Active Linear Regression

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Abstract

We consider the problem of active linear regression where a decision maker has to choose between several covariates to sample in order to obtain the best estimate ˆβ of the parameter β⋆ of the linear model, in the sense of minimizing E∥ ˆβ − β⋆∥2. Using bandit and convex optimization techniques we propose an algorithm to define the sampling strategy of the decision maker and we compare it with other algorithms. We provide theoretical guarantees of our algorithm in different settings, including a O(T−2) regret bound in the case where the covariates form a basis of the feature space, generalizing and improving existing results. Numerical experiments validate our theoretical findings.

1 Introduction

This paper studies the problem of sequential active learning for the estimation of linear models. Active learning is becoming more and more useful nowadays due to the exponential growth of datasets and of the cost of labeling data that may be complex and require expert knowledge (e.g. medical images). It is therefore of crucial importance to choose wisely which data to collect and to label, based on the information gathered so far. In machine learning the decision maker has often been considered as passive in the sense that the dataset is seen as an input of the machine learning task on which the decision maker has no influence. However the learner should be able to appropriately select the data. Active learning specifically studies the best ways to perform data selection (Cohn et al., 1996). The computing cost is today one of the major limiting factors of a machine learning algorithms. However all examples in a dataset play not the same role and have not equal importance (Freund et al., 1997). Bordes et al. (2005) have for example proposed a SVM algorithm where example selection yields faster training and higher accuracy compared to classical passive SVM techniques. The setting of active learning has several applications in practice. It has for example been applied to the online marketing context where one wants to estimate the potential impact of new products on customers, or in online polling systems where the different options available do not have the same variance.

There exist different methods for active learning. One of the most common is the so-called “pool-based” active learning (McCallumzy and Nigamy, 1998), where the decision maker has access to a pool of examples and chooses which one to query and to label. One other technique is the “retraining-based” active learning (Yang and Loog, 2016) where the idea is to retrain the model on well-chosen examples, for instance the ones that had the higher uncertainty. Castro and Nowak (2008)
have proven general minimax bounds for active learning, for a general class of functions, with rates depending on noise conditions and on the regularity of the decision boundary. In this paper we will focus on the case of pool-based active learning applied to the specific problem of linear regression.

Linear models, though often too simple, are widely studied and used in practice. A very rich and thorough theory on linear regression is available in the offline setting and there have been several recent works on the problem of active learning in the linear case. For example Sugiyama and Rubens (2008) have studied the problem of active learning with model selection in the linear case. More recently Sabato and Munos (2014) and then Riquelme et al. (2017) have studied the precise setting of active linear regression with stratification and thresholding techniques. Another setting similar to ours is the one of Hazan and Karnin (2014) who consider the problem of active linear regression with a hard-margin criterion. In this paper we want to minimize the classical $\ell^2$-norm of the difference between the true parameter of the linear model and its estimator.

More precisely, we consider a decision maker with a limited experimental budget who must learn a latent linear model. To this end, the decision maker builds a predictor that aims at estimating the unknown parameter associated to the linear model. In order to construct it the decision maker chooses at each time step which point (also called “covariate”) to sample, and receives a noisy output from the linear model. The quality of the predictor is measured by the expected squared error of its predictions.

Our setting can also be seen under the scope of optimal experiment design (Pukelsheim, 2006) which consists in choosing which experiment to perform, in order to minimize an objective function within a budget constraint. In experiment design the distance of the produced hypothesis to the true one is measured by the covariance matrix of the error (Boyd and Vandenberghe, 2004). There are several criterion that can be used to minimize a covariance matrix, the most popular being A, D and E-optimality. Our setting is equivalent to A-optimal design. Several algorithms have been proposed (Gao et al., 2014; Yang et al., 2013; Sagnol, 2010) to solve offline the A-optimal design problem. In this paper we are considering an online version of it.

Antos et al. (2010) have introduced a particular instance of this problem where the environment providing the data is assumed to be stochastic and i.i.d. across rounds. More precisely, they studied this problem using the framework of stochastic multi-armed bandits by considering a set of $K$ probability distributions (called arms), associated with $K$ variances, the goal being to define an allocation strategy over arms so as to estimate their expected values uniformly well. Later, this setting has also been studied by Carpentier et al. (2011) who improve their results.

Both previous works are actually focusing on the case where covariates that can be sampled are the vectors of the canonical basis of $\mathbb{R}^d$. In this paper, our main contributions are the study of the more general and challenging case where covariates form any set of cardinality $d$, generalizing and improving previous results. We also go beyond this case by considering an extension to larger set of covariates. In order to solve the problem we propose and analyze two different algorithms taking inspiration from the convex optimization and the bandit literature. We prove optimal $O(T^{-\frac{2}{3}})$ regret bounds in the case of $d$ covariate vectors and provide a weaker guarantee for more than $d$ covariates. Finally we corroborate our theoretical findings with numerical experiments.

## 2 Setting and description of the problem

### 2.1 Motivations and description of the problem

Suppose that a decision maker has access to $K \in \mathbb{N}^*$ covariates $X_1, \ldots, X_K \in \mathbb{R}^d$ that can be successively sampled (each of them several times if needed). We consider a standard linear model that generates observations $Y$:

$$Y = X^\top \beta^* + \varepsilon \quad \text{with } \beta^* \in \mathbb{R}^d.$$ 

The objective of the decision maker is to accurately estimate the unknown parameter $\beta^*$ by repeatedly sampling points in $\{X_1, \ldots, X_K\}$. We assume that each covariate has a specific and unknown variance $\sigma_k^2$, i.e., if $X_k$ is queried for the $i$-th time, then the observation is

$$Y_k^{(i)} = X_k^\top \beta^* + \varepsilon_k^{(i)} \quad \text{where } \mathbb{E}[\varepsilon_k^{(i)}] = 0, \ Var[\varepsilon_k^{(i)}] = \sigma_k^2 > 0 \quad \text{and } \varepsilon_k^{(i)} \text{ is } \kappa^2\text{-subGaussian},$$

the different $\varepsilon_k^{(i)}$ being independent from each other. In order to come up with the best estimator $\hat{\beta}$ of $\beta^*$ within a time horizon $T \in \mathbb{N}^*$, the decision maker can either choose a fixed sampling policy
We denote by $\tilde{X}$ the renormalized quantities. Developed above, the norms of the covariates have a scaling role and those can be renormalized to lie on the sphere at no cost. We are therefore going to make that assumption: for all $k \in [K], \parallel X_k \parallel_2 = 1$. This indicates that a point with high variance should certainly be sampled more than a point with low variance. The major difficulty is, as we assume, that the variance $\sigma_k^2$ is unknown! So an active algorithm for linear regression must at the same time estimate $\sigma_k^2$ and use it to optimize the loss; the fact that this loss is global, and not cumulative, makes this tradeoff "exploration vs. exploitation" much more intricate than in standard multi-armed bandit.

Let us be more precise by defining properly the global loss of a sampling policy. We denote by $T_k \geq 1$ the number of samples of covariate $X_k$, hence $T = \sum_{k=1}^K T_k$. For each $k \in [K]$, the linear model yields the following

$$\frac{\sum_{i=1}^{T_k} Y(i)}{T_k} = X_k^T \beta^* + \frac{\sum_{i=1}^{T_k} \epsilon(i)}{T_k}.$$

We denote the renormalized quantities $\tilde{Y}_k = \frac{\sum_{i=1}^{T_k} Y(i)}{\sqrt{T_k}}$, $\tilde{X}_k = \frac{\sqrt{T_k}}{\sigma_k} X_k$ and $\tilde{\epsilon}_k = \frac{\sum_{i=1}^{T_k} \epsilon(i)}{\sigma_k \sqrt{T_k}}$ so

$$\forall k \in [K], \tilde{Y}_k = \tilde{X}_k^T \beta^* + \tilde{\epsilon}_k,$$

where $\mathbb{E}[\tilde{\epsilon}] = 0$ and $\text{Var}[\tilde{\epsilon}] = 1$.

We denote by $\mathbb{X} = (\tilde{X}_1^T, \ldots, \tilde{X}_K^T)^\top \in \mathbb{R}^{d \times K}$ the induced design matrix of the policy.

Under the assumption that $\mathbb{X}$ has full rank, the above Ordinary Least Squares (OLS) problem has an optimal unbiased estimator $\hat{\beta} = (\mathbb{X}^\top \mathbb{X})^{-1} \mathbb{X}^\top \tilde{Y}$. The ultimate objective is to upper-bound $\mathbb{E}\|\hat{\beta} - \beta^*\|^2$ which can be easily rewritten as follows:

$$\mathbb{E}\|\hat{\beta} - \beta^*\|^2 = \text{Tr}((\mathbb{X}^\top \mathbb{X})^{-1}) = \text{Tr}\left(\sum_{k=1}^d \tilde{X}_k \tilde{X}_k^\top \right)^{-1} = \frac{1}{T} \text{Tr}\left(\sum_{k=1}^d \frac{p_k X_k X_k^\top}{\sigma_k^2} \right)^{-1},$$

where we have denoted for every $k \in [K], p_k = T_k / T$ the proportion of times the covariate $k$ has been sampled. By definition, $p = (p_1, \ldots, p_K) \in \Delta^K$, the simplex of dimension $K - 1$. We are now able to introduce the appropriate loss function of active linear regression. Denote by $\Omega(p)$ the sequentially constructed average design matrix, i.e.,

$$\Omega(p) = \frac{\sum_{k=1}^d p_k X_k X_k^\top}{\sigma_k^2} = \mathbb{X}^\top \mathbb{X}.$$

The objective is to minimize over $p \in \Delta^K$ the loss function $L(p) = \text{Tr}(\Omega(p)^{-1})$ with $L(p) = +\infty$ if $\Omega(p)$ is not invertible. For the problem to be non-trivial, we require that the covariates span $\mathbb{R}^d$.

**Assumption 1.** The vectors $X_1, \ldots, X_K$ span $\mathbb{R}^d$. In particular, if $K = d$, they form a basis of $\mathbb{R}^d$.

