SPEED: Experimental Design for Policy Evaluation in Linear Heteroscedastic Bandits

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Abstract

In this paper, we study the problem of optimal data collection for policy evaluation in linear bandits. In policy evaluation, we are given a *target* policy and asked to estimate the expected reward it will obtain when executed in a multi-armed bandit environment. Our work is the first work that focuses on such optimal data collection strategy for policy evaluation involving heteroscedastic reward noise in the linear bandit setting. We first formulate an optimal design for weighted least squares estimates in the heteroscedastic linear bandit setting that reduces the MSE of the value of the target policy. We then use this formulation to derive the optimal allocation of samples per action during data collection. We then introduce a novel algorithm SPEED (**S**tructured **P**olicy **E**valuation **E**xperimental **D**esign) that tracks the optimal design and derive its regret with respect to the optimal design. Finally, we empirically validate that SPEED leads to policy evaluation with mean squared error comparable to the oracle strategy and significantly lower than simply running the target policy.

1. Introduction

Bandit policy optimization has been widely applied in diverse applications such as web marketing (Bottou et al., 2013), web search (Li et al., 2011), and healthcare recommendations (Zhou et al., 2017). In practice, before widely deploying a learned policy, it is necessary to have an accurate estimation of its performance (i.e., expected reward). To this effect, *policy evaluation* is often a critical step as it allows practitioners to determine if a learned policy truly represents improved task performance. While off-policy evaluation (OPE) has been extensively studied as a potential solution (Dudík et al., 2014; Li et al., 2015; Swaminathan et al., 2017; Wang et al., 2017; Su et al., 2020; Kallus et al., 2021; Cai et al., 2021), in practice, some amount of limited, online evaluation is often required before more widescale deployment. For instance, in web-marketing it is common to run an A/B test with a subset of all users before a potential new policy is deployed for all users (Kohavi and Longbotham, 2017).

When online policy evaluation is required, we desire methods that provide an accurate estimate of policy performance with a minimal amount of data collected. The default choice for online policy evaluation is to simply run the target policy and average the resulting rewards. However, this approach is sub-optimal when the space of actions is large or different actions have reward distributions with different variances.

In this paper, we formulate a new experimental design for allocating action samples so as to obtain minimal mean squared error policy evaluation. Specifically, we consider optimal policy evaluation under the following linear heteroscedastic bandit model. Let $\mathcal{A}$ be a set of *actions*. Each $a \in A$ is associated with a vector $\mathbf{x}(a) \in \mathbb{R}^d$. The expected *reward* of action a is a linear function $\boldsymbol{\theta}_*^\top \mathbf{x}(a)$, for some $\boldsymbol{\theta}_* \in \mathbb{R}^d$. Often the variance of the reward is assumed to be the same for all actions, but in this paper, we depart from this assumption. We suppose that the variance is governed by a quadratic function of the form $\mathbf{x}(a)^T \boldsymbol{\Sigma}_* \mathbf{x}(a)$, for some symmetric positive definite matrix $\boldsymbol{\Sigma}_* \in \mathbb{R}^{d \times d}$. This assumption allows us to capture problems in which both the mean reward and the variance may depend on the action taken, but both vary smoothly in $\mathbf{x}(a)$.

We briefly contrast our studied setting with other work. Recently, there has been an increasing focus on theoretically optimal data collection for bandit policy evaluation. In policy evaluation, the usual metric of algorithm performance is regret with respect to the mean squared error of an oracle algorithm that has knowledge of the variances of different reward distributions (i.e., knows Σ^*). In recent times there has been an increasing focus on studying data collection for policy evaluation in bandit settings (Zhu and Kveton, 2021; 2022; Wan et al., 2022) and there has been some the-

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oretical progress (Chaudhuri et al., 2017; Fontaine et al., 2021). Several works (Antos et al., 2008; Carpentier and Munos, 2012; Carpentier et al., 2015; Fontaine et al., 2021) have shown that when $d = A$ a regret of $\widetilde{O}(An^{-3/2})$ is possible where n is the total budget of actions that can be tried and $\widetilde{O}$ hides logarithmic factors. These works have also shown that simply running the target policy to take actions results in a slower decrease of regret at the rate of $\widetilde{O}(An^{-1})$. The work of Zhu and Kveton (2022); Wan et al. (2022) studies the same setting under safety constraints and provides asymptotic error bounds. However, none of the above works provides a finite-time regret guarantee for data collection for policy evaluation in the heteroscedastic linear bandit setting.

The closest works to our own (Antos et al., 2008; Carpentier and Munos, 2012; Carpentier et al., 2015; Fontaine et al., 2021) either consider unstructured settings or assume that $d = A$. As many real-world bandit applications have $d \ll A$, a natural question arises as to how to build an algorithm for policy evaluation in the heteroscedastic linear bandit setting with unknown $\boldsymbol{\theta}_*$ and $\boldsymbol{\Sigma}_*$ that can leverage the structure. Further, we want the regret of such an algorithm to decrease at a faster rate than $\widetilde{O}(n^{-1})$ (the on-policy regret rate) and to scale with the dimension d instead of actions as $A \gg d$. Note that the regret should scale at least by d^2 because the learner needs to probe in d^2 dimensions to estimate $\boldsymbol{\Sigma}_* \in \mathbb{R}^{d\times d}$ (Wainwright, 2019). Thus, the goal of our work is to answer the question:

Can we design an algorithm to collect data for policy evaluation that adapts to the variance of each action, and its regret degrades at a faster rate than $\widetilde{O}(d^2 n^{-1})$?

In this paper, we answer this question affirmatively. We note that heteroscedasticity is also studied for policy improvement setup (Kirschner and Krause, 2018; Zhou and Gu, 2022; Zhou et al., 2021; Zhang et al., 2021; Zhao et al., 2022). In these prior works the reward variances are time-dependent as opposed to the quadratic structure studied in this paper. Note that policy improvement requires a different approach than policy evaluation. These works build tight confidence sets around the unknown model parameter $\boldsymbol{\theta}_*$ by employing weighted ridge regression involving an estimated upper bound to the time-dependent variances. However, in our setting, the variances of each action share the unknown low dimensional co-variance matrix $\boldsymbol{\Sigma}_*$. Hence we deviate from these approaches and employ an alternating OLS-WLS estimation to learn the underlying parameter $\boldsymbol{\Sigma}_*$. We discuss more related works and motivations in Appendix A.1.

We make the following novel contributions to the growing literature on online policy evaluation:

1. We are the first to formulate the policy evaluation problem for heteroscedastic linear bandit setting where the variance of each action $\mathbf{x}(a) \in \mathbb{R}^d$ depends on the lower dimensional co-variance matrix $\boldsymbol{\Sigma}_* \in \mathbb{R}^{d\times d}$ such that variance $\sigma^2(a) = \mathbf{x}(a)^\top \boldsymbol{\Sigma}_* \mathbf{x}(a)$. This is a more general heteroscedastic linear bandit setting than studied in Chaudhuri et al. (2017); Kirschner and Krause (2018); Fontaine et al. (2021), and different than time-dependent variance model of Zhang et al. (2021); Zhao et al. (2022).

2. We characterize our loss in this setting and show that the optimal design, denoted as **P**olicy **E**valuation (PE) Optimal design to minimize this loss is different than A-, D-, E-, G-, T-, V-optimality (Pukelsheim, 2006). We establish several key properties of this novel PE-Optimal design and discuss how we can solve this optimization problem efficiently.

3. Finally we propose the agnostic algorithm, SPEED, that tracks this optimal design and analyze its MSE. We then bound the regret of SPEED compared to an oracle strategy that follows the optimal design with the knowledge of $\boldsymbol{\Sigma}_*$. We show that the regret scales as $O(\frac{d^3 \log(n)}{n^{3/2}})$ which is an improvement over the regret for the stochastic non-structured bandit setting which scales as $O(\frac{A \log(n)}{n^{3/2}})$ (Carpentier and Munos, 2011; 2012; Carpentier et al., 2015; Fontaine et al., 2021). Hence, we answer positively to our main query. We also prove the first lower bound for this setting that scales as $\Omega(\frac{d^2 \log(n)}{n^{3/2}})$. Finally, we complement our theoretical findings with experiments on real-life data sets.

2. Preliminaries

We define $[m] := [1, 2, \ldots, m]$. The setting consists of A actions, indexed by $a \in [A]$, and consists of features $\mathbf{x}(a) \in \mathbb{R}^d$ such that the dimension $d^2 \ll A$. Denote by $\Delta(\mathcal{A})$ the probability simplex over the action space $\mathcal{A}$ and a policy $\pi \in \Delta(\mathcal{A})$ as a mapping $\pi : a \to [0, 1]$ such that $\sum_a \pi(a) = 1$. We denote the total available budget as n.

We study the linear bandit setting where the expected reward for each action is assumed to be a linear function (Mason et al., 2021; Jamieson and Jain, 2022). Specifically, at each round $t \in [n]$, the selected action a_t is associated with a feature vector $\mathbf{x}(a_t) \in \mathbb{R}^d$, and the rewards satisfy: $R_t(a_t) = \mathbf{x}(a_t)^\top \boldsymbol{\theta}_* + \eta$, where $\boldsymbol{\theta}_* \in \mathbb{R}^d$ is the *unknown* reward parameter, and η is zero-mean noise with variance $\sigma^2(a)$. We assume that the variance $\sigma^2(a)$ has a lower-dimensional structure such that $\sigma^2(a) = \mathbf{x}(a)^\top \boldsymbol{\Sigma}_* \mathbf{x}(a)$ where $\boldsymbol{\Sigma}_* \in \mathbb{R}^{d\times d}$ is an *unknown* variance parameter and we further assume that η is bounded between $-B$ to B. Observe that the variance depends on the action features, which is called the heteroscedastic noise model (Greene, 2002; Chaudhuri et al., 2017) and differs from the unknown time-dependent variance model of Zhang et al. (2021); Zhao et al. (2022). Moreover, Chaudhuri et al. (2017) only consider the special case of our setting when $\boldsymbol{\Sigma}_*$ is identity, such that $\sigma^2(a) = \mathbf{x}(a)^\top \mathbf{x}(a)$. We also assume that the norms of

the features are bounded such that $H_L^2 \leq \|\mathbf{x}(a)\|^2 \leq H_U^2$ for all $a \in \mathcal{A}$. In our heteroscedastic linear bandit setting selecting any action gives information about $\boldsymbol{\theta}_*$ and also gives information about the noise covariance matrix $\boldsymbol{\Sigma}_*$.

