ X_{i_1}^T \beta < \ldots < X_{i_K}^T \beta \} \right].
\]

sFrom Assumption 6, we have

\[
\mathbb{E} \left[ X_1X_1^T \mathbb{1} \{ X_{i_1}^T \beta < \ldots < X_{i_K}^T \beta \} \right] \leq C_X \mathbb{E} \left[ (X_{i_1}X_{i_1}^T + X_{i_K}X_{i_K}^T) \mathbb{1} \{ X_{i_1}^T \beta < \ldots < X_{i_K}^T \beta \} \right].
\]
Then it follows that
\[
E\left[ X_1X_1^\top \right] \approx \sum_{(i_1,...,i_K) \in T_{\text{min}}^1} E\left[ X_{i_1}X_{i_1}^\top 1 \{ X_{i_1}^\top \beta < \cdots < X_{i_K}^\top \beta \} \right] \\
+ \sum_{(i_1,...,i_K) \in T_{\text{max}}^1} E\left[ X_{i_K}X_{i_K}^\top 1 \{ X_{i_1}^\top \beta < \cdots < X_{i_K}^\top \beta \} \right] \\
+ \sum_{(i_1,...,i_K) \in T_{\text{mid}}^1} C_X E\left[ (X_{i_1}X_{i_1}^\top + X_{i_K}X_{i_K}^\top ) 1 \{ X_{i_1}^\top \beta < \cdots < X_{i_K}^\top \beta \} \right]
\]
\[ \approx \sum_{(i_1,...,i_K) \in T_{\text{min}}^1} C_X E\left[ (X_{i_1}X_{i_1}^\top + X_{i_K}X_{i_K}^\top ) 1 \{ X_{i_1}^\top \beta < \cdots < X_{i_K}^\top \beta \} \right] \\
+ \sum_{(i_1,...,i_K) \in T_{\text{mid}}^1} C_X E\left[ (X_{i_1}X_{i_1}^\top + X_{i_K}X_{i_K}^\top ) 1 \{ X_{i_1}^\top \beta < \cdots < X_{i_K}^\top \beta \} \right] \\
+ \sum_{(i_1,...,i_K) \in T_{\text{max}}^1} C_X E\left[ (X_{i_1}X_{i_1}^\top + X_{i_K}X_{i_K}^\top ) 1 \{ X_{i_1}^\top \beta < \cdots < X_{i_K}^\top \beta \} \right].
\]

Since \( T_{\text{min}}^1, T_{\text{mid}}^1 \) and \( T_{\text{max}}^1 \) are disjoint sets, we can write
\[
E\left[ X_iX_i^\top 1 \{ X_i = \arg \min_{X \in \mathcal{X}} X^\top \beta \} \right] = \sum_{(i_1,...,i_K) \in T_{\text{min}}^1} E\left[ X_{i_1}X_{i_1}^\top 1 \{ X_{i_1}^\top \beta < \cdots < X_{i_K}^\top \beta \} \right] \\
+ \sum_{(i_1,...,i_K) \in T_{\text{max}}^1} E\left[ X_{i_1}X_{i_1}^\top 1 \{ X_{i_1}^\top \beta < \cdots < X_{i_K}^\top \beta \} \right] \\
+ \sum_{(i_1,...,i_K) \in T_{\text{mid}}^1} E\left[ X_{i_1}X_{i_1}^\top 1 \{ X_{i_1}^\top \beta < \cdots < X_{i_K}^\top \beta \} \right].
\]
We can also express \( E\left[ X_iX_i^\top 1 \{ X_i = \arg \max_{X \in \mathcal{X}} X^\top \beta \} \right] \) similarly. Therefore, we have
\[
E\left[ X_1X_1^\top \right] \approx C_X \sum_{i=1}^K \left( E\left[ X_iX_i^\top 1 \{ X_i = \arg \min_{X \in \mathcal{X}} X^\top \beta \} \right] + E\left[ X_iX_i^\top 1 \{ X_i = \arg \max_{X \in \mathcal{X}} X^\top \beta \} \right] \right) \\
\approx C_X (1 + \nu) \sum_{i=1}^K E\left[ X_iX_i^\top 1 \{ X_i = \arg \max_{X \in \mathcal{X}} X^\top \beta \} \right].
\]
Then, summing \( E\left[ X_jX_j^\top \right] \) over all \( j = 1, ..., K \) gives
\[
E[X^\top X] = \sum_{j=1}^K E\left[ X_jX_j^\top \right] \approx KC_X (1 + \nu) \sum_{i=1}^K E\left[ X_iX_i^\top 1 \{ X_i = \arg \max_{X \in \mathcal{X}} X^\top \beta \} \right].
\]
Hence,
\[
\sum_{i=1}^K E\left[ X_iX_i^\top 1 \{ X_i = \arg \max_{X \in \mathcal{X}} X^\top \beta \} \right] \approx \frac{1}{C_X(1 + \nu)} \cdot \frac{1}{K} E[X^\top X] \approx (2C_X\nu)^{-1} \Sigma.
\]
D.3 Proposition 1