As developed above, the norms of the covariates have a scaling role and those can be renormalized to lie on the sphere at no cost. We are therefore going to make that assumption: $\forall k \in [K], \parallel X_k \parallel_2 = 1$. Notice also that $L$ is convex on the simplex $\Delta^d$, thus continuous in its relative interior $\Delta^d$.

**Proposition 1.** $L$ is strictly convex on $\Delta^d$ and continuous in its relative interior $\Delta^d$.

The proof is delayed to Appendix B. Proposition 1 implies that $L$ has a unique minimum $p^*$ in $\Delta^d$:

$$p^* = \arg\min_{p \in \Delta^d} L(p)$$

Finally, we evaluate the performance of a sampling policy in term of “regret”, i.e., the difference in loss between the optimal sampling policy and the policy in question.
Definition 1. Let \( p_T \) denotes the sampling proportions after \( T \) samples of a policy. Its regret is then

\[
R(T) = \frac{1}{T} (L(p_T) - L(p^*))
\]

We will construct active sampling algorithms that minimize this regret. A key concept is the gradient of \( L \) that can be computed as follows. Since

\[
\nabla_k \Omega(p) = X_k X_k^T / \sigma_k^2,
\]

it follows

\[
\frac{\partial L}{\partial p_k}(p) = -\text{Tr} \left( \Omega(p)^{-2} X_k X_k^T \right) = -\frac{1}{\sigma_k^2} \text{Tr} \left( X_k^T \Omega(p)^{-1} \Omega(p)^{-1} X_k \right) = -\left\| \Omega(p)^{-1} X_k / \sigma_k \right\|_2^2.
\]

We are first going to focus on the case \( K = d \). The more general case is considered in Section 5.

### 3 A naive randomized algorithm

We propose now the naive Algorithm 1 for the setting described above. It works as follows: at each round \( t \), lower confidence estimates of the variances are constructed, providing an optimistic estimate \( \hat{L} \) of the objective function \( L \). Then, the algorithm minimizes this estimate (this can be done with \( A \)-optimal design algorithms (Gao et al., 2014)). Finally the covariate \( X_k \) is sampled with probability \( \hat{p}_{t,k} \). Then feedback is collected and estimates are updated.

**Algorithm 1 Naive randomized algorithm**

**Require:** \( d, T, \delta \) confidence parameter

1: for \( 1 \leq t \leq 2d \) do
2: Sample covariate \( X_t \) modulo \( d \)
3: end for
4: \( p_{2d} \leftarrow (1/d, \ldots, 1/d) \)
5: Compute empirical variances \( \hat{\sigma}_1^2, \ldots, \hat{\sigma}_d^2 \)
6: for \( 2d + 1 \leq t \leq T \) do
7: Compute \( \hat{p}_t \in \text{argmin} \hat{L} \), where \( \hat{L} \) is the same function as \( L \), but with variances replaced by lower confidence estimates of the variances.
8: Draw \( \pi(t) \) randomly according to probabilities \( \hat{p}_t \) and sample covariate \( X_{\pi(t)} \)
9: Update \( p_{t+1} = p_t + \frac{1}{T}\alpha(t+1) - p_t \) and \( p_{t+1} \)
10: end for

**Proposition 2.** Algorithm 1 has final sampling proportions \( p_T \) such that

\[
R(T) = \frac{1}{T} (L(p_T) - L(p^*)) = O_{\Gamma, \sigma_k} \left( \sqrt{\log T} \right).
\]

The proof of this slow rate of convergence is differed to Appendix E.

### 4 A faster first-order algorithm

In this section, we improve the “slow” rates of Algorithm 1 with a different approach based on convex optimization techniques, namely the Frank-Wolfe algorithm (Berthet and Perchet, 2017).

#### 4.1 Description of the algorithm

The main algorithm is described in Algorithm 2 and uses the following idea: the arm sampled maximizes the norm of a proxy of the gradient of \( L \), corrected by some a positive error term \( \alpha(t, T_k) \). We explain in the following subsections how to choose it wisely.
Algorithm 2 Frank-Wolfe algorithm

Require: \( d, T, \delta \) confidence parameter

Require: \( N_1, \ldots, N_d \) of sum \( N \)

1: Sample each covariate \( X_k \) \( N_k \) times
2: \( p_N \leftarrow (N_1/N, \ldots, N_d/N) \)
3: Compute empirical variances \( \hat{\sigma}^2_1, \ldots, \hat{\sigma}^2_d \)
4: for \( N + 1 \leq t \leq T \) do
   5: Compute \( \nabla L(p_t) \)
   6: for \( k \in [d] \) do
   7: \( \hat{G}_k \leftarrow \nabla_k \hat{L}(p_t) - \alpha(T_k, t) \)
   8: end for
   9: \( \pi(t) \leftarrow \text{argmin}_{k \in [d]} \hat{G}_k \) and sample covariate \( X_{\pi(t)} \)
   10: Update \( p_{t+1} = p_t + \frac{1}{t+1} (e_{\pi(t+1)} - p_t) \) and update \( \hat{\sigma}^2_{\pi(t)} \)
11: end for

\( N_1, \ldots, N_d \) are the number of times each covariate is sampled at the beginning of the algorithm. This phase is needed to ensure that \( L \) is smooth. More details about that will be given with Lemma 1.

4.2 Concentration of the gradient of the loss

The cornerstone of the algorithm (and obviously its analysis) is to guarantee that the estimates of the gradients concentrate around their true value.

To simplify notations, we denote them by

\[
G_k = \frac{\partial L}{\partial p_k}(p) = -\left\| \Omega(p)^{-1} X_k / \sigma_k \right\|^2_2 \quad \text{and} \quad \hat{G}_k = -\left\| \hat{\Omega}(p)^{-1} X_k / \hat{\sigma}_k \right\|^2_2,
\]

and we can claim the following concentration arguments (whose proof is delayed to Appendix C).

Theorem 1. For every \( k \in [K] \), after having gathered \( T_k \leq T \) samples of covariates \( X_k \), the following holds with probability at least \( 1 - \delta \):

\[
G_k - \hat{G}_k \leq 678 K \sigma_{\max} / \sigma_{\min}^3 \left( \frac{1}{\sigma_k \lambda_{\min}(\Gamma)} \max_{j \in [K]} \sigma_j^2 \right)^{1/2} \cdot (\log(4TK/\delta))^{3/2} \cdot \max \left( \log(4TK/\delta) / T_k, \sqrt{\log(4TK/\delta)} / T_k \right),
\]

where \( \Gamma \) is the Gram matrix of \( X_1, \ldots, X_K \), \( \lambda_{\min}(\Gamma) \) is the smallest eigenvalue of \( \Gamma \), \( \sigma_{\max} \) and \( \sigma_{\min} \) are respectively the maximal and minimal values of \( \sigma_i \).

4.3 Analysis of the convergence of the algorithm

In convex optimization, there are several classical assumptions that can be leveraged to derive fast convergence rates. Those assumptions are typical strong convexity, positive distance from the boundary of the constraint set, and smoothness of the objective function, \( i.e. \) that it is gradient-Lipschitz. We prove in the following that the loss \( L \) satisfies them, up to the smoothness because its gradient explodes on the boundary of \( \Delta^d \). However, \( L \) is smooth on the relative interior of the simplex. Consequently we will circumvent this smoothness issue by using a technique detailed in (Fontaine et al., 2019) consisting in pre-sampling every arm a linear number of times in order to force \( p \) to be far from the boundaries of the simplex. But this requires a bit of analysis first.

The following computations and claims claims will allow us to recover classical regularity assumptions of \( L \), which are critical for our Frank-Wolfe based algorithm. These claims are proved in Appendix D. We will use the following useful notations.

\[
X_0 = \begin{pmatrix} \cdots & X_1^\top & \cdots \\ \vdots & \vdots & \vdots \\ \cdots & X_d^\top & \cdots \end{pmatrix} \quad \text{and} \quad \Gamma = X_0 X_0^\top = \text{Gram}(X_1, \ldots, X_d).
\]
The diagonal coefficients of $\Omega(p)^{-1}$ have the following explicit form

$$
\forall i \in [d], \quad (\Omega(p))_{ii}^{-1} = \sum_{j=1}^{d} \frac{\sigma_j^2 \text{Cof}(X_0)^2}{\det(X_0)^j} 1/p_j,
$$

where $\text{Cof}(G)$ is the cofactor matrix of $G$. This property translates into a simpler expression for $L$:

$$
L(p) = \frac{1}{\det(X_0)} \sum_{k=1}^{d} \frac{\sigma_k^2 \text{Cof}(X_0)^k}{p_k}.
$$

With this expression, the optimal proportion $p^*$ can be computed with the following closed form:

$$
p_k^* = \frac{\sigma_k \sqrt{\text{Cof}(G)^k}}{\sum_{i=1}^{d} \sigma_i \sqrt{\text{Cof}(G)^i}}.
$$

This yields that $L$ is strongly convex on $\Delta^d$, with strong convexity parameter

$$
\mu = 2 \det(G)^{-1} \min_i \text{Cof}(G)_i \sigma_i^2.
$$

Moreover, this also implies that $p^*$ is far away from the boundary of $\Delta^d$. Indeed, if $\eta \doteq \text{dist}(p^*, \partial \Delta^d)$ denotes this distance, then

$$
\eta = \sqrt{\frac{d}{d - 1} \sum_{i=1}^{d} \sigma_i \sqrt{\text{Cof}(G)^i}}.
$$

All these results are proved in Appendix D. It remains to recover the smoothness of $L$. This is done using a pre-sampling phase described with Lemma 1 which is proved in (Fontaine et al., 2019).

**Lemma 1.** If there exists $\alpha \in (0, 1/2)$ and $p^o \in \Delta^d$ such that $p^* \succeq \alpha p^o$ (component-wise) then the decision maker can safely sample arm $i$ at most $\alpha p^o T$ times (for all $i \in [d]$) at the beginning of the algorithm without changing the convergence results.