The value of a policy π is defined as $v(\pi) := \mathbb{E}[R_t]$ where the expectation is taken over $a_t \sim \pi, R_t \sim R(a_t)$. Finally, recall that in the policy evaluation problem, we are given a fixed, target policy π and asked to estimate $v(\pi)$. Estimating $v(\pi)$ requires a dataset of actions and their associated rewards, $\mathcal{D} := \{(a_1, r_1, ..., a_n, r_n)\}$, which is collected by executing some policy. We refer to the policy that collects $\mathcal{D}$ as the *behavior policy*, denoted by $\mathbf{b} \in \triangle(\mathcal{A})$. We then define the value estimate of a policy π as Y_n, where n is the sample budget. The exact nature of the value estimate for the linear bandit setting will be made clear in Appendix B. Our goal is to choose a behavior policy that minimizes the mean squared error (MSE) defined as $\mathbb{E}_{\mathcal{D}}[(Y_n - v(\pi))^2]$, where the expectation is over the collected data set $\mathcal{D}$. In this paper, we use the terms MSE and loss interchangeably.

We now state the assumption on the boundedness on the variance of each action $a \in [A]$. Let the singular value decomposition of $\boldsymbol{\Sigma}_*$ be $\mathbf{UDP}^\top$ with orthogonal matrices $\mathbf{U}, \mathbf{P}^\top$ and $\mathbf{D} = \operatorname{diag}(\lambda_1, \ldots, \lambda_d)$ where λ_i denotes a singular value. It follows that $\sigma^2_{\min} \leq \sigma^2(a) \leq \sigma^2_{\max}$ where $\sigma^2_{\min} = \min_i |\lambda_i| H_L^2$ and $\sigma^2_{\max} = \max_i |\lambda_i| H_U^2$ (see Remark C.4).

Assumption 2.1. We assume that $\boldsymbol{\Sigma}_*$ has its minimum and maximum eigenvalues bounded such that for every action $a \in [A]$ the following holds $\sigma^2_{\min} \leq \sigma^2(a) \leq \sigma^2_{\max}$.

3. Optimal Design for Policy Evaluation

In this section, we first derive an expression for policy evaluation error in terms of the behavior sampling proportion $\mathbf{b} \in \triangle(\mathcal{A})$, target policy π, and action features $\mathbf{x}(a) \in \mathbb{R}^d$. We call this expression "optimal design" (Pukelsheim, 2006) as minimizing it results in minimizing the error for policy evaluation. We then analyze the error incurred by an oracle that has access to problem-dependent parameters. Suppose we have a budget of n samples to divide between the actions, and let $T_n(1), T_n(2), \ldots, T_n(A)$ be the number of samples allocated to actions $1, 2, \ldots, A$ at the end of n rounds. In a linear bandit, we can define the value estimate of a *target policy* as $Y_n := \sum_a \mathbf{w}(a)^\top \widehat{\boldsymbol{\theta}}_n$ where, $\mathbf{w}(a) := \pi(a)\mathbf{x}(a)$ is the expected features under the target policy, and $\widehat{\boldsymbol{\theta}}_n$ is an unbiased estimate of $\boldsymbol{\theta}_*$ computed with n samples in $\mathcal{D}$. As $\widehat{\boldsymbol{\theta}}_n$ is an unbiased estimate, we have that $\mathbb{E}_{\mathcal{D}}[Y_n] = \sum_{a=1}^A \mathbf{w}(a)^\top \boldsymbol{\theta}_* = v(\pi)$. Since we have an unbiased estimator of $v(\pi)$, minimizing the MSE is equivalent to minimizing the variance of $\min \mathbb{E}_{\mathcal{D}}\big[(Y_n - \mathbb{E}[Y_n])^2\big] = \min \mathbb{E}_{\mathcal{D}}\big[\big(\sum_{a=1}^A \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\big)^2\big]$ where the minimization is with respect to the data distribution $\mathcal{D}$, which is governed by observing rewards to actions determined by a *behavior policy*. In general, the behavior policy may be different from the target policy and it may even be non-stationary over the n rounds of data collection.

$$\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}} = \sum_{a \in \mathcal{A}} \mathbf{b}(a) \left(\tfrac{\mathbf{x}(a)}{\sigma(a)}\right) \left(\tfrac{\mathbf{x}(a)}{\sigma(a)}\right)^\top = \sum_{a \in \mathcal{A}} \mathbf{b}(a) \widetilde{\mathbf{x}}(a) \widetilde{\mathbf{x}}(a)^\top \tag{1}$$

where, $\widetilde{\mathbf{x}}(a) = \mathbf{x}(a)/\sigma(a)$. Observe that our design matrix in (1) captures the information about the action features $\mathbf{x}(a)$, and variance $\sigma^2(a)$ and weights them by the sampling proportion $\mathbf{b}(a)$. Then in the following proposition, we exactly characterize the loss with respect to the design matrix $\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}}$, target policy $\pi(a)$ and action features $\mathbf{x}(a)$. Define $\mathbf{V} = \sum_a \mathbf{w}(a)\mathbf{w}(a)^\top$.

Proposition 1. *Let $\widehat{\boldsymbol{\theta}}_n$ be the estimate of $\boldsymbol{\theta}_*$ after observing n samples and define $\mathbf{w}(a) = \pi(a)\mathbf{x}(a)$. Define the design matrix as $\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}} = \sum_{a=1}^A \mathbf{b}(a) \left(\frac{\mathbf{x}(a)}{\sigma(a)}\right) \left(\frac{\mathbf{x}(a)}{\sigma(a)}\right)^\top$. Then the loss is given by*

$$\mathbb{E}_{\mathcal{D}}[\big(\sum_{a=1}^A \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_\star)\big)^2] = \frac{1}{n}\big(\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b},\boldsymbol{\Sigma}} \mathbf{w}(a')\big) =: \mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma}).$$

Proof (Overview) The key idea is to show that the linear model yields for each action $a \in [A], \widetilde{Y}_n(a) = \widetilde{\mathbf{x}}_n(a)^\top \boldsymbol{\theta}^\star + \widetilde{\eta}_n(a)$ where we define

$$\widetilde{Y}_n(a) = \sum_{t=1}^{T_n(a)} \frac{R_t(a)}{\sigma(a)\sqrt{T_n(a)}}, \widetilde{\mathbf{x}}_n(a) = \frac{\sqrt{T_n(a)}\mathbf{x}(a)}{\sigma(a)}, \widetilde{\eta}_n(a) = \sum_{t=1}^{T_n(a)} \frac{\eta_t(a)}{\sigma(a)\sqrt{T_n(a)}}$$

with $\eta_t(a)$ being the noise and $T_n(a)$ is the number of samples of action a. Next observe that using the independent noise assumption we have that $\mathbb{E}[\widetilde{\eta}_n(a)] = 0$ and $\mathbf{Var}[\widetilde{\eta}_n(a)] = 1$. Let $\mathbf{X} = \big(\widetilde{\mathbf{x}}_n(1)^\top, \cdots, \widetilde{\mathbf{x}}_n(A)^\top\big)^\top \in \mathbb{R}^{A \times d}$ the induced design matrix of the policy and $\mathbf{Y} = [\widetilde{Y}_n(1), \widetilde{Y}_n(2), \ldots, \widetilde{Y}_n(A)]^\top$. The above ordinary least squares (OLS) problem has an optimal unbiased estimator $\widehat{\boldsymbol{\theta}}_n = \big(\mathbf{X}^\top \mathbf{X}\big)^{-1} \mathbf{X}^\top \mathbf{Y}$ (Fontaine et al., 2021). Substituting the definition of $\widehat{\boldsymbol{\theta}}_n$ yields the desired expression of the loss as stated in the proposition. The detailed proof is given in Appendix C.2. ■

Observe that the loss in our setting depends on the inverse of the design matrix denoted by $\mathbf{A}^{-1}_{\mathbf{b},\boldsymbol{\Sigma}}$, the target policy, as well as action features of the cross product of all arms $a, a' \in \mathcal{A}$. Hence, minimizing the loss is equivalent to minimizing the quantity $1/n(\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b},\boldsymbol{\Sigma}} \mathbf{w}(a'))$. We call this the PE-Optimal design. Further note that this design is different than a number of different prior notions of optimality such as D-, E-, T-, or G-optimality (Pukelsheim, 2006; Fedorov, 2013; Jamieson and Jain, 2022). None

of these previously proposed designs capture the objective of minimal MSE policy evaluation. For example, G-optimality (as used by (Katz-Samuels et al., 2020; Mason et al., 2021; Katz-Samuels et al., 2021)) minimizes the worst-case error of $\max_{\mathbf{x}(a)} \mathbb{E}_{\mathcal{D}}[(\mathbf{x}(a)^\top(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*))^2]$ by minimizing the quantity $\max_{\mathbf{x}(a)} \mathbf{x}(a)^\top \mathbf{A}_{\mathbf{b}}^{-1}\mathbf{x}(a)$ for homoscedastic noise. The E-optimal design minimizes $\max_{\|\mathbf{u}\|\leq 1} \mathbb{E}_{\mathcal{D}}[(\mathbf{u}^\top(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*))^2]$ by minimizing the minimum eigenvalue of the inverse of design matrix (Mukherjee et al., 2022b) and the A-optimal design minimizes $\mathbb{E}_{\mathcal{D}}[(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)^2]$ by minimizing the trace of the inverse of design matrix (Fontaine et al., 2021).