**Proposition 1** In the case of independent arms, both a multivariate Gaussian distribution and a uniform distribution on a unit sphere satisfy Assumption 6 with $C_X = O(1)$. For an arbitrary distribution, it holds with $C_X = (K - 1) / K_0$ where $K_0 = [(K - 1) / 2]$.

The proof of Proposition 1 involves the following few technical lemmas.

**Lemma 11** Suppose each $X_i \in \mathbb{R}^d$ is i.i.d. Gaussian with mean $\mu$ and covariance matrix $\Gamma$. For any permutation $(i_1, \ldots, i_K)$ of $(1, \ldots, K)$, any integer $k \in \{2, \ldots, K - 1\}$ and fixed $\beta$, 

$$
\mathbb{E} \left[ X_{i_k} X_{i_k}^T 1 \{ X_{i_1}^T \beta < \ldots < X_{i_k}^T \beta \} \right] \leq \mathbb{E} \left[ X_{i_k} X_{i_k}^T 1 \{ X_{i_1}^T \beta < \ldots < X_{i_k}^T \beta \} \right] + \mathbb{E} \left[ X_{i_1} X_{i_1}^T 1 \{ X_{i_1}^T \beta < \ldots < X_{i_k}^T \beta \} \right].
$$

**Proof** It suffices to show that for any $y \in \mathbb{R}^d$

$$
\mathbb{E} \left[ (X_{i_k}^T y)^2 1 \{ X_{i_1}^T \beta < \ldots < X_{i_k}^T \beta \} \right] \leq \mathbb{E} \left[ (X_{i_1}^T y)^2 1 \{ X_{i_1}^T \beta < \ldots < X_{i_k}^T \beta \} \right] + \mathbb{E} \left[ (X_{i_k}^T y)^2 1 \{ X_{i_1}^T \beta < \ldots < X_{i_k}^T \beta \} \right].
$$

Now, we can write 

$$
y = \tilde{\beta}^T y + \sum_{j=1}^{d-1} g_j g_j^T y := \beta w_0 + \sum_{j=1}^{d-1} g_j g_j^T y.
$$

where $w_0 = \beta^T y$ and $\tilde{\beta} = \beta / \|\beta\|$ and $[\tilde{\beta}, g_1, \ldots, g_{d-1}]$ form an orthonormal basis. For $i \in [N]$, we can write 

$$
X_i^T y = (X_i^T \tilde{\beta}) w_0 + X_i^T \left( \sum_{j=1}^{d-1} g_j g_j^T \right) y = (X_i^T \tilde{\beta}) w_0 + \left( \sum_{j=1}^{d-1} g_j g_j^T \right) X_i^T y.
$$