We have proved that $p_k^*$ is bounded away from 0 and thus a pre-sampling would be possible. However, this requires to have some estimate of each $\sigma_k^2$. The good news is that those estimate must be accurate up to some multiplicative factor (and not additive factor) so that a logarithmic number of samples of each arm is enough to get valid lower/upper bounds (see Corollary 1). Indeed, the estimate $\bar{\sigma}_k^2$ obtained satisfies, for each $k \in [d]$, that $\sigma_k^2 \in [\bar{\sigma}_k^2/2, 3\bar{\sigma}_k^2/2]$. Consequently we know that

$$
\forall k \in [d], p_k^* \geq \frac{1}{\sqrt{3} \sum_{i=1}^{d} \sigma_i \sqrt{\text{Cof}(G)^i}} \geq \frac{1}{2} p^o, \quad \text{where } p^o = \frac{\sigma_k \sqrt{\text{Cof}(G)^k}}{\sum_{i=1}^{d} \sigma_i \sqrt{\text{Cof}(G)^i}}.
$$

This will let us use Lemma 1 and with a pre-sampling stage as prescribed, $p$ is forced to remain far away from the boundaries of the simplex in the sense that $p_{t+1} \geq p_t^o/2$ at each stage $t$ subsequent to the pre-sampling, and for all $i \in [d]$. Consequently, this logarithmic phase of estimation plus linear phase of pre-sampling ensure that in the remaining of the process, $L$ is actually smooth.

**Lemma 2.** With the pre-sampling of Lemma 1, $L$ is smooth with constant $C_S$ where

$$
C_S \leq 432 \frac{\sigma_{\max}^2 \left( \sum_{k=1}^{d} \sigma_k \sqrt{\text{Cof}(G)^k} \right)^3}{\det(G) \sigma_{\min}^3 \sqrt{\text{min}_k \text{Cof}(G)^k}}.
$$

We can now state our main theorem whose proof is delayed to Appendix F; it relies on the analysis of Frank-Wolfe algorithm (Berthet and Perchet, 2017).

**Theorem 2.** Applying Algorithm 2 after having pre-sampled each arm $k \in [d]$ at most $p_k^o T/2$ times gives the following bound on the regret

$$
R(T) = \frac{1}{T} (L(p_T) - L(p^*)) = O_{\Gamma, \sigma_k} \left( \frac{\log(T)^2}{T^2} \right).
$$

The notation $O_{\Gamma, \sigma_k}$ means that there is a hidden constant depending on $\Gamma$ and on the $\sigma_k$. The explicit dependency on these parameters is given in the proof.
5 Discussion and Generalization to $K > d$

We discuss in this section the case where the number $K$ of covariate vectors is greater than $d$.

5.1 Discussion of the case $K > d$

It may be possible that the optimal $p^*$ lies on the boundary of the simplex $\Delta^K$ meaning that some arms should not be sampled. This can be easily seen if we consider that there exist two covariate points that are equal and that have different variances. The point with the lowest variance should be sampled while the point with the highest one should not. All the difficulty of an algorithm for the case where $K > d$ is to be able to detect which covariate should be sampled and which one should not.

In optimal design of experiments (Pukelsheim, 2006), this setting is called A-optimal design. It consists precisely in the following constraint minimization problem given $v_1, \ldots, v_p \in \mathbb{R}^d$:

$$\min \text{Tr} \left( \sum_{j=1}^{p} \lambda_j v_j v_j^\top \right)^{-1} \quad \text{under constraints} \quad \forall j \in \{1, \ldots, p\}, \lambda_j \geq 0 \quad \text{and} \quad \sum_{j=1}^{p} \lambda_j = 1 \quad (\text{P})$$

It is known (Pukelsheim (2006)) that the dual problem of A-optimal design consists in finding the smallest ellipsoid, in some sense, containing all the points $v_j$:

$$\max \text{Tr}(\sqrt{W})^2 \quad \text{under constraints} \quad W \succ 0^2 \quad \text{and} \quad \forall j \in \{1, \ldots, p\}, v_j^\top W v_j \leq 1 \quad (\text{D})$$

In our case the role of the ellipsoid can be easily seen with the KKT conditions.

**Proposition 3.** The points $X_k/\sigma_k$ lie within the ellipsoid defined by the matrix $\Omega(p^*)^{-2}$.

This geometric interpretation shows that the points with high variance are likely to be in the interior of the ellipsoid (because $X_k/\sigma_k$ is close from the origin) and therefore will not be sampled. Nevertheless since the variances are unknown one is not easily able to find which point has to be sampled. Figures illustrating the geometric interpretation can be found in Appendix H.

5.2 A theoretical upper-bound and a lower bound

We derive here a bound for the convergence rate of Algorithm 2 in the case where $K > d$.

**Theorem 3.** Applying Algorithm 2 with $K > d$ covariate points gives the following (certainly non-tight) bound on the regret:

$$R(T) = \frac{1}{T} \left( L(p_T) - L(p^*) \right) = O \left( \frac{\log(T)}{T^{5/4}} \right).$$

One can ask whether this result is optimal, and if it is possible to obtain a bound that is as good as the one obtained in Theorem 2. The following theorem proves a lower bound on the regret that shows that we cannot do as good as in the case where there are $d$ covariates. However the upper and lower bounds of Theorems 3 and 4 (proved in Appendix G) do not match. It is still an open question whether we can obtain better rates than $T^{-5/4}$.

**Theorem 4.** For any algorithm, there exists a set of parameters such that $R(T) \gtrsim \frac{1}{T^{3/2}}$.

6 Simulations

We finally present numerical experiments to validate our findings. We compare several algorithms for the problem of active linear regression. The first one is the most naive algorithm, that samples equally each covariate. We run also simulations for Algorithm 1 and Algorithm 2 that are described above. Finally we implement also a Thompson sampling algorithm to see how it performs on our problem.

We begin by quickly describing the Thompson sampling algorithm. We choose Normal Inverse Gamma distributions as priors for the mean and variance of each of the arms, since they are the

\footnote{\(W \succ 0\) means here that $W$ is symmetric positive definite.}
conjugate priors for gaussian likelihood with unknown mean and variance. At each time step $t$, for each arm $k \in [K]$, a value of $\hat{\sigma}_k$ is sampled from the prior distribution. An approximate value of $\nabla_k L(p)$ is computed with the $\hat{\sigma}_k$ values. The arm with the lowest gradient value is chosen and sampled. The value of this arm updates the hyperparameters of the prior distributions.

We run our experiments on synthetic data, with horizon time $T = 10^6$ and we average the results over 25 rounds. We consider covariate vectors in $\mathbb{R}^3$ of unit norm. We first present plots in the case where we consider 3 covariate vectors. We also plot the results in log–log scale in order to see the convergence speed which is given by the slope of the plot. Results on Figure 1 show that Frank-Wolfe and Thompson sampling have regret $O(1/T^2)$ as expected.

![Figure 1: Case of $K = 3$ covariates in $\mathbb{R}^3$](image)

- slope for naive: $-1.0$
- slope for randomized: $-1.9$
- slope for Frank-Wolfe & Thompson: $-2.0$

We see that Thompson sampling performs well on low-dimensional data. However the computation time for Thompson sampling is approximately 200 times slower as the Frank-Wolfe algorithm (due to the sampling of complex Normal Inverse Gamma distributions) and therefore inefficient in practice.

Figure 1 shows that Algorithm 1 performs nearly as well as Algorithm 2. However the step of minimization of $\hat{L}$ (line 7 of Algorithm 1) is very time-consuming in the case where $K > d$ (since there is no close form for $p^\star$) and leads to approximate results. Consequently Algorithm 1 is not suited for the case $K > d$. For this case we conduct similar experiments, with one additional covariate. Solving the problem with known variances shows that one covariate should not be sampled, i.e. $p^\star \in \partial \Delta^K$. However results presented in Figure 2 show that our algorithm performs well.

![Figure 2: Case of $K = 4$ covariates in $\mathbb{R}^3$](image)

- slope for naive: $-1.0$
- slope for Frank-Wolfe: $-1.9$
- slope for Thompson: $-1.9$

However the good results presented on Figure 2 are due to the fact that it is “easy” for the algorithm to detect that one covariate should not be sampled, in the sense that this covariate clearly lies in the interior of the ellipsoids mentioned in Section 5.1 and Appendix H. If we consider a more challenging
setting with two covariates that are equal but with variances separated with $1/\sqrt{T}$ we obtain the rates described in Figure 3. We see that we have an experimental convergence rate of $T^{-1.36}$ which is much slower than the rates of Figure 2, and between the rates proved in Theorems 3 and Theorem 4.

![Figure 3: Case of $K = 4$ covariates in $\mathbb{R}^3$ in a challenging setting](image)

(a) Regret as a Function of $T$

(b) Regret as a Function of $T$ in log–log scale

slope for naive: $-1.0$  slope for Frank-Wolfe: $-1.36$

7 Conclusion

We have proposed an algorithm mixing bandit and convex optimization techniques to solve the problem of active linear regression. This algorithm has proven fast and optimal rates $\tilde{O}(T^{-2})$ in the case of $d$ covariates that can be sampled in $\mathbb{R}^d$. One cannot obtain such fast rates in the more general case of $K > d$ covariates. We have therefore provided weaker results in this very challenging setting and conducted more experiments showing that the problem is indeed more difficult.

References

Antos, A., Grover, V., and Szepesvári, C. (2010). Active learning in heteroscedastic noise. *Theoretical Computer Science*, 411(29-30):2712–2728.

Berthet, Q. and Perchet, V. (2017). Fast rates for bandit optimization with upper-confidence frank-wolfe. In *Advances in Neural Information Processing Systems*, pages 2225–2234.

Bordes, A., Ertekin, S., Weston, J., and Bottou, L. (2005). Fast kernel classifiers with online and active learning. *Journal of Machine Learning Research*, 6(Sep):1579–1619.

Boyd, S. and Vandenberghe, L. (2004). *Convex optimization*. Cambridge university press.

Carpentier, A., Lazaric, A., Ghavamzadeh, M., Munos, R., and Auer, P. (2011). Upper-confidence-bound algorithms for active learning in multi-armed bandits. In *International Conference on Algorithmic Learning Theory*, pages 189–203. Springer.