We now state a few more notations for ease of exposition. Using Proposition 1 we define the optimal behavior policy when the co-variance matrix $\boldsymbol{\Sigma}_*$ is known as

$$\mathbf{b}^* := \arg\min_{\mathbf{b}} \mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma}_*). \tag{2}$$

where the loss $\mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma}_*)$ is defined in Proposition 1. We define the optimal loss (with the knowledge of $\boldsymbol{\Sigma}_*$) as:

$$\mathcal{L}_n(\pi, \mathbf{b}^*, \boldsymbol{\Sigma}_*) = \min_{\mathbf{b}} \mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma}_*). \tag{3}$$

Now an agnostic algorithm does not know the true co-variance matrix $\boldsymbol{\Sigma}_*$ and must estimate the covariance matrix $\widehat{\boldsymbol{\Sigma}}_\Gamma$ after conducting exploration for Γ rounds. Define the optimal behavior policy for an arbitrary co-variance matrix $\widehat{\boldsymbol{\Sigma}}_\Gamma$ and target policy π as $\widehat{\mathbf{b}}^* = \arg\min_{\mathbf{b}} \mathcal{L}_n(\pi, \mathbf{b}, \widehat{\boldsymbol{\Sigma}}_\Gamma)$ and the agnostic loss as

$$\mathcal{L}_n(\pi, \widehat{\mathbf{b}}^*, \widehat{\boldsymbol{\Sigma}}_\Gamma) = \min_{\mathbf{b}} \mathcal{L}_n(\pi, \mathbf{b}, \widehat{\boldsymbol{\Sigma}}_\Gamma) \tag{4}$$

3.1. Computation of $\mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma})$

In this section, we digress a bit to discuss the computational aspect of $\mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma})$. Note that our loss function leads to a new type of design (PE-Optimal design) and so the natural question to ask is *how to optimize this loss function w.r.t.* $\mathbf{b}$*?* We show in Proposition 2 that the loss $\mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma})$ for any arbitrary design proportion $\mathbf{b} \in \triangle(\mathcal{A})$ is strictly convex with respect to the proportion $\mathbf{b}$. The proposition and its proof are given in Appendix C.3. Next in Proposition 3 we show that the gradient of the loss function is bounded. The proposition and its proof are given in Appendix C.4. We first state an assumption that $\lambda_{\min}\left(\sum_{a=1}^{A} \mathbf{w}(a)\mathbf{w}(a)^\top\right) > 0$ which is required for proving Proposition 3.

Assumption 3.1. (Distribution of π) We assume that the set of actions a such that $\pi(a)>0$, spans $\mathbb{R}^d$ and $\mathbb{R}^{d\times d}$.

Note that this is a realistic assumption as if the target policy never takes an action that is needed to cover some dimension then we do not need to identify $\boldsymbol{\theta}_*$ in that dimension. Using Proposition 2 and Proposition 3 we can effectively solve the PE-Optimal design with gradient descent approaches (Lacoste-Julien and Jaggi, 2013; Berthet and Perchet, 2017). We capture this convergence guarantee with the assumption of the existence of an approximation oracle.

Assumption 3.2. (Approximation Oracle) We assume access to an approximation oracle. Given a convex loss function $\mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma})$ with minimizer $\mathbf{b}^*$, the approximation oracle returns a proportion $\widehat{\mathbf{b}}^* = \arg\min_{\mathbf{b}} \mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma})$ such that $|\mathcal{L}_n(\pi, \widehat{\mathbf{b}}^*, \boldsymbol{\Sigma}) - \mathcal{L}_n(\pi, \mathbf{b}^*, \boldsymbol{\Sigma})| \leq \epsilon$.

Therefore from Proposition 2, and 3 and using Assumption 3.1, and 3.2 we can get a computationally efficient solution to $\mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma})$. In the next section, we discuss the loss of an oracle.

4. Agnostic Algorithm SPEED and Regret Analysis

In this section, we first present the agnostic algorithm and then analyze its regret.

4.1. Details of Algorithm SPEED

In practice, $\boldsymbol{\Sigma}_*$ is unknown and so the oracle behavior policy cannot be directly computed. Instead, we must first conduct a small amount of exploration to estimate $\boldsymbol{\Sigma}_*$ and then use the estimate in place of $\boldsymbol{\Sigma}_*$ in (1). Specifically, we define the forced exploration phase as the first Γ rounds in which the algorithm conducts exploration to estimate $\boldsymbol{\Sigma}_*$. To conduct forced exploration we apply Principal Component Analysis (PCA) on the feature matrix $\mathbf{X}$ and choose the most significant d directions (directions having the highest variance). Then we choose one random action from each of these d significant directions and sample them uniform randomly for Γ rounds. Since the algorithm explores first and then uses the estimate to compute the PE-Optimal design, it can be viewed as an explore-then-commit algorithm (Rusmevichientong and Tsitsiklis, 2010; Lattimore and Szepesvári, 2020b). As we consider a structured setting we call this algorithm **S**tructured **P**olicy **E**valuation **E**xperimental **D**esign (SPEED). After $\Gamma = \sqrt{n}$ rounds, SPEED estimates the covariance matrix $\widehat{\boldsymbol{\Sigma}}_\Gamma$ as follows:

$$\widehat{\boldsymbol{\Sigma}}_\Gamma = \min_{\mathbf{S}} \sum_{t=1}^{\Gamma} \left[\langle \mathbf{x}(I_t)\mathbf{x}(I_t)^\top, \mathbf{S}\rangle - (R(I_t) - \mathbf{x}(I_t)^\top \widehat{\boldsymbol{\theta}}_t)^2\right]^2 \tag{5}$$

where $\widehat{\boldsymbol{\theta}}_t$ is the ordinary least square estimate of $\boldsymbol{\theta}_*$. A similar Similar covariance estimation technique has been proposed before for the active regression setting though only for the case when $\boldsymbol{\Sigma}_*$ has rank 1 (Chaudhuri et al., 2017). The estimate of the covariance matrix $\widehat{\boldsymbol{\Sigma}}_\Gamma$ is then fed to the oracle optimizer (Assumption 3.2) to compute the sampling proportion $\widehat{\mathbf{b}}$. Finally, actions are chosen according to $\widehat{\mathbf{b}}$ for the remaining $n - \Gamma$ rounds and then $\widehat{\boldsymbol{\theta}}_n$ is computed. Full pseudocode is given in Algorithm 1.

Algorithm 1 Structured Policy Evaluation Experimental Design (SPEED)

1: **Input:** Finite set of actions $\mathcal{A}$, target policy π, budget n.
2: Conduct forced exploration for $\Gamma = \sqrt{n}$ rounds and estimate $\widehat{\mathbf{\Sigma}}_\Gamma$ using (5).
3: Let $\widehat{\mathbf{b}} \in \triangle(\mathcal{A})$ be the minimizer of $\mathcal{L}_n(\pi, \mathbf{b}, \widehat{\mathbf{\Sigma}}_\Gamma)$.
4: Pull each action a exactly $T_n(a) = \left\lfloor \widehat{\mathbf{b}}(a)(n-\Gamma) \right\rfloor$ times. Set $\mathcal{H}(a) := \{I_t, R(I_t)\}_{t=\Gamma}^{T_n(a)}$ by selecting $I_t = a$ according to $\widehat{\mathbf{b}}(a)$. Set $\mathcal{D} \leftarrow \cup_a \mathcal{H}(a)$.
5: Construct the policy weighted least squares estimator $\widehat{\boldsymbol{\theta}}_n$ using $\mathcal{D}$ using only the observations from step 4.
6: **Output:** $\mathcal{D}$ and $\widehat{\boldsymbol{\theta}}_n$.

4.2. Regret Analysis of SPEED

In this section we first state our regret definition and then analyze the regret of the agnostic algorithm SPEED. The regret for the agnostic algorithm for the estimated behavior policy $\widehat{\mathbf{b}}$ is given by

$$\mathcal{R}_n = \overline{\mathcal{L}}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*). \tag{6}$$

where $\overline{\mathcal{L}}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma)$ is the loss of the agnostic algorithm and $\mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*)$ is the oracle loss defined in (3). We now state the main theorem for the regret of SPEED.

Theorem 1. ***(Regret of Algorithm 1, informal)*** *The regret of Algorithm 1 for $n \geq O(\frac{d^4 \log^2(A/\delta)}{\sigma^4_{\min}})$ running PE-Optimal design in Equation (4) is given by $\mathcal{R}_n = O\left(\frac{d^3 \log(n)}{n^{3/2}}\right)$.*

Discussion (Regret): Theorem 1 states that the regret of Algorithm 1 scales as $O(d^3 \log(n)/n^{3/2})$ where d is the dimension of $\boldsymbol{\theta}_*$. Note that our regret bound depends on the underlying feature dimension d instead of actions A, and scales as $\widetilde{O}(d^3 n^{-3/2})$ which gives a positive answer to the main question of whether such a result is possible. In the case where $d^3 < A$, we have a tighter bound than Carpentier and Munos (2011). Furthermore, the result of Carpentier and Munos (2011; 2012); Carpentier et al. (2015) cannot be easily extended to take advantage of structure in the linear bandit setting. Finally, note that we improve upon the A-optimal design studied in Fontaine et al. (2021), as their regret depends on actions A and scales as $O(\frac{A \log n}{n^{3/2}})$.

Proof (Overview) of Theorem 1: We now outline the key steps for proving Theorem 1.

Step 1(Concentration of (OLS-WLS): We now state a concentration lemma that is key to proving the regret of SPEED. This lemma is novel for our proof because we must estimate the underlying covariance matrix $\mathbf{\Sigma}_*$ using OLS estimator for Γ rounds. Then use the estimation $\widehat{\mathbf{\Sigma}}_\Gamma$ in WLS estimator. We define the variance concentration good event till Γ using our forced exploration as:

$$\xi^{var}_\delta(\Gamma) := \left\{\forall a, |\mathbf{x}(a)^\top (\widehat{\mathbf{\Sigma}}_\Gamma - \mathbf{\Sigma}_*)\mathbf{x}(a)| < \frac{2Cd^2 \log(A/\delta)}{\Gamma}\right\} \tag{7}$$

Lemma 4.1. ***(OLS-WLS Concentration Lemma)*** *After Γ samples of exploration, we can show that $\mathbb{P}\left(\xi^{var}_\delta(\Gamma)\right) \geq 1 - 8\delta$ where, $C > 0$ is a constant.*

Proof (Overview) of Lemma 4.1: We have an initial estimate $\widehat{\boldsymbol{\theta}}_\Gamma$ of $\boldsymbol{\theta}_*$ and the squared residual $y_t := (\mathbf{x}_t^\top \widehat{\boldsymbol{\theta}}_\Gamma - r_t)^2$ that SPEED obtains by estimating of $\mathbf{\Sigma}_*$ via $\min_{\mathbf{S} \in \mathbb{R}^{d \times d}} \sum_{t=1}^{\Gamma} (\langle \mathbf{x}_t \mathbf{x}_t^\top, \mathbf{S} \rangle - y_t)^2$. Let $\zeta_\Gamma := \widehat{\boldsymbol{\theta}}_\Gamma - \boldsymbol{\theta}_*$ then we can show that $y_t = \mathbf{x}_t^\top \mathbf{\Sigma}_* \mathbf{x}_t + \epsilon_t$ and the noise ϵ_t can be bounded by $\epsilon_t \leq \underbrace{2(\eta_t^2 - \mathbb{E}\left[\eta_t^2\right])}_{\textbf{Part A}} + \underbrace{2\left(\mathbf{x}_t^\top \zeta_\Gamma\right)^2}_{\textbf{Part B}}$.