Then we define the following two random variables 

$$
U_i := X_i^T \tilde{\beta}, \quad V_i := G X_i
$$

where $G = \sum_{j=1}^{d-1} g_j g_j^T$. Then we have 

$$
\begin{bmatrix} U_i \\ V_i \end{bmatrix} \sim \mathcal{N} \left( \begin{bmatrix} \mu^T \tilde{\beta} \\ G \mu \end{bmatrix}, \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \right)
$$

where 

$$
A_{11} = \tilde{\beta}^T \Gamma \tilde{\beta} \in \mathbb{R}
$$

$$
A_{12} = A_{21} = \tilde{\beta}^T \Gamma G^T \in \mathbb{R}^{1 \times d}
$$

$$
A_{22} = GTG^T \in \mathbb{R}^{d \times d}.
$$
Then, we know from Lemma 15 that the conditional distribution \(V_i \mid U_i\) of a multivariate normal distribution is also a multivariate normal distribution. In particular, 

\[
V_i \mid U_i = u_i \sim \mathcal{N} \left( G\mu + A_{21}A_{11}^{-1}(u_i - \mu^\top \beta), B \right)
\]

where \(B = A_{22} - A_{21}A_{11}^{-1}A_{12}\). Therefore, given \(U_{ik} = u_{ik}\), we can write 

\[
X_{ik}^\top y = u_{ik}w_0 + V_{ik}^\top y \\
= u_{ik}w_0 + \left( G\mu + A_{21}A_{11}^{-1}(u_{ik} - \mu^\top \beta) + B^{1/2}Z \right)^\top y.
\]

where \(Z \sim \mathcal{N}(0, I_d)\) and \(Z \perp U_{ik}\). Rearranging gives 

\[
X_{ik}^\top y = u_{ik} \left( w_0 + A_{11}^{-1}A_{12}y \right) + \left( G\mu - A_{21}A_{11}^{-1}\mu^\top \beta \right)^\top y + Z^\top B^{1/2}y.
\]

Hence, \(X_{ik}^\top y\) is a linear function of \(u_{ik}\). Then it follows that

\[
\left( X_{ik}^\top y \right)^2 = \left[ u_{ik} \left( w_0 + A_{11}^{-1}A_{12}y \right) + \left( G\mu - A_{21}A_{11}^{-1}\mu^\top \beta \right)^\top y + Z^\top B^{1/2}y \right]^2
\]

\[
\leq \max \left\{ \left[ u_{i1} \left( w_0 + A_{11}^{-1}A_{12}y \right) + \left( G\mu - A_{21}A_{11}^{-1}\mu^\top \beta \right)^\top y + Z^\top B^{1/2}y \right] \right\}^2
\]

\[
\leq \left[ u_{i1} \left( w_0 + A_{11}^{-1}A_{12}y \right) + \left( G\mu - A_{21}A_{11}^{-1}\mu^\top \beta \right)^\top y + Z^\top B^{1/2}y \right]^2
\]

\[
+ \left[ u_{iK} \left( w_0 + A_{11}^{-1}A_{12}y \right) + \left( G\mu - A_{21}A_{11}^{-1}\mu^\top \beta \right)^\top y + Z^\top B^{1/2}y \right]^2.
\]

Therefore, it follows that

\[
\mathbb{E} \left[ (X_{ik}^\top y)^2 \mathbb{1}_{\{X_{i1}^\top \beta < ... < X_{iK}^\top \beta\}} \right]
\]

\[
\leq \mathbb{E} \left[ (X_{i1}^\top y)^2 \mathbb{1}_{\{X_{i1}^\top \beta < ... < X_{iK}^\top \beta\}} \right] + \mathbb{E} \left[ (X_{ik}^\top y)^2 \mathbb{1}_{\{X_{i1}^\top \beta < ... < X_{iK}^\top \beta\}} \right].
\]

Hence,

\[
\mathbb{E} \left[ X_{ik}^\top X_{ik}^\top \mathbb{1}_{\{X_{i1}^\top \beta < ... < X_{iK}^\top \beta\}} \right] \leq \mathbb{E} \left[ (X_{i1}^\top X_{i1}^\top + X_{ik}^\top X_{ik}^\top )\mathbb{1}_{\{X_{i1}^\top \beta < ... < X_{iK}^\top \beta\}} \right].
\]