Castro, R. M. and Nowak, R. D. (2008). Minimax bounds for active learning. *IEEE Transactions on Information Theory*, 54(5):2339–2353.

Chafaï, D., Guédon, O., Lecué, G., and Pajor, A. (2012). *Interactions between compressed sensing random matrices and high dimensional geometry*. Citeseer.

Cohn, D. A., Ghahramani, Z., and Jordan, M. I. (1996). Active learning with statistical models. *Journal of artificial intelligence research*, 4:129–145.

Fontaine, X., Berthet, Q., and Perchet, V. (2019). Regularized contextual bandits. In Chaudhuri, K. and Sugiyama, M., editors, *Proceedings of Machine Learning Research*, volume 89 of *Proceedings of Machine Learning Research*, pages 2144–2153. PMLR.

Freund, Y., Seung, H. S., Shamir, E., and Tishby, N. (1997). Selective sampling using the query by committee algorithm. *Machine learning*, 28(2-3):133–168.
Gao, W., Chan, P. S., Ng, H. K. T., and Lu, X. (2014). Efficient computational algorithm for optimal allocation in regression models. *Journal of Computational and Applied Mathematics, 261*:118–126.

Hazan, E. and Karnin, Z. (2014). Hard-margin active linear regression. In *International Conference on Machine Learning*, pages 883–891.

Maurer, A. and Pontil, M. (2009). Empirical bernstein bounds and sample variance penalization. *arXiv preprint arXiv:0907.3740*.

McCallumzy, A. K. and Nigamy, K. (1998). Employing em and pool-based active learning for text classification. In *Proc. International Conference on Machine Learning (ICML)*, pages 359–367. Citeseer.

Pukelsheim, F. (2006). *Optimal design of experiments*. SIAM.

Riquelme, C., Johari, R., and Zhang, B. (2017). Online active linear regression via thresholding. In *Thirty-First AAAI Conference on Artificial Intelligence*.

Sabato, S. and Munos, R. (2014). Active regression by stratification. In Ghahramani, Z., Welling, M., Cortes, C., Lawrence, N. D., and Weinberger, K. Q., editors, *Advances in Neural Information Processing Systems 27*, pages 469–477. Curran Associates, Inc.

Sagnol, G. (2010). *Optimal design of experiments with application to the inference of traffic matrices in large networks: second order cone programming and submodularity*. PhD thesis, École Nationale Supérieure des Mines de Paris.

Sugiyama, M. and Rubens, N. (2008). Active learning with model selection in linear regression. In *Proceedings of the 2008 SIAM International Conference on Data Mining*, pages 518–529. SIAM.

Vershynin, R. (2018). *High-dimensional probability: An introduction with applications in data science*, volume 47. Cambridge University Press.

Wainwright, M. J. (2019). *High-dimensional statistics: A non-asymptotic viewpoint*, volume 48. Cambridge University Press.

Wang, Q. and Chen, W. (2017). Improving regret bounds for combinatorial semi-bandits with probabilistically triggered arms and its applications. In *Neural Information Processing Systems*.

Whittle, P. (1958). A multivariate generalization of tchebichev’s inequality. *The Quarterly Journal of Mathematics*, 9(1):232–240.

Yang, M., Biedermann, S., and Tang, E. (2013). On optimal designs for nonlinear models: a general and efficient algorithm. *Journal of the American Statistical Association*, 108(504):1411–1420.

Yang, Y. and Loog, M. (2016). Active learning using uncertainty information. In *2016 23rd International Conference on Pattern Recognition (ICPR)*, pages 2646–2651. IEEE.
A Concentration Arguments

In this section we present results on the concentration of the variance for subgaussian random variables. Traditional results on the concentration of the variances (Maurer and Pontil, 2009; Carpentier et al., 2011) are obtained in the bounded setting. We propose results in a more general framework. Let us begin with some definitions.

Definition 2 (Sub-gaussian random variable). A random variable $X$ is said to be $\kappa^2$-sub-gaussian if
\[ \forall \lambda \geq 0, \quad \exp(\lambda(X - \mathbb{E}X)) \leq \exp(\lambda^2\kappa^2/2). \]

And we define its $\psi_2$-norm as
\[ \|X\|_{\psi_2} = \inf \{ t > 0 \mid \mathbb{E}[\exp(X^2/t^2)] \leq 2 \}. \]

We can bound the $\psi_2$-norm of a subgaussian random variable as stated in the following lemma that we prove in Appendix B.

Lemma 3 ($\psi_2$-norm). If $X$ is a centered $\kappa^2$-sub-gaussian random variable then
\[ \|X\|_{\psi_2} \leq 2\sqrt{2}/\sqrt{3}\kappa. \]

Proof. A proposition from (Wainwright, 2019) shows that for all $\lambda \in [0, 1)$, a sub-gaussian variable $X$ verifies
\[ \mathbb{E}\left(\frac{\lambda X^2}{2\kappa^2}\right) \leq \frac{1}{\sqrt{1 - \lambda}}. \]

Taking $\lambda = 3/4$ and defining $u = \frac{2\sqrt{2}}{\sqrt{3}}\kappa$ gives
\[ \mathbb{E}(X^2/u^2) \leq 2. \]

Consequently $\|X\|_{\psi_2} \leq u$. \qed

A wider class of random variables is the class of sub-exponential random variables that are defined as follows.

Definition 3 (Sub-exponential random variable). A random variable $X$ is said to be sub-exponential if there exists $K > 0$ such that
\[ \forall 0 \leq \lambda \leq 1/K, \quad \mathbb{E}[\exp(\lambda|X|)] \leq \exp(K\lambda). \]

And we define its $\psi_1$-norm as
\[ \|X\|_{\psi_1} = \inf \{ t > 0 \mid \mathbb{E}[\exp(|X|/t)] \leq 2 \}. \]

A result from (Vershynin, 2018) gives the following lemma, that makes a connection between subgaussian and subexponential random variables.

Lemma 4. A random variable $X$ is sub-gaussian if and only if $X^2$ is sub-exponential, and we have
\[ \|X^2\|_{\psi_1} = \|X\|_{\psi_2}^2. \]

We now want to obtain a concentration inequality on the empirical variance of a sub-gaussian random variable. We give use the following notations to define the empirical variance.

Definition 4. We define the following quantities for $n$ i.i.d repetitions of the random variable $X$.
\[ \mu = \mathbb{E}[X] \quad \text{and} \quad \hat{\mu} = \frac{1}{n} \sum_{i=1}^n X_i \]
\[ \mu^{(2)} = \mathbb{E}[X^2] \quad \text{and} \quad \hat{\mu}^{(2)} = \frac{1}{n} \sum_{i=1}^n X_i^2. \]

The variance and empirical variance are defined as follows
\[ \sigma^2 = \mu^{(2)} - \mu^2 \quad \text{and} \quad \hat{\sigma}^2 = \hat{\mu}^{(2)} - \hat{\mu}^2. \]
Here is the main theorem of the section, giving the concentration bound.

**Theorem 5.** If the random variable $X$ is centered and $\kappa^2$-sub-gaussian we have the following concentration on its empirical variance, with probability at least $1 - \delta$,

$$|\hat{\sigma}^2 - \sigma^2| \leq \frac{8}{3} \kappa^2 \cdot \max \left( \frac{\log(4/\delta)}{cn}, \sqrt{\frac{\log(4/\delta)}{cn}} \right) + 2\kappa^2 \frac{\log(4/\delta)}{n}$$

where $c = \frac{e - 1}{2e(2e - 1)} \approx 0.07$.

**Proof.** We have

$$|\hat{\sigma}^2 - \sigma^2| = |\hat{\mu}^{(2)} - \hat{\mu}^2 - (\mu^{(2)} - \mu^2)|$$

$$\leq |\hat{\mu}^{(2)} - \mu^{(2)}| + |\hat{\mu}^2 - \mu^2|$$

$$\leq |\hat{\mu}^{(2)} - \mu^{(2)}| + |\hat{\mu} - \mu||\hat{\mu} + \mu|$$

$$\leq |\hat{\mu}^{(2)} - \mu^{(2)}| + |\hat{\mu}|^2$$

since $\mu = 0$.

We now apply Hoeffding’s inequality to the $X_t$ variables that are $\kappa^2$-subgaussian, to get

$$\mathbb{P} \left( \frac{1}{n} \sum_{i=1}^{n} X_i - \mu > t \right) \leq \exp \left( - \frac{n^2 t^2}{2n\kappa^2} \right) = \exp \left( - \frac{nt^2}{2\kappa^2} \right).$$

And finally

$$\mathbb{P} \left( |\hat{\mu} - \mu| > \kappa \frac{2 \log(2/\delta)}{n} \right) \leq \delta.$$

Consequently with probability at least $1 - \delta$, $|\hat{\mu}|^2 \leq 2\kappa^2 \frac{\log(2/\delta)}{n}$.

The variables $X_t^2$ are sub-exponential random variables. We can apply Bernstein’s inequality as stated in (Chafaï et al., 2012) to get for all $t > 0$:

$$\mathbb{P} \left( \left| \frac{1}{n} \sum_{i=1}^{n} X_i^2 - \mu^{(2)} \right| > t \right) \leq 2 \exp \left( -cn \min \left( \frac{t^2}{\sigma^2}, \frac{t}{m} \right) \right)$$

$$\leq 2 \exp \left( -cn \min \left( \frac{t^2}{s^2}, \frac{t}{m} \right) \right).$$

with $c = \frac{e - 1}{2e(2e - 1)}$, $s^2 = \frac{1}{n} \sum_{i=1}^{n} \|X_i^2\|_{\psi_1}^2 \leq m^2$ and $m = \max_{i=1 \leq i \leq n} \|X_i^2\|_{\psi_1}$.

Inverting the inequality we obtain

$$\mathbb{P} \left( |\hat{\mu}^{(2)} - \mu^{(2)}| > m \cdot \max \left( \frac{\log(2/\delta)}{cn}, \sqrt{\frac{\log(2/\delta)}{cn}} \right) \right) \leq \delta.$$

And finally, with probability at least $1 - \delta$,

$$|\hat{\sigma}^2 - \sigma^2| \leq m \cdot \max \left( \frac{\log(4/\delta)}{cn}, \sqrt{\frac{\log(4/\delta)}{cn}} \right) + 2\kappa^2 \frac{\log(4/\delta)}{n}.$$

Using Lemmas 4 and 3 we obtain that $m \leq 8\kappa^2 / 3$.