For the part A, observe that η_t^2 is a sub-exponential random variable as $\eta_t \sim \mathcal{SG}(0, \mathbf{x}_t^\top \mathbf{\Sigma}_* \mathbf{x}_t)$. Hence we can use sub-exponential concentration inequality from Lemma C.2 (Appendix C.1) to bound it. For part B first recall that $\zeta_\Gamma := \widehat{\boldsymbol{\theta}}_\Gamma - \boldsymbol{\theta}_*$ and we use Lemma C.3 (Appendix C.1) to bound it. Combining the two parts give the desired concentration inequality. The proof is in Appendix D.2. ■

Step 2 (Agnostic loss $\overline{\mathcal{L}}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma)$): In this step we bound the agnostic loss $\overline{\mathcal{L}}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma)$. The Lemma 4.1 leads to Corollary D.5 (Appendix D.4) which shows that for $n \geq 16C^2 d^4 \log^2(A/\delta)/\sigma^4_{\min}$ we have that $\mathcal{L}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) \leq (1 + 2C_\Gamma(\delta)) \sum_{a,a'} \mathbf{w}(a) \mathbf{A}^{-1}_{\widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma} \mathbf{w}(a')$, where $C_\Gamma(\delta) = \frac{2Cd^2 \log(A/\delta)}{\sigma^2_{\min} \Gamma}$. Note that Fontaine et al. (2021) does not require this approach as the variances of each action do not share a common structure. Similarly, this approach differs from the time-dependent variance model of Zhang et al. (2021); Zhao et al. (2022). Now observe that for an agnostic algorithm, the loss function is defined as $\mathcal{L}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma)$. However, $\mathcal{L}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) \neq \sum_{a,a'} \mathbf{w}(a) \mathbf{A}^{-1}_{\widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma} \mathbf{w}(a')$. We denote $\overline{\mathcal{L}}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) := \mathbb{E}\left[\left(\mathbf{z}^\top (\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*)\right)^2\right]$ where $\widehat{\boldsymbol{\theta}}_{n-\Gamma}$ is the estimation of $\boldsymbol{\theta}_*$ after $n - \Gamma$ samples. We now bound the quantity $\overline{\mathcal{L}}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma)$ using Proposition 7. In it, we show that $\mathbb{E}\left[\left(\mathbf{z}^\top (\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*)\right)^2\right. \leq (1 + 2C_\Gamma(\delta)) \mathbf{z}^\top (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{z} = \frac{(1+2C_\Gamma(\delta))}{n-\Gamma} \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma} \mathbf{w}(a')$

Step 3 (Regret Decomposition): Define the regret as in (6). Then recall that $\mathbf{b}^* \in \triangle(\mathcal{A})$ is the optimal design in (2) and $\widehat{\mathbf{b}}^* = \arg\min_{\mathbf{b}} \mathcal{L}_n(\pi, \mathbf{b}, \widehat{\mathbf{\Sigma}}_\Gamma)$ is the agnostic design. Define $\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) := \frac{(1+2C_\Gamma(\delta))}{n-\Gamma} \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma} \mathbf{w}(a')$. Then we can show that the regret can be decomposed into three parts: $\mathcal{R}_n = \underbrace{\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma)}_{\textbf{Approximation error}}$

$$+\underbrace{\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma)}_{\textbf{Comparing two diff loss}}$$

$$+\underbrace{\mathcal{L}_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*)}_{\textbf{Estimation error of } \mathbf{\Sigma}_*}.$$

For the approximation error we need access to an oracle (Assumption 3.2) that gives ϵ approximation error. Then setting $\epsilon = \frac{1}{\sqrt{n}}$ we have that the estimation error is upper bounded by $n^{-3/2}$. For comparing two different loss parts, we use the definition of $C_\Gamma(\delta)$ to bound it as $O(\frac{d^2 \log(A/\delta)}{n^{3/2}})$ as shown in (24) in Appendix D.3.

Now observe that the third quantity (estimation error of $\mathbf{\Sigma}_*$) contains $\mathcal{L}_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma)$ that depends on the design matrix $\mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma}$ which in turn depends on the estimation of $\widehat{\mathbf{\Sigma}}_\Gamma$. Similarly $\mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*)$ in the third quantity depends on the design matrix $\mathbf{A}^{-1}_{\mathbf{b}^*, \mathbf{\Sigma}_*}$ which in turn depends on the true $\mathbf{\Sigma}_*$. Hence, we now bound the concentration of the loss under $\mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma}$ against the design matrix $\mathbf{A}^{-1}_{\mathbf{b}^*, \mathbf{\Sigma}_*}$ in the following lemma.

Lemma 4.2. ***(Loss Concentration of design matrix)*** *Let $\widehat{\mathbf{\Sigma}}_\Gamma$ be the empirical estimate of $\mathbf{\Sigma}_*$, and $\mathbf{V} = \sum_{a,a'} \mathbf{w}(a)\mathbf{w}(a')^\top$. We have that for any arbitrary proportion $\mathbf{b}$ the following*

$$\mathbb{P}\Big(\Big|\sum_{a,a'} \mathbf{w}(a)^\top (\mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma} - \mathbf{A}^{-1}_{\mathbf{b}^*, \mathbf{\Sigma}_*})\mathbf{w}(a')\Big| \leq \frac{2CB^* d^3 \log(A/\delta)}{\Gamma}\Big) \geq 1 - \delta$$

where B^* is a problem-dependent quantity and $C > 0$ is a universal constant.

Proof (Overview) of Lemma 4.2: We can decompose $|\sum_{a,a'} \mathbf{w}(a)^\top (\mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma} - \mathbf{A}^{-1}_{\mathbf{b}^*, \mathbf{\Sigma}_*})\mathbf{w}(a')| \leq \|\mathbf{u}\| \underbrace{\Big\|\mathbf{A}_{\mathbf{b}^*, \mathbf{\Sigma}_*} - \mathbf{A}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma}\Big\|}_{\Delta} \|\mathbf{v}\|$ where, $\|\mathbf{u}\| = \|\mathbf{A}^{-1}_{\mathbf{b}^*, \mathbf{\Sigma}_*}\mathbf{w}\|$ and $\|\mathbf{v}\| = \|\mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}\|$. First, observe that $\|\mathbf{u}\|$ is a problem-dependent quantity. Then to bound Δ we bound the $\|\widehat{\mathbf{\Sigma}}_\Gamma - \mathbf{\Sigma}_*\| \leq \frac{2Cd^2 \log(A/\delta)}{\Gamma}$. Finally to bound $\|\mathbf{v}\|$ we need to bound $\widehat{\sigma}^2_\Gamma(a) \leq \sigma^2(a) + \frac{2Cd^2 \log(A/\delta)}{\Gamma}$ where $\widehat{\sigma}^2_\Gamma(a)$ is the empirical variance of $\sigma^2(a)$. Combining everything yields the desired result. The proof is in Appendix D.4 ■

One of our key technical contributions in Lemma 4.2 is to show that the concentration of the two losses $\mathcal{L}_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma)$, and $\mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*)$ scales with d^3 instead of the number of actions A. In contrast a similar loss concentration in Fontaine et al. (2021) scales with A. Now using Lemma 4.2, setting the exploration factor $\Gamma = \sqrt{n}$, and $\delta = \frac{1}{n}$ we can show that the estimation error is upper bounded by $\frac{B^* C d^3 \log(n)}{n^{3/2}} + \frac{d^2}{n^2}\mathbf{Tr}(\sum_{a,a'} \mathbf{w}(a)\mathbf{w}(a')^\top)$. Combining everything we have the regret of SPEED as $O(\frac{B^* d^3 \log(n)}{n^{3/2}})$. The full proof of Theorem 1 is in Appendix D.5. ■.

Theorem 1 upper bounds the regret of our agnostic algorithm SPEED compared to an oracle algorithm with knowledge of $\mathbf{\Sigma}_*$. To quantify the tightness of our upper bound, we now turn to whether we can lower bound the regret of SPEED. For our final theoretical result, we consider a slightly different notion of regret: $\mathcal{R}'_n := \mathcal{L}_n(\pi, \widehat{\mathbf{b}}, \mathbf{\Sigma}_*) - \mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*)$. This notion of regret captures how sub-optimal the estimated $\widehat{\mathbf{b}}$ is compared to $\mathbf{b}^*$ and *not* additional error incurred by using an estimate of $\mathbf{\Sigma}_*$ in the WLS estimator. We conjecture that $\mathcal{R}'_n$ is indeed a lower bound to $\mathcal{R}_n$ as we have established in Proposition 1 that the minimum variance estimator is the WLS estimator using $\mathbf{\Sigma}_\star$. Intuitively, $\mathcal{L}_n(\pi, \widehat{\mathbf{b}}, \mathbf{\Sigma}_*)$ is a lower bound to $\overline{\mathcal{L}}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma)$ as estimation error will likely only increase when using $\widehat{\mathbf{\Sigma}}_\Gamma$ in place of $\mathbf{\Sigma}_*$ in the WLS estimator. We leave proving that $\mathcal{R}'_n$ is a lower bound to $\mathcal{R}_n$ in future work.