**Lemma 12** Suppose \(X \in \mathbb{R}^d\) is uniformly distributed on the unit sphere \(S^{d-1}\) and \(K = o(d)\). For fixed vector \(\beta \in \mathbb{R}^d\) and a given integer \(k \in \{2, ..., K - 1\}\),

\[
\mathbb{E} \left[ X_{ik}^\top X_{ik}^\top \mathbb{1}_{\{X_{i1}^\top \beta < ... < X_{iK}^\top \beta\}} \right] \leq C_X \mathbb{E} \left[ (X_{i1}^\top X_{i1}^\top + X_{ik}^\top X_{ik}^\top )\mathbb{1}_{\{X_{i1}^\top \beta < ... < X_{iK}^\top \beta\}} \right].
\]

where \(C_X = \mathcal{O}(1)\).
Proof Here, we instead show directly

\[
\mathbb{E}[XX^\top] \preceq C \left( \mathbb{E}\left[ XX^\top 1 \{ X = \arg \max_{X_i \in \{X_1, \ldots, X_K\}} X_i^\top \beta \} \right] + \mathbb{E}\left[ XX^\top 1 \{ X = \arg \min_{X_i \in \{X_1, \ldots, X_K\}} X_i^\top \beta \} \right] \right)
\]

for some constant \( C \). It can be shown that if \( C = \mathcal{O}(1) \), then the claim holds with \( C_X = \mathcal{O}(1) \). Suppose \( X \in \mathbb{R}^d \) is uniformly distributed on the unit sphere \( S^{d-1} := \{ s \in \mathbb{R}^d : \| s \|_2 = 1 \} \). Then by Lemma 2 in Cambanis et al. (1981), we can write for each \( X_i \),

\[
X_i \sim \left( B_i U_{i,1}, (1 - B_i^2)^{1/2} U_{i,2} \right)
\]

where \( B_i \sim \text{beta}(\frac{1}{2}, \frac{d-1}{2}) \), \( U_{i,1} = \pm 1 \) with probability \( \frac{1}{2} \), \( U_{i,2} \sim \text{unif}(S^{d-2}) \). \( U_{i,1} \), \( U_{i,2} \) and \( B_i \) are independent of each other. Similar to the analysis of the Gaussian case, we can normalize \( \beta \) so that \( \beta = \frac{\beta}{\| \beta \|} \). Without loss of generality, assume that \( \beta = [1, 0, \ldots, 0]^\top \). That is, only the first element is non-zero. We can do this since \( X \) is spherical and rotation invariant. Then we can write

\[
\mathbb{E}\left[ XX^\top 1 \{ X = \arg \max_{X_i \in \{X_1, \ldots, X_K\}} X_i^\top \beta \} \right] = \mathbb{E}\left[ XX^\top 1 \{ X = \arg \max_{X_i \in \{X_1, \ldots, X_K\}} X_i^{(1)} \} \right]
\]

where \( X_i^{(1)} \) is the first element of \( X_i \). Similarly,

\[
\mathbb{E}\left[ XX^\top 1 \{ X = \arg \min_{X_i \in \{X_1, \ldots, X_K\}} X_i^\top \beta \} \right] = \mathbb{E}\left[ XX^\top 1 \{ X = \arg \min_{X_i \in \{X_1, \ldots, X_K\}} X_i^{(1)} \} \right].
\]

Now, from the definition of \( X \), for \( B \sim \text{beta}(\frac{1}{2}, \frac{d-1}{2}) \) we have

\[
X_i X_i^\top \mathbb{E}\left[ XX^\top \right] = \mathbb{E}\left[ \begin{array}{cc} B_i^2 & B_i \sqrt{1 - B_i^2} U_{i,1} U_{i,2}^\top \\ B_i \sqrt{1 - B_i^2} U_{i,1} U_{i,2} & (1 - B_i^2) U_{i,2} U_{i,2}^\top \end{array} \right].
\]