This gives the expected result. □
We now state a corollary of this result.

**Corollary 1.** Under the same conditions as Theorem 5, for a logarithmic number of samples \( n \), we have
\[
|\hat{\sigma}^2 - \sigma^2| \leq \frac{1}{2} \sigma^2.
\]

### B Proof of preliminary easy results

#### B.1 Proof of Proposition 1

**Proof.** Let \( p, q \in \Delta^d \), so that \( \Omega(p) \) and \( \Omega(q) \) are invertible, and \( \lambda \in [0, 1] \). We have \( L(p) = \text{Tr}(\Omega(p)^{-1}) \) and \( L(\lambda p + (1 - \lambda)q) = \text{Tr}(\Omega(\lambda p + (1 - \lambda)q)^{-1}) \), where
\[
\Omega(\lambda p + (1 - \lambda)q) = \sum_{k=1}^{d} \frac{\lambda p_k + (1 - \lambda)q_k}{\sigma_k^2} X_k X_k^T
= \lambda \Omega(p) + (1 - \lambda)\Omega(q).
\]

It is well-known (Whittle, 1958) that the inversion is strictly convex on the set of positive definite matrices. Consequently,
\[
\Omega(\lambda p + (1 - \lambda)q)^{-1} = (\lambda \Omega(p) + (1 - \lambda)\Omega(q))^{-1} < \lambda \Omega(p)^{-1} + (1 - \lambda)\Omega(q)^{-1}.
\]

Taking the trace this gives
\[
L(\lambda p + (1 - \lambda)q) < \lambda L(p) + (1 - \lambda)L(q).
\]

Hence \( L \) is convex. \( \square \)

#### B.2 Proof of Lemma 5

**Lemma 5.** Let \( S \) be a symmetric positive definite matrix and \( D \) a diagonal matrix with strictly positive entries \( d_1, \ldots, d_n \). Then
\[
\lambda_{\min}(DSD) \geq \min_i (d_i)^2 \lambda_{\min}(S).
\]

**Proof.** Let us note \( \chi \) the characteristic polynomial of \( DSD \). We have \( \chi(X) = \det(XI_n - DSD) \). And the eigenvalues of \( DSD \) are the roots of \( \chi \).

We have \( \chi(X) = \det(XI_n - DSD) = \det(D^{-1}) \det(XD - DSD^2) = \det(XI_n - S^{1/2}D^2S^{1/2}) \), which shows that \( DSD \) and \( S^{1/2}D^2S^{1/2} \) have the same eigenvalues.

Consequently,
\[
\lambda_{\min}(DSD) = \lambda_{\min}(S^{1/2}D^2S^{1/2})
= \inf_{x \neq 0} \frac{x^T S^{1/2}D^2S^{1/2} x}{x^T x}
= \inf_{x \neq 0} \frac{x^T S^{1/2}D^2S^{1/2} x}{x^T Sx} \inf_{x \neq 0} \frac{x^T Sx}{x^T x} \inf_{x \neq 0} \frac{x^T Sx}{x^T x}
\geq \inf_{x \neq 0} \frac{\|DS^{1/2}x\|^2}{\|S^{1/2}x\|^2} \lambda_{\min}(S)
\geq \lambda_{\min}(D)^2 \lambda_{\min}(S).
\]

\( \square \)
B.3 Proof of Proposition 3

Proof. We want to minimize $L$ on the simplex $\Delta^K$. Let us introduce the Lagrangian function

$$L : (p_1, \ldots, p_K, \lambda, \mu_1, \ldots, \mu_K) \in \mathbb{R}^K \times \mathbb{R} \times \mathbb{R}^K_+ \mapsto L(p) + \lambda \sum_{k=1}^{K} p_k - (\mu, p)$$

Applying Karush-Kuhn-Tucker theorem gives that $p^*$ verifies

$$\forall k \in [d], \quad \frac{\partial L}{\partial p_k}(p^*) = 0.$$

Consequently

$$\forall k \in [d], \quad \left\| \Omega(p^*)^{-1} \frac{X_k}{\sigma_k} - \lambda - \mu_k \leq \lambda. \right\|$$

This shows that the points $X_k/\sigma_k$ lie within the ellipsoid defined by the equation $x^\top \Omega(p^*)^{-2} x \leq \lambda$. 

C Proof of Theorem 1

C.1 Insights and intermediary results

We give here the main ingredients and propositions needed for the proof.

We compute now

$$G_i - \hat{G}_i = \left\| \hat{\Omega}(p)^{-1} \frac{X_i}{\hat{\sigma}_i} - \Omega(p)^{-1} \frac{X_i}{\sigma_i} \right\|^2 \leq \left\| \hat{\Omega}(p)^{-1} \frac{X_i}{\sigma_i} - \Omega(p)^{-1} \frac{X_i}{\sigma_i} \right\|^2 \left\| \Omega(p)^{-1} \frac{X_i}{\sigma_i} + \Omega(p)^{-1} \frac{X_i}{\sigma_i} \right\|_2$$

Let us now note

$$A = \hat{\Omega}(p) \hat{\sigma}_i \quad \text{and} \quad B = \Omega(p) \sigma_i$$

We have, supposing that $\|X_k\|_2 = 1$,

$$\left\| \hat{\Omega}(p)^{-1} \frac{X_k}{\sigma_k} - \Omega(p)^{-1} \frac{X_k}{\sigma_k} \right\|_2 = \left\| (A^{-1} - B^{-1}) X_k \right\|_2 \leq \left\| A^{-1} - B^{-1} \right\|_2 \|X_k\|_2 \leq \left\| A^{-1} (B - A) B^{-1} \right\|_2 \leq \left\| A^{-1} \right\|_2 \left\| B^{-1} \right\|_2 \left\| B - A \right\|_2.$$ 

One of the quantity to bound is $\left\| B^{-1} \right\|_2$. We have

$$\left\| B^{-1} \right\|_2 = \rho(B^{-1}) = \frac{1}{\min(\text{Sp}(B))}.$$ 

We know that $\text{Sp}(B) = \sigma, \text{Sp}(\Omega(p))$. Therefore we need to find the smallest eigenvalue $\lambda$ of $\Omega(p)$. Since the matrix is invertible we know $\lambda > 0$.

We prove the following lemma in Appendix B.

**Lemma 6.** Let $X = (X_1, \cdots, X_k)^\top$. We have

$$\lambda_{\min}(\Omega(p)) \geq \min_{k \in [K]} \frac{p_k}{\sigma_k^2} \lambda_{\min}(X^\top X).$$
Proof. Let us note for all \( k \in [K] \), \( \alpha_k = \frac{\sqrt{p_k}}{\sigma_k} \) and \( Y_k = \alpha_k X_k \).

Let \( D = \begin{pmatrix} \alpha_1 & \cdots & \alpha_K \end{pmatrix} \).

We note also \( Y = \begin{pmatrix} Y_1^T & \cdots & Y_K^T \end{pmatrix} = \begin{pmatrix} \alpha_1 & \cdots & \alpha_K \end{pmatrix} \begin{pmatrix} X_1^T & \cdots & X_K^T \end{pmatrix} = DX \). We have

\[
\Omega(p) = \sum_{k=1}^K \frac{p_k}{\sigma_k^2} X_k X_k^T = \sum_{k=1}^K \frac{p_k}{\sigma_k^2} \alpha_k \alpha_k X_k X_k = Y^T Y = X^T D^2 X.
\]

And finally,

\[
\lambda_{\min}(\Omega(p)) = \lambda_{\min}(X^T D^2 X)
\]

\[
= \inf_{x \neq 0} \frac{x^T X^T D^2 X x}{x^T x}
\]

\[
= \inf_{x \neq 0} \frac{x^T X^T D^2 X x}{x^T X^T X x} \frac{x^T X^T X x}{x^T x}
\]

\[
\geq \inf_{x \neq 0} \frac{\|D X x\|_2^2}{\|X x\|_2^2} \lambda_{\min}(X^T X)
\]

\[
\geq \lambda_{\min}(D)^2 \lambda_{\min}(X^T X)
\]

\[
\geq \min_{k \in [K]} \frac{p_k}{\sigma_k^2} \lambda_{\min}(X^T X).
\]

We notice that the smallest eigenvalue of \( X^T X \) is linked to the smallest non-zero eigenvalue of the Gram matrix of \( (X_1, \ldots, X_d) \). A more precise result is given in the

Lemma 7. Let \( \Omega = \sum_{k=1}^K X_k X_k^T = X^T X \). Then Sp(\( \Omega \)) \cup \{0\} = Sp(Gram(X_1, \ldots, X_K)) \) where Gram(X_1, \ldots, X_K) is the Gram matrix of X_1, \ldots, X_K.

Proof. Let \( x \) be an eigenvector associated to the eigenvalue \( \lambda \) of \( \Omega \). Then

\[
\lambda x = \Omega x = \sum_{k=1}^K X_k (X_k, x).
\]

And for all \( i \in [K] \), if we note \( U_i = \langle x, X_i \rangle \) we have

\[
\lambda U_i = \lambda \langle x, X_i \rangle = \Omega \langle x, X_i \rangle = \sum_{k=1}^K \langle X_k, X_i \rangle \langle X_k, x \rangle = (\text{Gram}(X_1, \ldots, X_K) U)_i.
\]

Finally \( GU = \lambda U \) and \( U \) is an eigenvector associated to the eigenvalue \( \lambda \) of \( G = \text{Gram}(X_1, \ldots, X_K) \).