Theorem 2. ***(Lower Bound)*** *Let $|\mathbf{\Theta}|=2^d$, $\boldsymbol{\theta}_* \in \mathbf{\Theta}$. Then any δ-PAC policy $\mathbf{b}$ satisfies $\mathcal{R}'_n = \mathcal{L}_n(\pi, \widehat{\mathbf{b}}, \mathbf{\Sigma}_*) - \mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*) \geq \Omega\big(\frac{d^2 \lambda_d(\mathbf{V}) \log(n)}{n^{3/2}}\big)$ for the environment in (28).*

Proof (Overview:) The proof follows the change of measure argument (Lattimore and Szepesvári, 2020b). We follow the proof technique of Huang et al. (2017); Mukherjee et al. (2022b). We reduce our linear bandit problem to the hypothesis testing setting and state a worst-case environment as in (28). We then show that the regret of any δ-PAC algorithm against an oracle in this environment must scale as $\Omega(\log n / n^{3/2})$. The proof is given in Appendix E. ■

From the above result, the upper bound of SPEED regret $\mathcal{R}_n$ matches the lower bound of regret $\mathcal{R}'_n$ in n but suffers an additional factor of d.

In Appendix C we show that the SPEED outperforms the on-policy algorithm and several other baselines.

5. Conclusions and Future Directions

We proposed SPEED for optimal data collection for policy evaluation in linear bandits with heteroscedastic reward noise. We formulated a novel optimal design problem, PE-Optimal design, for which the optimal behavior policy is the solution that will produce minimal MSE policy evaluation when using a weighted least square estimate of the hidden reward parameters $\boldsymbol{\theta}_*$ and $\mathbf{\Sigma}_*$. We showed the regret of SPEED degrades at the rate of $\widetilde{O}(d^3 n^{-3/2})$ and matches the lower bound of $\widetilde{O}(d^2 n^{-3/2})$ except a factor of d. In contrast the Onpolicy suffers a regret of $\widetilde{O}(n^{-1})$ (Carpentier et al., 2015). We showed empirically that our design outperforms other optimal designs. In future work, we intend to extend the result to a more general class of hard problems such as collecting data to minimize the MSE of multiple target policies under a generalized linear bandit setting.

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A. Appendix

A.1. Related Works and Motivations

Our work is most closely related to existing work on data collection for policy evaluation. Perhaps the most natural choice of behavior policy is to simply run the target policy, i.e., on-policy data collection (Sutton and Barto, 2018). The works in adaptive importance sampling for bandits (Oosterhuis and de Rijke, 2020; Tucker and Joachims, 2022) and MDPs (Hanna et al., 2017; Ciosek and Whiteson, 2017; Bouchard et al., 2016) have shown how to lower the variance of Monte Carlo estimation through the choice of behavior policy. In contrast to these works, we consider estimating $v(\pi)$ by estimating the reward distributions rather than using Monte Carlo estimation. Such *certainty-equivalence* estimators take advantage of the setting's structure and are thus typically of lower variance than Monte Carlo estimators (Sutton and Barto, 2018). The work of Wan et al. (2022) studies a different estimator for reducing the variance of the importance sampling in constrained MDP setting whereas we study certainty equivalence estimator. Another set of work has studied sample allocation for stratified Monte Carlo estimators – a problem that is formally equivalent to behavior policy selection for policy evaluation in the bandit setting with linearly independent arms (Antos et al., 2008; Carpentier et al., 2015). This line of work was recently extended to tabular, tree-structured MDPs by Mukherjee et al. (2022a). In contrast, we consider the structured linear bandit setting which incorporates generalization across actions.

Our work is closely related to optimal experimental design and active learning literature. We formulate determining the optimal behavior policy in the bandit setting as an optimal design problem. In contrast to prior work, we introduce a new type of optimality that is tailored to the policy evaluation problem. We are also, to the best of our knowledge, the first to consider both heteroscedastic noise and weighted least squares estimators in formulating our design. The heteroscedastic noise model and weighted least squares estimator have been considered by (Chaudhuri et al., 2017) in the active learning literature and in linear bandit setting by Kirschner and Krause (2018) using information directed sampling. In contrast to these works (and the active learning setting in general), we aim to minimize the weighted error $\sum_{a\in\mathbf{A}} \pi(a)\mathbf{x}(a)^\top(\boldsymbol{\theta}^* - \widehat{\boldsymbol{\theta}})^2$ whereas in the active learning setting the goal is to minimize $\|\boldsymbol{\theta}^* - \widehat{\boldsymbol{\theta}}\|^2$ which results in A-optimal design (Fontaine et al., 2021; Pukelsheim, 2006). Moreover the regret bounds in Fontaine et al. (2021) holds for $d = |\mathcal{A}|$. (Riquelme et al., 2017) extends the results of (Carpentier and Munos, 2011) to a different linear regression setting than ours but under homoscedastic noise model

Data collection for policy evaluation is also related to the problem of exploration for policy learning in MDPs or best-arm identification in bandits. In those contexts, the aim of exploration is to find the optimal policy and the exploration-exploitation trade-off describes the tension between reducing uncertainty and focusing on known promising actions. In bandits, the exploration-exploitation trade-off is often navigated under the "**O**ptimism in the **F**ace of **U**ncertainty" principle using techniques such as UCB (Lai and Robbins, 1985; Auer et al., 2002; Abbasi-Yadkori et al., 2011) or Thompson Sampling (Thompson, 1933; Agrawal and Goyal, 2012). In contrast to the standard exploration problem, we focus on evaluating a fixed policy. Instead of balancing exploration and exploitation, a behavior policy for policy evaluation should take actions that reduce uncertainty about $v(\pi)$ with emphasis on actions that have high probability under π. Also, note that heteroscedastic bandits have been studied from the perspective of policy improvement (Kirschner and Krause, 2018; Zhao et al., 2022) however, in this paper we focus on optimal data collection for policy evaluation.

B. Loss of the Oracle

B.1. Oracle Loss

Recall from Section 1, that our final goal is to control the regret that compares the loss of an agnostic algorithm against the loss of an oracle. In this section, we develop our theory for optimal data collection by considering an oracle for the heteroscedastic linear bandit setting. We consider an oracle that has knowledge of $\boldsymbol{\Sigma}_*$ but does not know $\boldsymbol{\theta}_*$. Our goal is to identify the sampling proportion $\mathbf{b}^*$ that such an oracle would select such that taking actions according to $\mathbf{b}^*$ minimizes the loss. After observing n samples, let the *weighted* least square estimate be:

$$\widehat{\boldsymbol{\theta}}_n \coloneqq \arg\min_{\boldsymbol{\theta}} \sum_{t=1}^{n} \frac{1}{\sigma^2(I_t)} (R(I_t) - \mathbf{x}(I_t)^\top \boldsymbol{\theta})^2 \tag{8}$$

where I_t is the action sampled at round t and $\sigma^2(I_t)$ is the variance of action I_t. Also note that this is an unbiased estimator of $\boldsymbol{\theta}_*$ (see Remark C.5). We prove in Proposition 5 (see Appendix C.6) that if the oracle estimates $\widehat{\boldsymbol{\theta}}_n$ using the weighted least square estimate in (8) then it can minimize the loss $\mathcal{L}_n^*(\pi, \mathbf{b}^*, \boldsymbol{\Sigma}_*)$. Now the oracle uses the weighted least square

estimate in (8) to estimate $\widehat{\boldsymbol{\theta}}_n$, knows $\boldsymbol{\Sigma}_*$, and has access to the oracle approximator to solve the PE-Optimal design. Then the following proposition bounds the loss of the oracle after n samples.

Proposition 6. ***(Oracle Loss)*** *Let the oracle sample each action a for $\lceil n\mathbf{b}^*(a)\rceil$ times, where $\mathbf{b}^*$ is the solution to (2). Define $\lambda_1(\mathbf{V})$ as the maximum eigenvalue of $\sum_{a,a'} \mathbf{w}(a)\mathbf{w}(a')^\top$. Then the loss is given by $\mathcal{L}_n^*(\pi, \mathbf{b}^*, \boldsymbol{\Sigma}_*) \leq O\left(\frac{d\lambda_1(\mathbf{V})\log n}{n}\right) + O\left(\frac{1}{n}\right)$.*

Proof (Overview) Note that the oracle knows the $\boldsymbol{\Sigma}_*$ and uses $\widehat{\boldsymbol{\theta}}_n$ in (8) to estimate $\boldsymbol{\theta}_*$. We use Corollary 1 to show that $\mathcal{L}_n(\pi, \mathbf{b}^*, \boldsymbol{\Sigma}_*) \leq \lambda_1(\mathbf{V})d$ where $\mathbf{V} = \sum_{a,a'} \mathbf{w}(a)\mathbf{w}(a')^\top$. The proof follows by showing that $(\sum_{a=1}^{A} \mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*))^2$ is a sub-exponential variable. Then using sub-exponential concentration inequality in Lemma C.2 (Appendix C.1) and setting $\delta = O(1/n^2)$ we can bound the expected loss with high probability. The full proof is given in Appendix D.1. ■

Connection to prior work: We can interpret the result of Proposition 6 in the following way: Consider the basic stochastic bandit setting which is a special case of our setting where $\mathbf{x}(a)$ is a one-hot vector in $\mathbb{R}^A$. In this case, from Proposition 6 we know that that $\mathbf{b}^* = \arg\min_{\mathbf{b}} \sum_a \frac{\pi^2(a)\sigma^2(a)}{\lceil \mathbf{b}(a)n\rceil}$. This captures the optimal number of times the actions should be pulled weighted by the target policy and their variance. Solving for $\mathbf{b}^*$, we obtain $\mathbf{b}^*(a) \propto \pi^2(a)\sigma^2(a)$. Note that this solution matches the optimal sampling proportion given by Antos et al. (2008); Carpentier and Munos (2011; 2012); Carpentier et al. (2015) for the simple bandit setting. Moreover, the loss of their oracle decreases at the rate of $\widetilde{O}(An^{-1})$ whereas we decrease at the rate of $\widetilde{O}(dn^{-1})$. Our oracle loss scales with d instead of d^2 as it knows the $\boldsymbol{\Sigma}_*$ and does not need to explore d^2 directions. So we obtain an equivalence between the solution of PE-Optimal design and the solution from prior work in the basic bandit setting while considering a strictly more general setting.