By the independence of \( U_{1,2} \), \( U_{2,2} \), and \( B_i \), we have

\[
\mathbb{E}[XX^\top] = \mathbb{E}\left[ \begin{array}{cc} B^2 & 0 \\ 0 & \frac{1}{d-1}(1 - B^2) I_{d-1} \end{array} \right].
\]

By the definitions of \( B_i \) and \( U_{i,1} \), it follows that

\[
\mathbb{E}\left[ XX^\top 1 \{ B = \max_{i \in \{B_{1,\ldots,B_K}\}} B_i \} \right] \preceq \mathbb{E}\left[ XX^\top 1 \{ X = \arg \max_{X_i \in \{X_1, \ldots, X_K\}} X_i^{(1)} \} \right] + \mathbb{E}\left[ XX^\top 1 \{ X = \arg \min_{X_i \in \{X_1, \ldots, X_K\}} X_i^{(1)} \} \right].
\]

Since \( \mathbb{E}[B^2] = \frac{(a+1)\alpha}{(\alpha+\beta+1)(\alpha+\beta)} \) for \( B \sim \text{beta}(\alpha, \beta) \), we have \( \mathbb{E}[B^2] = \frac{3}{d(d+2)} \) and \( \frac{1 - \mathbb{E}[B^2]}{d-1} = \frac{d+3}{d(d+2)} \) using \( \alpha = \frac{1}{2} \) and \( \beta = \frac{d-1}{2} \). Clearly, \( \lambda_{\min} (\mathbb{E}[XX^\top]) = \frac{3}{d(d+2)} \). Similarly, for the matrix \( \mathbb{E}\left[ XX^\top 1 \{ B = \max_i B_i \} \right] \), we have

\[
\mathbb{E}\left[ XX^\top 1 \{ B = \max_i B_i \} \right] = \mathbb{E}\left[ \begin{array}{cc} B^2 \mathbb{1}\{ B = \max_i B_i \} & 0 \\ 0 & \frac{1}{d-1}(1 - B^2) \mathbb{1}\{ B = \max_i B_i \} I_{d-1} \end{array} \right].
\]
Note that $\mathbb{E}[B^2 1\{B = \max_i B_i\}] = \sum_{j=1}^K \mathbb{E}[B_j^2 1\{B_j = \max_i B_i\}] \geq \mathbb{E}[B^2]$. Then, we need to show

$$C(1 - \mathbb{E}[B^2 1\{B = \max_i B_i\}]) \geq 1 - \mathbb{E}[B^2]$$

for some $C$. Note that $\mathbb{E}[B^2 1\{B = \max_i B_i\}] \leq N \mathbb{E}[B^2]$. Hence, we can show

$$C \geq \frac{1 - \mathbb{E}[B^2]}{1 - N \mathbb{E}[B^2]} = \frac{1 - \frac{3}{d(d+2)}}{1 - \frac{3K}{d(d+2)}} = \frac{d^2 + d - 3}{d^2 + d - 3K}.$$

Since $K = o(d)$, we have $C = O(1)$. Hence,

$$\mathbb{E}[XX^\top] \preceq C \mathbb{E}\left[XX^\top 1\{B = \max_i B_i\}\right]_{B_i \in \{B_1, \ldots, B_K\}} \preceq C \left(\mathbb{E}\left[XX^\top 1\{X = \arg \max X_i^{(1)}\}\right] + \mathbb{E}\left[XX^\top 1\{X = \arg \min X_i^{(1)}\}\right]\right) = C \left(\mathbb{E}\left[XX^\top 1\{X = \arg \max X_i^{\top \beta}\}\right] + \mathbb{E}\left[XX^\top 1\{X = \arg \min X_i^{\top \beta}\}\right]\right)$$

which implies $C_X = O(1)$.