This directly gives the following

Proposition 4.

\[
\|B^{-1}\|_2 \leq \frac{1}{\sigma_i \lambda_{\min}(G)} \max_{k \in [K]} \frac{\sigma_k^2}{p_k}.
\]
We jump now to the bound of $\|A^{-1}\|_2$. We could obtain a similar bound to the one of $\|B^{-1}\|_2$ but it would contain $\hat{\sigma}_k$ values. Since we do not want a bound containing estimates of the variances, we prove the

**Proposition 5.**

$$\|A^{-1}\|_2 \leq 2 \|B^{-1}\|_2.$$ 

**Proof.** We have, if we note $H = A - B$, $\|A^{-1}\|_2 = \|(A + B)^{-1}\|_2 \leq \|B^{-1}\|_2 \|(I_n + B^{-1}H)^{-1}\|_2 \leq 2 \|B^{-1}\|_2$ from a certain rank. \qed

Let us now bound $\|B - A\|_2$. We have

$$\|B - A\|_2 = \left\| \sum_{k=1}^K p_k \frac{X_k X_k^\top}{\sigma_k^2} - \sum_{k=1}^K p_k \frac{X_k X_k^\top}{\hat{\sigma}_k^2} \right\|_2$$

$$= \left\| \sum_{k=1}^K p_k \frac{X_k X_k^\top}{\sigma_k^2} \left( \frac{\sigma_k^2}{\hat{\sigma}_k^2} - \frac{\hat{\sigma}_k^2}{\hat{\sigma}_k^2} \right) \right\|_2$$

$$\leq \sum_{k=1}^K p_k \left| \frac{\sigma_k}{\hat{\sigma}_k} - \frac{\hat{\sigma}_k}{\sigma_k} \right| \|X_k\|_2^2$$

$$\leq \sum_{k=1}^K p_k \left| \frac{\sigma_k}{\hat{\sigma}_k} - \frac{\hat{\sigma}_k}{\sigma_k} \right| .$$

The next step is now to use Theorem 5 in order to bound the difference $\left| \frac{\sigma_k}{\hat{\sigma}_k} - \frac{\hat{\sigma}_k}{\sigma_k} \right|$. 

**Proposition 6.** With the notations introduced above, we have

$$\|B - A\|_2 \leq 113K\sigma_{\max}^2 \kappa_{\max}^2 \cdot \max \left( \frac{\log(4TK/\delta)}{Tk}, \sqrt{\frac{\log(4TK/\delta)}{Tk}} \right).$$

**Proof.** Corollary 1 gives that for all $k \in [K]$, $\frac{1}{2}\sigma_k^2 \leq \hat{\sigma}_k^2 \leq \frac{3}{2}\sigma_k^2$.

A consequence of Theorem 5 is that for all $k \in [K]$, if we note $T_k$ the (random) number of samples of covariate $k$, we have, with probability at least $1 - \delta$,

$$\forall k \in [K], \left| \sigma_k^2 - \hat{\sigma}_k^2 \right| \leq \frac{8}{3}\kappa_k^2 \cdot \max \left( \frac{\log(4TK/\delta)}{cTk}, \sqrt{\frac{\log(4TK/\delta)}{cTk}} \right) + 2\kappa_k^2 \log(4TK/\delta) \frac{Tk}{cTk}.$$ 

We note $\Delta_k$ the r.h.s of the last equation. We begin by establishing a simple upper bound of $\Delta_k$. Using the fact that $\sqrt{1/c} \leq 1/c$ and that $8/(3c) \leq 38$, we have

$$\Delta_k \leq \frac{8}{3c} \kappa_k^2 \cdot \max \left( \frac{\log(4TK/\delta)}{Tk}, \sqrt{\frac{\log(4TK/\delta)}{Tk}} \right) + 2\kappa_k^2 \frac{\log(4TK/\delta)}{Tk}$$

$$\leq 38\kappa_k^2 \cdot \max \left( \frac{\log(4TK/\delta)}{Tk}, \sqrt{\frac{\log(4TK/\delta)}{Tk}} \right) + 2\kappa_k^2 \frac{\log(4TK/\delta)}{Tk}$$

$$\leq 40\kappa_k^2 \cdot \max \left( \frac{\log(4TK/\delta)}{Tk}, \sqrt{\frac{\log(4TK/\delta)}{Tk}} \right).$$

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Let $k \in [K]$. We have
\[
\frac{\sigma_i - \hat{\sigma}_i}{\sigma_k^2} = \frac{\sigma_i^2 - \hat{\sigma}_i^2}{\sigma_k^2 \sigma_k^2} = \frac{\sigma_i^2 - \sigma_i \sigma_k^2 + \sigma_i \sigma_k^2 - \hat{\sigma}_i^2}{\sigma_k^2 \sigma_k^2}
\leq \frac{\sigma_i (\hat{\sigma}_i^2 - \sigma_i^2)}{\sigma_k^2 \sigma_k^2} + \frac{\sigma_i - \hat{\sigma}_i}{\sigma_k^2}
\leq \frac{\sigma_i (\hat{\sigma}_i^2 - \sigma_i^2)}{\sigma_k^2 \sigma_k^2} + \frac{\sigma_i^2 - \hat{\sigma}_i^2}{\sigma_k^2 \sigma_k^2}
\leq \frac{\sigma_i (\hat{\sigma}_i^2 - \sigma_i^2)}{\sigma_k^2 \sigma_k^2} + \frac{\sigma_i^2 - \hat{\sigma}_i^2}{\sigma_k^2 \sigma_k^2}
\leq \frac{\sigma_i^2 - \sigma_k^2}{\sigma_k^2 \sigma_k^2} \frac{\sigma_i}{\sigma_k^2} + \frac{\sigma_i^2 - \hat{\sigma}_i^2}{\sigma_k^2 \sigma_k^2}
\leq \Delta_k \frac{2 \sigma_{\max}}{\sigma_{\min}^4} + \Delta_i \frac{2 \sqrt{\sigma}}{\sigma_{\min}}.
\]
Finally we have, using the fact that $T \geq T_k$ for all $k \in [K].$
\[
\| B - A \|_2 \leq \sum_{k=1}^{K} p_k \left| \frac{\sigma_i}{\sigma_k} - \frac{\hat{\sigma}_i}{\sigma_k} \right| \leq \frac{2 \sigma_{\max}}{\sigma_{\min}^4} \left( \sum_{k=1}^{K} p_k \Delta_k + \sqrt{2} \sum_{k=1}^{K} p_k \Delta_i \right)
\leq \frac{2 \sigma_{\max}}{\sigma_{\min}^4} \left( \sum_{k=1}^{K} \frac{T_k}{T} 40 \kappa_k^2 \cdot \max \left( \log \left( \frac{4TK/\delta}{T} \right), \log \left( \frac{4TK/\delta}{T} \right) \right) + \sqrt{2} \Delta_i \right)
\leq \frac{2 \sigma_{\max}}{\sigma_{\min}^4} \left( \sum_{k=1}^{K} 40 \kappa_k^2 \cdot \max \left( \log \left( \frac{4TK/\delta}{T} \right), \log \left( \frac{4TK/\delta}{T} \right) \right) + \sqrt{2} \Delta_i \right)
\leq \frac{2 \sigma_{\max}}{\sigma_{\min}^4} \left( \sum_{k=1}^{K} 80 \sigma_k^2 \cdot \max \left( \log \left( \frac{4TK/\delta}{T} \right), \log \left( \frac{4TK/\delta}{T} \right) \right) + \sqrt{2} \Delta_i \right)
\leq \left( K + \sqrt{2} \right) \frac{80 \sigma_{\max}}{\sigma_{\min}^4} \kappa_{\max}^2 \cdot \max \left( \log \left( \frac{4TK/\delta}{T} \right), \log \left( \frac{4TK/\delta}{T} \right) \right).
\]

The last quantity to bound to end the proof is $\left\| \hat{\Omega}(p)^{-1} \frac{X_k}{\sigma_k} + \Omega(p)^{-1} \frac{X_k}{\sigma_k} \right\|_2$.

**Proposition 7.** We have
\[
\left\| \hat{\Omega}(p)^{-1} \frac{X_k}{\sigma_k} + \Omega(p)^{-1} \frac{X_k}{\sigma_k} \right\|_2 \leq 3 \| B^{-1} \|_2.
\]

**Proof.** We have
\[
\left\| \hat{\Omega}(p)^{-1} \frac{X_k}{\sigma_k} + \Omega(p)^{-1} \frac{X_k}{\sigma_k} \right\|_2 = \left\| (A^{-1} + B^{-1}) X_k \right\|_2
\leq \left\| A^{-1} + B^{-1} \right\|_2 \left\| X_k \right\|_2
\leq \left\| A^{-1} - B^{-1} \right\|_2 + 2 \left\| B^{-1} \right\|_2.
\]
For $T$ sufficiently large we have $\left\| \hat{\Omega}(p)^{-1} \frac{X_k}{\sigma_k} + \Omega(p)^{-1} \frac{X_k}{\sigma_k} \right\|_2 \leq 3 \left\| B^{-1} \right\|_2$. \qed

Combining Propositions 4, 5, 6 and 7 we obtain that $G_i - \hat{G}_i \leq 6 \left\| B^{-1} \right\|_2 B - A \right\|_2$ and

$$G_i - \hat{G}_i \leq 678 K \sigma_{\text{max}} \left( \frac{1}{\sigma_1 \lambda_{\min}(\text{Gram})} \max_k \sigma_k^2 \right)^{3} \cdot \kappa_{\text{max}} \max \left( \frac{\log(4TK/\delta)}{T_i}, \frac{\sqrt{\log(4TK/\delta)}}{T_i} \right)$$

which proves Theorem 1.

D Preliminary claims for the fast rates

D.1 Preliminary lemmas

Lemma 8. The diagonal coefficients of $\Omega(p)^{-1}$ can be computed as follows:

$$\forall i \in [d], \Omega(p)^{-1}_{ii} = \sum_{j=1}^{d} \frac{\sigma_j^2 \text{Cof}(X_0^\top)}{\det(X_0^\top)} \frac{1}{p_j}.$$  

Proof. We suppose that $\forall i \in [d], p_i \neq 0$ so that $\Omega(p)$ is invertible.