C. Experiments

We now conduct numerical experiments to show that SPEED decreases MSE faster than other baselines. As baselines, we compare against Onpolicy, Oracle , A-Optimal (Fontaine et al., 2021), G-Optimal (Wan et al., 2022). The Onpolicy algorithm simply runs the target policy to collect data and evaluate π, whereas the Oracle (as discussed in Section 3) is similar to SPEED but knows $\boldsymbol{\Sigma}_*$. Of these baselines, A-Optimal , and G-Optimal are the closest in relation to our work. We experiment with A-Optimal design because this criterion minimizes the average variance of the estimates of the regression coefficients and is most closely aligned with our goal. Note that Fontaine et al. (2021) considers policy improvement. The work of Wan et al. (2022) considers data collection under safety constraints using Inverse Propoensity Weighting. The G-Optimal implement this variant. In our unconstrained policy evaluation setting their approach boils down to just G-optimal design (Pukelsheim, 2006). Further experimental details are in Appendix F.

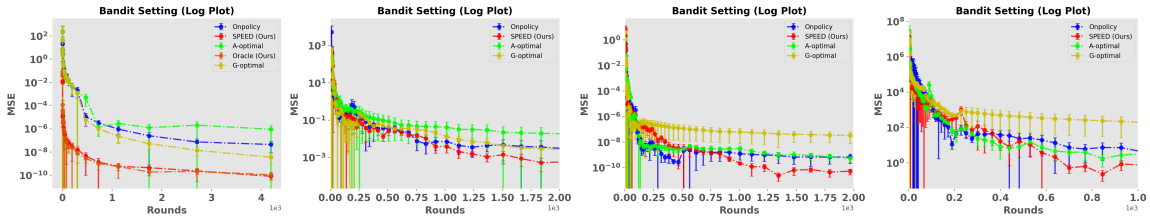

Figure 1. (Left) MSE plot for the Unit ball. (Middle-left) MSE plot for the Movielens dataset. (Middle-Right) MSE plot for Red Wine Quality dataset. (Right) MSE plot for Air Quality dataset. The vertical axis gives MSE and the horizontal axis is the number of rounds. The vertical axis is log-scaled and confidence bars show one standard error.

Unit Ball: We perform this experiment on a set of 5 actions that are arranged in a unit ball in $\mathbb{R}^2$ to show that SPEED allocates proportion to the most informative action (weighted by their variance). Figure 1 (Left) shows that SPEED outperforms Onpolicy, G-Optimal , and A-Optimal . We also show Oracle in this setting to show how quickly SPEED converges to it. However, for settings based on real-life data, we do not have such oracles.

Movielens Dataset: Consider a startup that wants to recommend movies to users based on their ratings. They have access to a target policy and want to evaluate it on a limited informative dataset before deploying it for full public use. We use real-world Movielens 1M dataset (Lam and Herlocker, 2016) datasets for this experiment. We apply low-rank factorization to the rating matrix to obtain 5-dimensional representations of users and movies. We then fit a weighted least square estimate of $\boldsymbol{\theta}^*$ and $\boldsymbol{\Sigma}_*$. We generate the reward using this $\boldsymbol{\theta}^*$ and $\boldsymbol{\Sigma}_*$. Then we use SPEED and other baselines to generate the small informative dataset to evaluate the target policy and this experiment is shown in Figure 1 (Left). SPEED initially conducts

forced exploration to estimate $\boldsymbol{\theta}_*$, $\boldsymbol{\Sigma}_*$ and incurs slightly higher MSE but the MSE decreases faster than other baselines as the number of rounds increases.

Red Wine Quality: We use a similar motivation as before to conduct this experiment. However, we now consider an online wine company that wants to recommend wines to users and wants to evaluate a target policy before full deployment. We perform this experiment on real-world dataset *Red Wine Quality* from UCI datasets (Cortez et al., 2009). The dataset consists of 1600 samples (actions) of red wine with each sample a having feature $\mathbf{x}(a) \in \mathbb{R}^{11}$ and their ratings. We fit a weighted least square estimate to the original dataset and get an estimate of $\boldsymbol{\theta}^*$ and $\boldsymbol{\Sigma}_*$. We generate the reward using this $\boldsymbol{\theta}^*$ and $\boldsymbol{\Sigma}_*$. Then we use SPEED to generate the informative dataset to evaluate the target policy. Figure 2 (Middle-Right) shows that SPEED outperforms other baselines as horizon increases.

Air Quality: We now consider a setting where a government agency wants to record air quality and notify the public. However, it wants to evaluate a target policy on a limited informative dataset before full deployment. We perform this experiment on real-world dataset *Air-Quality* from UCI datasets (De Vito et al., 2008). The dataset consists of 1500 samples (actions) with each sample a having feature $\mathbf{x}(a) \in \mathbb{R}^6$ and their air quality value. We fit a weighted least square estimate to the original dataset and get an estimate of $\boldsymbol{\theta}^*$ and $\boldsymbol{\Sigma}_*$. We generate the reward using this $\boldsymbol{\theta}^*$ and $\boldsymbol{\Sigma}_*$. Then we use SPEED and other baselines (which do not know $\boldsymbol{\theta}^*$ and $\boldsymbol{\Sigma}_*$) to generate the informative dataset to evaluate the target policy and this experiment is shown in Figure 1 (Right) Figure 2 (Bottom-Right) shows that SPEED MSE decreases faster than other baselines as the number of rounds increases.

C.1. Probability Tools

Lemma C.1. ***(Kiefer and Wolfowitz, 1960)*** *Assume that $\mathcal{A} \subset \mathbb{R}^d$ is compact and $\operatorname{span}(\mathcal{A}) = \mathbb{R}^d$. Let $\pi : \mathcal{A} \to [0,1]$ be a distribution on $\mathcal{A}$ so that $\sum_{a\in\mathcal{A}} \pi(a) = 1$ and $\mathbf{V}(\pi) \in \mathbb{R}^{d\times d}$ and $g(\pi) \in \mathbb{R}$ be given by*

$$\mathbf{V}(\pi) = \sum_{a\in\mathcal{A}} \pi(a) a a^\top, \quad g(\pi) = \max_{a\in\mathcal{A}} \|a\|^2_{\widetilde{\mathbf{X}}(\pi)^{-1}}$$

Then the following are equivalent:

(a) π^* is a minimizer of g.

(b) π^* is a maximizer of $f(\pi) = \log\det \mathbf{V}(\pi)$.

(c) $g(\pi^*) = d$.

Furthermore, there exists a minimizer π^* of g such that $|\operatorname{Supp}(\pi^*)| \le d(d+1)/2$.

Lemma C.2. ***(Sub-Exponential Concentration)*** *Suppose that X is sub-exponential with parameters (ν, α). Then*

$$\mathbb{P}[X \ge \mu + t] \le \begin{cases} e^{-\frac{t^2}{2\nu^2}} & \text{if } 0 \le t \le \frac{\nu^2}{\alpha} \\ e^{-\frac{1}{2\alpha}} & \text{if } t > \frac{\nu^2}{\alpha} \end{cases}$$

which can be equivalently written as follows:

$$\mathbb{P}[X \ge \mu + t] \le \exp\left\{-\frac{1}{2}\min\left\{\frac{t}{\alpha}, \frac{t^2}{\nu^2}\right\}\right\}.$$

Lemma C.3. ***(Restatement of Theorem 2.2 in (Rigollet and Hütter, 2015))*** *Assume that the linear model holds where the noise $\varepsilon \sim \mathrm{subG}_n(\sigma^2)$. Then the least squares estimator $\hat{\theta}^{\mathrm{LS}}$ satisfies*

$$\mathbb{E}\left[\mathrm{MSE}\left(\mathbf{X}\hat{\theta}^{\mathrm{LS}}\right)\right] = \frac{1}{n}\mathbb{E}\left|\mathbf{X}\hat{\theta}^{\mathrm{LS}} - \mathbf{X}\theta^*\right|_2^2 \lesssim \sigma^2 \frac{r}{n}$$

where $r = \operatorname{rank}\left(\mathbf{X}^\top\mathbf{X}\right)$. Moreover, for any $\delta > 0$, with probability at least $1-\delta$, it holds

$$\mathrm{MSE}\left(\mathbf{X}\hat{\theta}^{\mathrm{LS}}\right) \lesssim \sigma^2 \frac{r + \log(1/\delta)}{n}$$

C.2. Formulation for PE-Optimal Design to Reduce MSE

Proposition 1. *Let $\widehat{\boldsymbol{\theta}}_n$ be the estimate of $\boldsymbol{\theta}_*$ and define $\mathbf{w}(a) = \pi(a)\mathbf{x}(a)$. Define the design matrix as $\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}} = \sum_{a=1}^{A} \mathbf{b}(a) \left(\frac{\pi(a)\mathbf{x}(a)}{\sigma(a)}\right) \left(\frac{\pi(a)\mathbf{x}(a)}{\sigma(a)}\right)^\top$. Then the mean squared error is given by*

$$\mathbb{E}\left[\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2\right] = \frac{1}{n}\left(\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}}^{-1} \mathbf{w}(a')\right).$$

Proof. Let $T_n(a) \geq 0$ be the number of samples of $\mathbf{x}(a)$, hence $n = \sum_{a=1}^{A} T_n(a)$. For each $a \in [A]$, the linear model yields:

$$\frac{1}{T_n(a)} \sum_{t=1}^{T_n(a)} R_t(a) = \mathbf{x}(a)^\top \boldsymbol{\theta}_* + \frac{1}{T_n(a)} \sum_{t=1}^{T_n(a)} \eta_t(a).$$