**Lemma 13** Consider i.i.d. arbitrary distribution $p_X$. Fix some vector $\beta \in \mathbb{R}^d$. For a given integer $k \in \{2, \ldots, K-1\}$,

$$\mathbb{E}\left[X_k X_k^\top 1\{X_1^\top \beta < \ldots < X_k^\top \beta < \ldots < X_K^\top \beta\}\right] \preceq C_{K,k} \mathbb{E}\left[(X_1 X_1^\top + X_K X_K^\top) 1\{X_1^\top \beta < \ldots < X_K^\top \beta\}\right]$$

where $C_X = \binom{K-1}{(K-1)/2}$ assuming $K$ is odd — if $K$ is even, we can use $\lceil (K-1)/2 \rceil$.

**Proof** First notice that

$$\mathbb{E}\left[X_k X_k^\top 1\{X_1^\top \beta < \ldots < X_k^\top \beta < \ldots < X_K^\top \beta\}\right] = \mathbb{E}_V\left[V V^\top \mathbb{E}_{X_1/K,X_k} 1\{X_1^\top \beta < \ldots < X_{k-1}^\top \beta < V^\top \beta < X_{k+1}^\top \beta < \ldots < X_K^\top \beta\} \mid V\right]$$

where $X_{1:k}/X_k$ denotes $X_1, \ldots, X_{k-1}, X_{k+1}, \ldots, X_K$. Also,

$$\mathbb{E}\left[X_1 X_1^\top 1\{X_1^\top \beta < \ldots < X_K^\top \beta\}\right] = \mathbb{E}_V\left[V V^\top \mathbb{E}_{X_{1:k}} 1\{V^\top \beta < X_2^\top \beta < \ldots < X_K^\top \beta\} \mid V\right]$$

$$\mathbb{E}\left[X_K X_K^\top 1\{X_1^\top \beta < \ldots < X_K^\top \beta\}\right] = \mathbb{E}_V\left[V V^\top \mathbb{E}_{X_{k+1},K} 1\{X_1^\top \beta < \ldots < X_{K-1}^\top \beta < V^\top \beta\} \mid V\right]$$

Let $\psi(y) := \mathbb{P}(X^\top \beta \leq y)$ denote the CDF of $X^\top \beta$. Then

$$\mathbb{P}\left(X_1^\top \beta < \ldots < X_{k-1}^\top \beta < V^\top \beta < X_{k+1}^\top \beta < \ldots < X_K^\top \beta\right)$$

$$= \prod_{i=1}^{k-1} \mathbb{P}\left(X_i^\top \beta \leq V^\top \beta\right) \frac{1}{(k-1)!} \prod_{i=k+1}^{N} \mathbb{P}\left(X_i^\top \beta \geq V^\top \beta\right) \frac{1}{(K-k)!}$$