We know that $\Omega(p)^{-1} = \frac{\text{Com}(\Omega(p))^T}{\det(\Omega(p))}.$

$$\det(\Omega(p)) = \det \left( \sum_{k=1}^{d} \frac{p_k X_k X_k^\top}{\sigma_k^2} \right)$$

$$= \det(\sqrt{T^{-1} X^\top} \sqrt{T^{-1} X})$$

$$= T^{-d} \det(X^\top)^2$$

$$= T^{-d} \begin{vmatrix} \hat{X}_1 & \cdots & \hat{X}_d \\ \vdots & \ddots & \vdots \\ \hat{X}_1 & \cdots & \hat{X}_d \end{vmatrix}^2$$

$$= \frac{\sqrt{p_1}}{\sigma_1} X_1 \cdots \frac{\sqrt{p_d}}{\sigma_d} X_d$$

$$= \det(X_0)^2 \frac{p_1}{\sigma_1} \cdots \frac{p_d}{\sigma_d}.$$

We now compute $\text{Com}(\Omega(p))_{ii}$. We have $\text{Com}(\Omega(p)) = \text{Com}(T^{-1/2}X^\top T^{-1/2}X) = \text{Com}(T^{-1/2}X^\top) \text{Com}(T^{-1/2}X^\top)^\top.$

Let us note $M = T^{-1/2}X = \begin{pmatrix} \ldots \frac{\sqrt{p_1}}{\sigma_1} X_1^\top \ldots \\ \vdots \\ \frac{\sqrt{p_K}}{\sigma_K} X_K^\top \ldots \end{pmatrix}.$
Therefore
\[
\text{Com}(\Omega(p))_{ij} = \sum_{j=1}^{d} \text{Com}(M^T)_{ij}^2
\]
\[
= \sum_{j=1}^{d} \prod_{k \neq j} \frac{p_k}{\sigma_k^2} \text{Cof}(X_0^\top)_{ij}^2.
\]

Finally,
\[
\Omega(p)_{ii} = \sum_{j=1}^{d} \frac{\sigma_j^2 \text{Cof}(X_0^\top)_{ij}^2}{\det(X_0^\top X_0)} \frac{1}{p_j}.
\]

\[\square\]

**Lemma 9.** We have, for all \( p \in \Delta^d \),
\[
L(p) = \frac{1}{\det(X_0^\top X_0)} \sum_{k=1}^{d} \frac{\sigma_k^2}{p_k} \text{Com}(X_0 X_0^\top)_{kk}.
\]

**Proof.** Using Lemma 8 we obtain
\[
L(p) = \text{Tr}(\Omega(p)^{-1})
\]
\[
= \sum_{k=1}^{d} \Omega(p)_{kk}^{-1}
\]
\[
= \frac{1}{\det(X_0^\top X_0)} \sum_{k=1}^{d} \frac{\sigma_k^2}{p_k} \sum_{i=1}^{d} \text{Cof}(X_0^\top)_{ik}^2
\]
\[
= \frac{1}{\det(X_0^\top X_0)} \sum_{k=1}^{d} \frac{\sigma_k^2}{p_k} \text{Com}(X_0 X_0^\top)_{kk}.
\]

\[\square\]

**Lemma 10.** For all \( k \in [d] \), we have
\[
p_k^* = \frac{\sigma_k \sqrt{\text{Cof}(\Gamma)_{kk}}}{\sum_{i=1}^{d} \sigma_i \sqrt{\text{Cof}(\Gamma)_{ii}}},
\]
where \( \Gamma = \text{Gram}(X_1, \ldots, X_d) \).

**Proof.** We want to minimize \( L \) over the simplex. Using KKT conditions, we obtain that all \( \frac{\partial L(p)}{\partial p_k} \) have to be equal. Therefore there exists \( \lambda \) such that for all \( k \in [K] \),
\[
\frac{\text{Cof}(\Gamma)_{kk} \sigma_k^2}{\det(\Gamma) p_k^2} = \lambda
\]
and finally
\[
p_k^* = \frac{\sigma_k \sqrt{\text{Cof}(\Gamma)_{kk}}}{\sum_{i=1}^{d} \sigma_i \sqrt{\text{Cof}(\Gamma)_{ii}}} > 0.
\]

\[\square\]

**Lemma 11.** \( L \) is strongly convex on \( \Delta^d \), with strong convexity parameter
\[
\mu = \frac{2}{\det(\Gamma)} \min_i \text{Com}(\Gamma)_{ii} \sigma_i^2.
\]

**Proof.** We have, using Lemma 9, that \( \nabla^2 L(p) \) is a diagonal matrix and that for all \( i \in [d] \),
\[
\nabla^2 L(p)_{ii} = \frac{\text{Com}(\Gamma)_{ii} \sigma_i^2}{\det(\Gamma)} \geq \frac{2 \text{Com}(\Gamma)_{ii} \sigma_i^2}{\det(\Gamma)}.
\]

\[\square\]
Lemma 12. Let \( \eta = \text{dist}(p^*, \partial \Delta^d) \) be the distance from \( p^* \) to the boundary of the simplex. We have

\[
\eta = \sqrt{\frac{K}{K-1} \min_i \sigma_i \sqrt{\text{Cof}(\Gamma)_{ii}}}.
\]

Proof. This is immediate with Lemma 10 since \( \eta = \sqrt{\frac{K}{K-1} \min_i p_i^*} \). \( \Box \)

D.2 Proof of Lemma 2

Proof. We use the fact that for all \( i \in [d], p_i \geq p_i^o / 2 \). As in the proof of Lemma 11 we have that for all \( i \in [d] \),

\[
\nabla_{ii}^2 L(p) = \frac{\text{Cof}(\Gamma)_{ii} \sigma_i^2}{\text{det}(\Gamma)} \frac{2}{p_i^o} \leq 2 \frac{\text{Cof}(\Gamma)_{ii} \sigma_i^2}{\text{det}(\Gamma)(p_i^o / 2)^2}.
\]

We have \( p_i^o = \frac{\sigma_k \sqrt{\text{Cof}(\Gamma)_{kk}}}{\sum_{i=1}^d \sigma_i \sqrt{\text{Cof}(\Gamma)_{ii}}} \) which gives

\[
\nabla_{ii}^2 L(p) \leq 16 \frac{\sigma_{\max}^2 \left( \sum_{k=1}^d \sigma_k \sqrt{\text{Cof}(\Gamma)_{kk}} \right)^3}{\text{det}(\Gamma) \sigma_{\min}^3 \sqrt{\min_k \text{Cof}(\Gamma)_{kk}}} \doteq C_S.
\]

And consequently \( L \) is \( C_S \)-Lipschitz smooth.

We can obtain an upper bound on \( C_S \) using Corollary 1, which tells that \( \sigma_k / 2 \leq \sigma_k \leq 3\sigma_k / 2 \):

\[
C_S \leq 432 \frac{\sigma_{\max}^2 \left( \sum_{k=1}^d \sigma_k \sqrt{\text{Cof}(\Gamma)_{kk}} \right)^3}{\text{det}(\Gamma) \sigma_{\min}^3 \sqrt{\min_k \text{Cof}(\Gamma)_{kk}}}.
\]

\( \Box \)

E Proof of Proposition 2

Proof. We now conduct the analysis of Algorithm 1. Our strategy will be to convert the error \( L(p_T) - L(p^*) \) into a sum over \( t \in [T] \) of small errors. Notice first that the quantity

\[
\left\| \Omega(p)^{-1} X_k \right\|_2^2
\]

can be upper bounded by \( \frac{1}{\sigma_k \lambda_{\min}(G)} \max_{k \in [K]} \frac{\sigma_k^2}{0.5p_0} \), for \( p = p_T \). For \( p = \hat{p}_t \), we can also bound this quantity by \( \frac{4}{\sigma_k \lambda_{\min}(G)} \max_{k \in [K]} \frac{\sigma_k^2}{0.5p_0} \), using Lemma 1 to express \( \hat{p}_t \) with respect to lower estimates of the variances — and thus with respect to real variance thanks to Corollary 1. Then, from the convexity of \( L \), we have

\[
L(p_T) - L(p^*) = L(p_T) - L \left( \frac{1}{T} \sum_{t=1}^T \hat{p}_t \right) + L \left( \frac{1}{T} \sum_{t=1}^T \hat{p}_t \right) - L(p^*)
\]

\[
\leq \sum_k - \left\| \Omega(p_T)^{-1} X_k \right\|_2^2 \left( p_{k,T} - 1/T \sum_{t=1}^T \hat{p}_{k,t} \right) + 1/T \sum_{t=1}^T (L(\hat{p}_t) - L(p^*))
\]

Using Hoeffding inequality, \( \left| p_{k,T} - 1/T \sum_{t=1}^T \hat{p}_{k,t} \right| = 1/T \sum_{t=1}^T (1 \{ k \text{ is sampled at round } t \} - \hat{p}_{k,t}) \)

is bounded by \( \sqrt{\frac{\log(2/\delta)}{T}} \) with probability \( 1 - \delta \). It thus remains to bound the second term.
1/T \sum_{t=1}^{T} (L(\hat{p}_t) - L(p^*))$. First, notice that $L(p)$ is an increasing function of $\sigma_i$ for any $i$. If we define $\hat{L}$ be replacing each $\sigma_i^2$ by lower confidence estimates of the variances $\tilde{\sigma}_i^2$ (see Theorem 5), then

$$L(\hat{p}_t) - L(p^*) \leq L(\hat{p}_t) - \hat{L}(p^*) = L(\hat{p}_t) - \hat{L}(\hat{p}_t) + \hat{L}(p^*) \leq L(\hat{p}_t) - \hat{L}(\hat{p}_t).$$

Since the gradient of $L$ with respect to $\sigma^2$ is \( \left( \frac{2\mu_i}{\sigma_i^3} \| \Omega(p)^{-1} \|_2^2 \right)_i \), we can bound $L(\hat{p}_t) - \hat{L}(\hat{p}_t)$ by

$$1/\sigma_{\min}^3 \sup_k \| \Omega(\hat{p}_t)^{-1} X_k \|_2^2 \sum_i 2\hat{p}_i |\sigma_i^2 - \tilde{\sigma}_i^2|.$$ 

Since $\hat{p}_i$ is the probability of having a feedback from covariate $i$, we can use the probabilistically triggered arm setting of Wang and Chen (2017) to prove that $1/T \sum_{t=1}^{T} 2\hat{p}_i |\sigma_i^2 - \tilde{\sigma}_i^2| = \mathcal{O}\left( \sqrt{\frac{\log(T)}{T}} \right)$. Taking $\delta$ of order $T^{-1}$ gives the desired result.