We define the following:

$$\widetilde{Y}_n(a) = \sum_{t=1}^{T_n(a)} \frac{R_t(a)}{\sigma(a)\sqrt{T_n(a)}}, \qquad \widetilde{\mathbf{x}}_n(a) = \frac{\sqrt{T_n(a)}\mathbf{x}(a)}{\sigma(a)}, \qquad \widetilde{\eta}_n(a) = \sum_{t=1}^{T_n(a)} \frac{\eta_t(a)}{\sigma(a)\sqrt{T_n(a)}}$$

so that for all $a \in [A], \widetilde{Y}_n(a) = \widetilde{\mathbf{x}}_n(a)^\top \boldsymbol{\theta}_* + \widetilde{\eta}_n(a)$ where we can show the following regarding the expectation of $\widetilde{\eta}_n(a)$ as

$$\mathbb{E}[\widetilde{\eta}_n(a)] = \mathbb{E}\left[\sum_{t=1}^{T_n(a)} \frac{\eta_t(a)}{\sigma(a)\sqrt{T_n(a)}}\right] = \sum_{t=1}^{T_n(a)} \frac{\mathbb{E}\left[\eta_t(a)\right]}{\sigma(a)\sqrt{T_n(a)}} = 0$$

and the variance as

$$\mathbf{Var}\left[\widetilde{\eta}_n(a)\right] = \mathbf{Var}\left[\sum_{t=1}^{T_n(a)} \frac{\eta_t(a)}{\sigma(a)\sqrt{T_n(a)}}\right] \overset{(a)}{=} \sum_{t=1}^{T_n(a)} \mathbf{Var}\left[\frac{\eta_t(a)}{\sigma(a)\sqrt{T_n(a)}}\right] = \sum_{t=1}^{T_n(a)} \frac{\mathbf{Var}\left[\eta_t(a)\right]}{\sigma^2(a)T_n(a)} = \frac{T_n(a)\sigma^2(a)}{\sigma^2(a)T_n(a)} = 1$$

where, (a) follows as the noises are independent. We denote by $\mathbf{X} = \left(\widetilde{\mathbf{x}}_n(1)^\top, \cdots, \widetilde{\mathbf{x}}_n(A)^\top\right)^\top \in \mathbb{R}^{A\times d}$ the induced design matrix of the policy. Under the assumption that $\mathbf{X}$ has full rank, the above ordinary least squares (OLS) problem has an optimal unbiased estimator $\widehat{\boldsymbol{\theta}}_n = \left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\mathbf{Y}$, where $\mathbf{Y} = [\widetilde{Y}_n(1), \widetilde{Y}_n(2), \ldots, \widetilde{Y}_n(A)]^\top$. Let

$\eta = [\widetilde{\epsilon}_n(1), \widetilde{\epsilon}_n(2), \ldots, \widetilde{\epsilon}_n(A)]^\top$. Let $\mathbf{w}(a) = \pi(a)\mathbf{x}(a)$. Then the objective is to bound the loss as follows

$$
\begin{aligned}
&\mathbb{E}\left[\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top\widehat{\boldsymbol{\theta}}_n - \sum_{a=1}^{A}\mathbf{w}(a)^\top\boldsymbol{\theta}_*\right)^2\right] = \mathbb{E}\left[\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top\left(\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\mathbf{Y} - \boldsymbol{\theta}_*\right)\right)^2\right] = \mathbb{E}\left[\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top\left(\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\left(\mathbf{X}\boldsymbol{\theta}^\star + \eta\right) - \boldsymbol{\theta}_*\right)\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\eta\right)^2\right] \overset{(a)}{=} \mathbb{E}\left[\mathbf{Tr}\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\eta\eta^\top\mathbf{X}\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\sum_{a=1}^{A}\mathbf{w}(a)\right)\right] \\
&= \mathbf{Tr}\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\mathbb{E}\left[\eta\eta^\top\right]\mathbf{X}\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\sum_{a=1}^{A}\mathbf{w}(a)\right) \\
&\overset{(b)}{=} \mathbf{Tr}\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\mathbf{I}\mathbf{X}\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\sum_{a=1}^{A}\mathbf{w}(a)\right) \\
&= \mathbf{Tr}\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\sum_{a=1}^{A}\mathbf{w}(a)\right) = \mathbf{Tr}\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top\left(\sum_{a=1}^{A}\widetilde{\mathbf{x}}_n(a)\widetilde{\mathbf{x}}_n(a)^\top\right)^{-1}\sum_{a=1}^{A}\mathbf{w}(a)\right) \\
&= \frac{1}{n}\mathbf{Tr}\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top\left(\sum_{a=1}^{A}\frac{\mathbf{b}(a)\mathbf{x}(a)\mathbf{x}(a)^\top}{\sigma(a)^2}\right)^{-1}\sum_{a=1}^{A}\mathbf{w}(a)\right) \\
&\overset{(c)}{=} \frac{1}{n}\mathbf{Tr}\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top\left(\sum_{a=1}^{A}\mathbf{b}(a)\widetilde{\mathbf{x}}(a)\widetilde{\mathbf{x}}(a)^\top\right)^{-1}\sum_{a=1}^{A}\mathbf{w}(a)\right) \\
&= \frac{1}{n}\mathbf{Tr}\left(\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}}^{-1}\mathbf{w}(a')\right)
\end{aligned}
$$

where, in (a) we can introduce the trace operator as for any vector $\mathbf{x}$ we have $\mathbf{Tr}(\mathbf{x}^\top\mathbf{x}) = \|\mathbf{x}\|^2$, (b) follows as the matrix $\mathbb{E}[\eta\eta^\top]$ has all the non-diagonal element as 0 (since noises are independent and $\mathbf{Cov}(\widetilde{\epsilon}_n(a), \widetilde{\epsilon}_n(a')) = 0$) and the diagonal element are the $\mathbf{Var}[\widetilde{\epsilon}_n(a)] = 1$, and (c) follows as we redefine $\widetilde{\mathbf{x}}(a) = \mathbf{x}(a)/\sigma(a)$. □

C.3. Loss is convex

Proposition 2. *The loss function*

$$
\mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma}) = \frac{1}{n}\left(\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}}^{-1}\mathbf{w}(a')\right)
$$

for any arbitrary design proportion $\mathbf{b} \in \triangle(\mathcal{A})$ *and co-variance matrix* $\boldsymbol{\Sigma}$ *is strictly convex.*

Proof. Let $\mathbf{b}, \mathbf{b}' \in \triangle(\mathcal{A})$, so that $\mathbf{A}_{\mathbf{b}}$ and $\mathbf{A}_{\mathbf{b}'}$ are invertible. Recall that we have the loss for a design proportion $\mathbf{b}$ as

$$
\begin{aligned}
\mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma}) = \frac{1}{n}\left(\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}}^{-1}\mathbf{w}(a')\right) &\overset{(a)}{=} \frac{1}{n}\mathbf{Tr}\left(\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}}^{-1}\mathbf{w}(a')\right) = \frac{1}{n}\mathbf{Tr}\left(\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}}^{-1}\sum_{a,a'}\mathbf{w}(a)\mathbf{w}(a')^\top\right) \\
&= \frac{1}{n}\mathbf{Tr}\left(\mathbf{V}\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}}^{-1}\right)
\end{aligned}
$$

where, in (a) we can introduce the trace as the R.H.S. is a scalar quantity, $\mathbf{w}(a) = \pi(a)\mathbf{x}(a)$ and $\mathbf{V} = \sum_{a,a'} \mathbf{w}(a)\mathbf{w}(a')^\top$. Similarly for a $\lambda \in [0,1]$ we have

$$\mathcal{L}_n(\pi, \lambda\mathbf{b} + (1-\lambda)\mathbf{b}', \mathbf{\Sigma}) = \frac{1}{n}\mathbf{Tr}\left(\mathbf{A}^{-1}_{\mathbf{b},\mathbf{b}',\mathbf{\Sigma}} \sum_{a,a'} \mathbf{w}(a)\mathbf{w}(a')^\top\right) = \frac{1}{n}\mathbf{Tr}\left(\mathbf{V}\mathbf{A}^{-1}_{\mathbf{b},\mathbf{b}',\mathbf{\Sigma}}\right).$$

Let the matrix $\mathbf{A}_{\mathbf{b},\mathbf{b}',\mathbf{\Sigma}}$ be defined as

$$\mathbf{A}_{\mathbf{b},\mathbf{b}',\mathbf{\Sigma}} \coloneqq \lambda\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}} + (1-\lambda)\mathbf{A}_{\mathbf{b}',\mathbf{\Sigma}}.$$

Now observe that

$$\mathbf{A}_{\mathbf{b},\mathbf{b}',\mathbf{\Sigma}} = \lambda\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}} + (1-\lambda)\mathbf{A}_{\mathbf{b}',\mathbf{\Sigma}} = \sum_{a=1}^{A} \left(\lambda\mathbf{b}(a) + (1-\lambda)\mathbf{b}'(a)\right)\widetilde{\mathbf{x}}(a)\widetilde{\mathbf{x}}(a)^\top.$$

Also observe that this is a positive semi-definite matrix. Now using Lemma 1 from (Whittle, 1958) we can show that

$$(\lambda\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}} + (1-\lambda)\mathbf{A}_{\mathbf{b}',\mathbf{\Sigma}})^{-1} \prec \lambda\mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}} + (1-\lambda)\mathbf{A}^{-1}_{\mathbf{b}',\mathbf{\Sigma}}$$

for any positive semi-definite matrices $\mathbf{A}_{\mathbf{b}}, \mathbf{A}_{\mathbf{b}'}$, and $\lambda \in [0,1]$. Now taking the trace on both sides we get

$$\mathbf{Tr}\left(\lambda\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}} + (1-\lambda)\mathbf{A}_{\mathbf{b}',\mathbf{\Sigma}}\right)^{-1} \prec \mathbf{Tr}\lambda\mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}} + \mathbf{Tr}(1-\lambda)\mathbf{A}^{-1}_{\mathbf{b}',\mathbf{\Sigma}}.$$

Now using Lemma 2 from Whittle (1958) we can show that

$$\mathbf{Tr}\left(\lambda\mathbf{V}\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}} + (1-\lambda)\mathbf{V}\mathbf{A}_{\mathbf{b}',\mathbf{\Sigma}}\right)^{-1} \prec \mathbf{Tr}\lambda\mathbf{V}\mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}} + \mathbf{Tr}(1-\lambda)\mathbf{V}\mathbf{A}^{-1}_{\mathbf{b}',\mathbf{\Sigma}}.$$

for any positive semi-definite matrix $\mathbf{V}$. This implies that

$$\mathcal{L}_n(\pi, \lambda\mathbf{b} + (1-\lambda)\mathbf{b}', \mathbf{\Sigma}) < \lambda\mathcal{L}_n(\pi, \mathbf{b}, \mathbf{\Sigma}) + (1-\lambda)\mathcal{L}_n(\pi, \mathbf{b}', \mathbf{\Sigma}).$$