$$= \frac{1}{(k-1)! (K-k)!} \psi(V^\top \beta)^{k-1} \left(1 - \psi(V^\top \beta)\right)^{K-k}.$$
Likewise
\[
P\left(V^\top \beta < X_2^\top \beta < \cdots < X_K^\top \beta\right) = \frac{1}{(K-1)!} \left(1 - \psi(V^\top \beta)\right)^{K-1},
\]
\[
P\left(X_1^\top \beta < \cdots < X_{K-1}^\top \beta < V^\top \beta\right) = \frac{1}{(K-1)!} \psi(V^\top \beta)^{K-1}.
\]
Then, we need to show there exists \(C_{K,k}\) such that
\[
P\left(X_1^\top \beta < \cdots < X_{k-1}^\top \beta < V^\top \beta < X_{k+1}^\top \beta < \cdots < X_K^\top \beta\right)
\]
\[\leq C_{K,k} \left[P\left(V^\top \beta < X_2^\top \beta < \cdots < X_{K}^\top \beta\right) + P\left(X_1^\top \beta < \cdots < X_{K-1}^\top \beta < V^\top \beta\right)\right].
\]
That is,
\[
\frac{\psi(V^\top \beta)^{k-1} (1 - \psi(V^\top \beta))^{K-k}}{(k-1)!(K-k)!} \leq \frac{C_{K,k}}{(K-1)!} \left[\left(1 - \psi(V^\top \beta)\right)^{K-1} + \psi(V^\top \beta)^{K-1}\right].
\]
Hence,
\[
C_{K,k} \geq \binom{K-1}{k-1} \frac{\psi(V^\top \beta)^{k-1} (1 - \psi(V^\top \beta))^{K-k}}{(1 - \psi(V^\top \beta))^{K-1} + \psi(V^\top \beta)^{K-1}}.
\]
Since \(\psi(V^\top \beta) \in [0, 1]\), we have
\[
\frac{\psi(V^\top \beta)^{k-1} (1 - \psi(V^\top \beta))^{K-k}}{(1 - \psi(V^\top \beta))^{K-1} + \psi(V^\top \beta)^{K-1}} \leq 1
\]
for all \(K\) and \(k\). Hence, for \(C_{K,k} = \binom{K-1}{k-1}\),
\[
E\left[X_kX_k^\top \mathbb{1}\{X_1^\top \beta < \cdots < X_k^\top \beta < \cdots < X_K^\top \beta\}\right]
\]
\[\leq C_{K,k} E\left[(X_1X_1^\top + X_kX_k^\top)\mathbb{1}\{X_1^\top \beta < \cdots < X_K^\top \beta\}\right].
\]

Appendix E. Other lemmas

**Lemma 14 (Wainwright (2019), Theorem 2.19)** Let \(\{Z_\tau, \mathcal{F}_\tau\}_\tau\) be a martingale difference sequence, and suppose that \(Z_\tau\) is \(\sigma^2\)-sub-Gaussian in an adapted sense, i.e., for all \(\alpha \in \mathbb{R}\), \(E[e^{\alpha Z_\tau} | \mathcal{F}_{\tau-1}] \leq e^{\alpha^2 \sigma^2/2}\) almost surely. Then for all \(\gamma \geq 0\), \(P[|\sum_{\tau=1}^n Z_\tau| \geq \gamma] \leq 2 \exp[-\gamma^2/(2n\sigma^2)]\).

Note that Lemma 15 is a well-known result, but for the sake of completeness, we present its formal statement and proof.
Lemma 15 Let $X \in \mathbb{R}^d$ follow a multivariate Gaussian distribution with mean $\mu$ and covariance matrix $\Sigma$ and consider the partition of $X$ with

$$X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \sim \mathcal{N}\left( \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \right).$$

Then the conditional distribution of $X_1$ given $X_2$ is also a multivariate Gaussian distribution. In particular

$$X_1 \mid X_2 = x_2 \sim \mathcal{N}\left( \mu_1 + \Sigma_{12} \Sigma_{22}^{-1} (x_2 - \mu_2), \Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} \right).$$

**Proof** Define $Z = X_1 + AX_2$ where $A = -\Sigma_{12} \Sigma_{22}^{-1}$. Now we can write

$$\text{cov}(Z, X_2) = \text{cov}(X_1, X_2) + \text{cov}(AX_2, X_2)$$

$$= \Sigma_{12} + A \text{var}(X_2)$$

$$= \Sigma_{12} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{22}$$

$$= 0$$

Therefore $Z$ and $X_2$ are not correlated and, since they are jointly normal, they are independent. Now, clearly we have $\mathbb{E}(Z) = \mu_1 + A \mu_2$. Then

$$\mathbb{E}[X_1 \mid X_2] = \mathbb{E}[Z - AX_2 \mid X_2]$$

$$= \mathbb{E}[Z \mid X_2] - \mathbb{E}[AX_2 \mid X_2]$$

$$= \mathbb{E}[Z] - A X_2$$

$$= \mu_1 + A (\mu_2 - X_2)$$

$$= \mu_1 + \Sigma_{12} \Sigma_{22}^{-1} (X_2 - \mu_2).$$

For the covariance matrix, note that

$$\text{var}(X_1 \mid X_2) = \text{var}(Z - AX_2 \mid X_2)$$

$$= \text{var}(Z \mid X_2) + \text{var}(AX_2 \mid X_2) - A \text{cov}(Z, -X_2) - \text{cov}(Z, -X_2) A^\top$$