**F Proof of Theorem 2**

**Proof.** Theorem 1 gives that

$$|G_i - \hat{G}_i| \leq 678 K \frac{\sigma_{\max}}{\sigma_{\min}} \left( \frac{1}{\sigma_{\min}(\text{Gram})} \max_{k \in [K]} \frac{\sigma_k^2}{p_k} \right)^{\frac{3}{2}} \frac{1}{\lambda_{\min}(\Gamma)^3} \sqrt{\frac{\log(4TK/\delta)}{T_i}} \cdot \sqrt{\frac{\log(4TK/\delta)}{T_i}}.$$ 

Since each arm has been sampled at least a linear number of times we guarantee that $\log(4TK/\delta)/T_i \leq 1$ such that

$$|G_i - \hat{G}_i| \leq 678 K \left( \frac{\sigma_{\max}}{\sigma_{\min}} \right)^{\frac{3}{2}} \frac{1}{\lambda_{\min}(\Gamma)^3} \frac{1}{\lambda_{\min}(\Gamma)^3} \sqrt{\frac{\log(4TK/\delta)}{T_i}}.$$ 

Thanks to the presampling phase of Lemma 1, we know that $p_{\min} \geq p^2/2$. For the sake of clarity we note $C \approx 678 K \left( \frac{\sigma_{\max}}{\sigma_{\min}} \right)^{\frac{3}{2}} \frac{1}{\lambda_{\min}(\Gamma)^3} \frac{1}{\lambda_{\min}(\Gamma)^3} \sqrt{\frac{\log(4TK/\delta)}{T_i}}.$

Lemmas 11, 2 and 12 show that $L$ is $\mu$-strongly convex, $C_L$-smooth and that $\text{dist}(p^*, \partial \Delta^d) \geq \eta$. Consequently, since Lemma 1 shows that the pre-sampling stage does not affect the convergence result, we can apply Theorem 7 from (Berthet and Perchet, 2017) with the choice $\delta_T = 1/T^2$, which gives that

$$\mathbb{E}[L(p_T)] - L(p^*) \leq c_1 \frac{\sigma_i^2}{T} + c_2 \frac{\sigma_i^2}{T} + c_3 \frac{\sigma_i^2}{T},$$

with $c_1 = \frac{96C^2 K}{\mu^2 \eta^2}$, $c_2 = \frac{24C^2}{\mu^2 \eta^4}$ and $c_3 = \frac{3072^2 K}{\mu^2 \eta^2} \| L \|_\infty + \frac{\mu \eta^2}{2} + C_S$. With the presampling stage and Lemma 9, we can bound $\| L \|_\infty$ by

$$\| L \|_\infty \leq \frac{\sum_j \sigma_j^2 \text{Cof}(\Gamma)_{jj}}{\sigma_{\min} \sqrt{\text{Cof}(\Gamma)_{\min}}} \left( \sum_j \sigma_j \sqrt{\text{Cof}(\Gamma)_{jj}} \right).$$

We conclude the proof using the fact that $R(T) = \frac{1}{T} (L(p_T) - L(p^*))$. 

**G Proofs of Theorems in the case where $K > d$**

**G.1 Proof of Theorem 3**

**Proof.** In order to ensure that $L$ is smooth we pre-sample each covariate $n$ times. We note $\alpha = n/T \in (0,1)$. This forces $p_i$ to be greater than $\alpha$ for all $i$. Therefore $L$ is $C_S$-smooth with

$$C_S \leq \frac{2 \max_k \text{Cof}(\Gamma)_{kk} \sigma_{\max}^2}{\alpha^3 \text{det}(\Gamma)} \approx \frac{C}{\alpha^3}.$$
We use a similar analysis to the one of (Berthet and Perchet, 2017). Let us note \( \rho_t = L(p_t) - L(p^*) \) and \( \varepsilon_{t+1} = (e_{(t+1)}^\pi - e_{s_{t+1}}^\pi)^\top \nabla L(p_t) \) with \( e_{s_{t+1}}^\pi = \arg\max_{p \in \Delta K} p^\top \nabla L(p_t) \). Lemma 12 from (Berthet and Perchet, 2017) gives, for \( t \geq nK \),

\[
(t + 1)\rho_{t+1} \leq t\rho_t + \varepsilon_{t+1} + \frac{C_S}{t+1}.
\]

Summing for \( t \geq nK \) gives

\[
T\rho_T \leq nK\rho_{nK} + C_S \log(eT) + \sum_{t=nK}^{T} \varepsilon_t.
\]

We bound \( \sum_{t=nK}^{T} \frac{\varepsilon_t}{T} \) as in Theorem 3 of Berthet and Perchet (2017) by

\[
4\sqrt{\frac{3K \log(T)}{T}} + \left( \frac{\pi^2}{6} + K \right) \frac{2\| \nabla L \|_\infty + \| L \|_\infty}{T} = O \left( \frac{\log(T)}{T} \right).
\]

We are now interested in bounding \( \alpha(L(p_{nK}) - L(p^*)) \).

By convexity of \( L \) we have

\[
L(p_{nK}) - L(p^*) \leq \langle \nabla L(p_{nK}), p_{nK} - p^* \rangle \leq \| \nabla L(p_{nK}) \|_2 \| p_{nK} - p^* \|_2 \leq 2 \| \nabla L(p_{nK}) \|_2.
\]

We have also

\[
\frac{\partial L}{\partial p_k}(p_{nK}) = -\left\| \Omega(p_{nK})^{-1} X_k \sigma_k \right\|_2^2.
\]

Proposition 4 shows that

\[
\| \Omega(p)^{-1} \|_2 \leq \frac{1}{\lambda_{\min}(\Gamma)} \frac{\sigma_{\max}^2}{\min_k p_k}.
\]

In our case, \( \min_k p_{nK} = 1/K \). Therefore

\[
\| \Omega(p_{nK})^{-1} \|_2 \leq \frac{K \sigma_{\max}^2}{\lambda_{\min}(\Gamma)}.
\]

And finally we have

\[
\| \nabla L(p_{nK}) \|_2 \leq \frac{K}{\sqrt{\lambda_{\min}(\Gamma)}} \sigma_{\max} / \sigma_{\min}.
\]

We note \( C_1 \doteq \frac{2K^2}{\sqrt{\lambda_{\min}(\Gamma)}} \sigma_{\max} / \sigma_{\min} \). This gives

\[
L(p_T) - L(p^*) \leq \alpha C_1 + \frac{C \log(T)}{\alpha^3} + O \left( \frac{\log(T)}{T} \right).
\]

The choice of \( \alpha = T^{-1/4} \) finally gives

\[
L(p_T) - L(p^*) = O \left( \frac{\log(T)}{T^{1/4}} \right).
\]

G.2 Proof of Theorem 4

Proof. For simplicity we consider the case where \( d = 1 \) and \( K = 2 \). Let us suppose that there are two points \( X_1 \) and \( X_2 \) that can be sampled, with variances \( \sigma_1^2 = 1 \) and \( \sigma_2^2 = 1 + \Delta > 1 \), where \( \Delta \leq 1 \). We suppose also that \( X_1 = X_2 = 1 \) such that both points are identical.
The loss function associated to this setting is

\[ L(p) = \left( \frac{p_1}{\sigma_1^2} + \frac{p_2}{\sigma_2^2} \right)^{-1} = \frac{1 + \Delta}{p_2 + p_1(1 + \Delta)} = \frac{1 + \Delta}{1 + \Delta p_1}. \]

The optimal \( p \) has all the weight on the first covariate (of lower variance): \( p^\star = (1, 0) \) and \( L(p^\star) = 1. \)

Therefore \( L(p) - L(p^\star) = \frac{1 + \Delta}{1 + \Delta p_1} - 1 = \frac{p_2 \Delta}{1 + \Delta p_1} \geq \frac{\Delta}{2} p_2. \)

We see that we are now facing a classical 2-arm bandit problem: we have to choose between arm 1 giving expected reward 0 and arm 2 giving expected reward \( \Delta/2. \) Lower bounds on multi-armed bandits problems show that

\[ \mathbb{E}[L(p_T^\star) - L(p^\star)] \gtrapprox \frac{1}{\sqrt{T}}. \]

Thus we obtain

\[ R(T) \gtrapprox \frac{1}{T^{3/2}}. \]

\( \square \)

**H Geometric interpretation**

In this section we present figures detailing the geometric interpretation discussed in Subsection 5.1.

Geometrically the dual problem \( (D) \) is equivalent to finding an ellipsoid containing all data points \( X_k / \sigma_k \) such that the sum of the inverse of the semi-axis is maximized. The points that lie on the boundary of the ellipsoid are the one that have to be sampled. We see here that we have to sample the points that are far from the origin (after being rescaled by their standard deviation) because they cause less uncertainty.

We see that several cases can occur as shown on Figure 4. If one covariate is in the interior of the ellipsoid it is not sampled because of the KKT equations (see Proposition 3). However if all the points are on the ellipsoids some of them may not be sampled. It is the case on Figure 4b where \( X_1 \) is not sampled. This is due to the fact that a little perturbation of another point, for example \( X_3 \) can change the ellipsoid such that \( X_1 \) ends up inside the ellipsoid as shown on Figure 4d. This case can consequently be seen as a limit case.
Figure 4: Different minimal ellipsoids

(a) $p_1 = 0.21$  $p_2 = 0.37$  $p_3 = 0.42$

(b) $p_1 = 0$  $p_2 = 0.5$  $p_3 = 0.5$

(c) $p_1 = 0.5$  $p_2 = 0$  $p_3 = 0.5$

(d) $p_1 = 0$  $p_2 = 0.5$  $p_3 = 0.5$