$$= \text{var}(Z \mid X_2)$$

$$= \text{var}(Z)$$

Hence, it follows that

$$\text{var}(X_1 \mid X_2) = \text{var}(Z)$$

$$= \text{var}(X_1 + AX_2)$$

$$= \text{var}(X_1) + A \text{var}(X_2) A^\top + A \text{cov}(X_1, X_2) + \text{cov}(X_2, X_1) A^\top$$

$$= \Sigma_{11} + \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{22} \Sigma_{22}^{-1} \Sigma_{21} - 2 \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21}$$

$$= \Sigma_{11} + \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} - 2 \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21}$$

$$= \Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21}$$

\[\Box\]

7. If a random vector has a multivariate normal distribution then any two or more of its components that are uncorrelated are independent.
Appendix F. Additional Experiment Results

F.1 Details on Experimental Setup

For feature vectors drawn from the uniform distribution, we sample each feature vector \( X \) independently from a \( d \)-dimensional hypercube \([-1, 1]^d\). For elliptically distributed feature vectors, we construct each feature vector \( X \in \mathbb{R}^d \) following the definition in Theorem 1 of Cambanis et al. (1981):

\[
X = \mu + RAU^{(k)}
\]

where \( \mu \in \mathbb{R}^d \) is a mean vector, \( U^{(k)} \in \mathbb{R}^k \) is uniformly distributed on the unit sphere in \( \mathbb{R}^k \), \( R \in \mathbb{R} \) is a random variable independent of \( U^{(k)} \), and \( A \) is a \( d \times k \)-dimensional matrix with rank \( k \). We sample \( R \) from Gaussian distribution \( \mathcal{N}(0, 1) \), and sample each element of \( A \) uniformly in \([0, 1] \). We use zero mean \( \mu = 0_d \).

F.2 Additional Results for Two-Armed Bandits

Figure 4: The plots show the \( t \)-round cumulative regret of SA LASSO BANDIT (Algorithm 1), DR LASSO BANDIT (Kim and Paik 2019), and LASSO BANDIT (Bastani and Bayati, 2020) for \( K = 2 \), \( d \in \{100, 200\} \) and varying sparsity \( s_0 \in \{5, 10, 20\} \) under no correlation between arms, \( \rho^2 = 0 \).

Figure 4 shows the evaluations in two-armed bandits with independent arms whose features are drawn from a multivariate Gaussian distribution. Comparing the numerical results in Figure 4 with those in Figure 1 and Figure 2, we observe that the performance of DR LASSO BANDIT substantially deteriorates as correlation between arms decreases whereas the performances of SA LASSO BANDIT and LASSO BANDIT decrease more gracefully with a decrease in arm correlation. Throughout these experiments, our proposed algorithm, SA LASSO BANDIT, consistently exhibits the fastest convergence to the optimal action and robust performances under various instances.
F.3 Additional Results for K-Armed Bandits

Figure 5: The plots show the $t$-round regret of SA LASSO BANDIT (Algorithm 1), DR LASSO BANDIT (Kim and Paik, 2019), and LASSO BANDIT (Bastani and Bayati, 2020) for $K = 50$ and $s_0 = 10$. The first three rows are the results with features drawn from multivariate Gaussian distributions with varying levels of correlation between arms $\rho^2 \in \{0, 0.3, 0.7\}$. In the fourth row, features are drawn from a multi-dimensional uniform distribution. In the fourth row, features are drawn from a non-Gaussian elliptical distribution. For each row, we present evaluations for varying feature dimensions, $d \in \{100, 200, 400, 800\}$.