Hence, the loss function is convex. □

Remark C.4. ((**Bound on variance**) We can use singular value decomposition of $\mathbf{\Sigma}_*$ as $\mathbf{\Sigma}_* = \mathbf{U}\mathbf{D}\mathbf{P}^\top$ with orthogonal matrices $\mathbf{U}, \mathbf{P}^\top$ and $\mathbf{D} = \mathrm{diag}\left(\lambda_1, \ldots, \lambda_d\right)$ where λ_i denotes a singular value. Then we can bound $\mathbf{x}(a)^\top\mathbf{\Sigma}_*\mathbf{x}(a)$ as

$$\begin{aligned}\left\|\mathbf{x}(a)^\top\mathbf{\Sigma}_*\mathbf{x}(a)\right\| = \left\|\mathbf{x}(a)^\top\mathbf{U}\mathbf{D}\mathbf{P}^\top\mathbf{x}(a)\right\| &\overset{(a)}{=} \left\|\mathbf{u}^\top\mathbf{D}\mathbf{p}\right\| \leq \left\|\mathbf{u}^\top\right\| \max_i |\lambda_i| \left\|\mathbf{p}\right\| \\ &\overset{(b)}{=} \left\|\mathbf{x}(a)\right\| \max_i |\lambda_i| \left\|\mathbf{x}(a)\right\| = \max_i |\lambda_i| \left\|\mathbf{x}(a)\right\|^2\end{aligned}$$

where in (a) we have $\mathbf{u} = \mathbf{U}^\top\mathbf{x}(a)$, $\mathbf{p} = \mathbf{P}^\top\mathbf{x}(a)$ and (b) uses the fact that $\left\|\mathbf{U}^\top\mathbf{x}(a)\right\| = \left\|\mathbf{x}(a)\right\|$ for any orthogonal matrix $\mathbf{U}^\top$. Similarly we can show that $\left\|\mathbf{x}(a)^\top\mathbf{\Sigma}_*\mathbf{x}(a)\right\| \geq \min_i |\lambda_i| \left\|\mathbf{x}(a)\right\|^2$. Let $H_L^2 \leq \left\|\mathbf{x}(a)\right\|^2 \leq H_U^2$ for any $a \in [A]$. This implies that

$$\underbrace{\min_i |\lambda_i| H_L^2}_{\sigma^2_{\min}} \leq \min_i |\lambda_i| \left\|\mathbf{x}(a)\right\|^2 \leq \underbrace{\mathbf{x}(a)^\top\mathbf{\Sigma}_*\mathbf{x}(a)}_{\sigma^2(a)} \leq \max_i |\lambda_i| \left\|\mathbf{x}(a)\right\|^2 \leq \underbrace{\max_i |\lambda_i| H_U^2}_{\sigma^2_{\max}}$$

C.4. Loss Gradient is Bounded

Proposition 3. *Let $\mathbf{b}, \mathbf{b}' \in \triangle(\mathcal{A})$, so that $\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}$ and $\mathbf{A}_{\mathbf{b}',\mathbf{\Sigma}}$ are invertible and define $\mathbf{V} = \sum_{a,a'} \mathbf{w}(a)\mathbf{w}(a')^\top$. Then the gradient of the loss function is bounded such that*

$$\left\|\nabla_{\mathbf{b}(a)}\mathcal{L}(\pi, \mathbf{b}, \mathbf{\Sigma}) - \nabla_{\mathbf{b}(a)}\mathcal{L}(\pi, \mathbf{b}', \mathbf{\Sigma})\right\|_2 \leq C_\kappa$$

where, the

$$C_\kappa = \frac{\lambda_d(\mathbf{V})H_U^2}{\sigma^2(a)\left(\min_{a'\in\mathcal{A}} \frac{\mathbf{b}(a')}{\sigma(a')^2}\lambda_{\min}\left(\sum_{a=1}^{A} \mathbf{w}(a)\mathbf{w}(a)^\top\right)\right)^2} + \frac{\lambda_1(\mathbf{V})H_U^2}{\sigma^2(a)\left(\min_{a'\in\mathcal{A}} \frac{\mathbf{b}'(a')}{\sigma(a')^2}\lambda_{\min}\left(\sum_{a=1}^{A} \mathbf{w}(a)\mathbf{w}(a)^\top\right)\right)^2}.$$

Proof. Let $\mathbf{b}, \mathbf{b}' \in \triangle(\mathcal{A})$, so that $\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}$ and $\mathbf{A}_{\mathbf{b}',\mathbf{\Sigma}}$ are invertible. Observe that the gradient of the loss is given by

$$\begin{aligned}
\nabla_{\mathbf{b}(a)}\mathcal{L}(\pi, \mathbf{b}, \mathbf{\Sigma}) &= \nabla_{\mathbf{b}(a)}\mathbf{Tr}\left(\sum_{a,a'}\mathbf{w}(a)^\top \mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}\mathbf{w}(a')\right) \\
&\overset{(a)}{\leq} \lambda_1(\mathbf{V})\nabla_{\mathbf{b}(a)}\mathbf{Tr}(\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}) \\
&= -\lambda_1(\mathbf{V})\mathbf{Tr}\left(\left(\frac{\mathbf{w}(a)\mathbf{w}(a)^\top}{\sigma^2(a)}\right)\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-2}\right) \\
&= -\lambda_1(\mathbf{V})\frac{1}{\sigma^2(a)}\left\|\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}\mathbf{w}(a)\right\|_2^2
\end{aligned}$$

where, in (a) we denote $\mathbf{V} = \sum_{a,a'}\mathbf{w}(a)\mathbf{w}(a')^\top$. Similarly the gradient of the loss is lower bounded by

$$\nabla_{\mathbf{b}(a)}\mathcal{L}(\pi, \mathbf{b}, \mathbf{\Sigma}) \geq -\lambda_d(\mathbf{V})\frac{1}{\sigma^2(a)}\left\|\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}\mathbf{w}(a)\right\|_2^2$$

which yields a bound on the gradient difference as

$$\begin{aligned}
\|\nabla_{\mathbf{b}(a)}\mathcal{L}(\pi, \mathbf{b}, \mathbf{\Sigma}) - \nabla_{\mathbf{b}'(a)}\mathcal{L}(\pi, \mathbf{b}', \mathbf{\Sigma})\|_2 &\leq \left\|\lambda_d(\mathbf{V})\frac{1}{\sigma^2(a)}\left\|\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}\mathbf{w}(a)\right\|_2^2 - \lambda_1(\mathbf{V})\frac{1}{\sigma^2(a)}\left\|\mathbf{A}_{\mathbf{b}',\mathbf{\Sigma}}^{-1}\mathbf{w}(a)\right\|_2^2\right\|_2 \\
&\leq \left|\lambda_d(\mathbf{V})\frac{1}{\sigma^2(a)}\left\|\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}\mathbf{w}(a)\right\|_2^2\right| + \left|\lambda_1(\mathbf{V})\frac{1}{\sigma^2(a)}\left\|\mathbf{A}_{\mathbf{b}',\mathbf{\Sigma}}^{-1}\mathbf{w}(a)\right\|_2^2\right|.
\end{aligned}$$

So now we focus on the quantity

$$\left\|\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}\mathbf{w}(a)\right\|_2^2 \leq \|\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}\|_2^2\|\mathbf{w}(a)\|_2^2 \leq \|\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}\|_2^2 H_U^2.$$

Now observe that when $\mathbf{b}(a) \in \Delta(\mathcal{A})$ and initialized uniform randomly, then the optimization in (4) results in a non-singular $\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}$ if each action has been sampled at least once which is satisfied by SPEED. So now we need to bound the minimum eigenvalue of $\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}$ denoted as $\lambda_{\min}(\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}})$. Using Lemma 7 of Fontaine et al. (2021) we have that for all $\mathbf{b} \in \Delta(\mathcal{A})$,

$$\min_{a\in[A]}\frac{\mathbf{b}(a)}{\sigma(a)^2}\sum_{a=1}^{A}\mathbf{w}(a)\mathbf{w}(a)^\top \preccurlyeq \sum_{a=1}^{A}\frac{\mathbf{b}(a)}{\sigma(a)^2}\mathbf{w}(a)\mathbf{w}(a)^\top.$$

And finally

$$\min_{a\in[A]}\frac{\mathbf{b}(a)}{\sigma(a)^2}\lambda_{\min}\left(\sum_{a=1}^{A}\mathbf{w}(a)\mathbf{w}(a)^\top\right) \leq \lambda_{\min}(\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}})$$

This implies that

$$\lambda_{\min}(\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}) \leq \frac{1}{\min_{a\in[A]}\frac{\mathbf{b}(a)}{\sigma(a)^2}\lambda_{\min}\left(\sum_{a=1}^{A}\mathbf{w}(a)\mathbf{w}(a)^\top\right)}$$

Plugging everything back we get that

$$\begin{aligned}
\|\nabla_{\mathbf{b}(a)}\mathcal{L}(\pi, \mathbf{b}, \mathbf{\Sigma}) - \nabla_{\mathbf{b}'(a)}\mathcal{L}(\pi, \mathbf{b}', \mathbf{\Sigma})\|_2 \leq &\frac{\lambda_d(\mathbf{V})H_U^2}{\sigma^2(a)\left(\min_{a'\in\mathcal{A}}\frac{\mathbf{b}(a')}{\sigma(a')^2}\lambda_{\min}\left(\sum_{a=1}^{A}\mathbf{w}(a)\mathbf{w}(a)^\top\right)\right)^2} \\
&+ \frac{\lambda_1(\mathbf{V})H_U^2}{\sigma^2(a)\left(\min_{a'\in\mathcal{A}}\frac{\mathbf{b}'(a')}{\sigma(a')^2}\lambda_{\min}\left(\sum_{a=1}^{A}\mathbf{w}(a)\mathbf{w}(a)^\top\right)\right)^2}.
\end{aligned}$$

The claim of the lemma follows. □

C.5. Kiefer-Wolfowitz Equivalence

We now introduce a Kiefer-Wolfowitz type equivalence (Kiefer and Wolfowitz, 1960) for the quantity $\mathbf{Tr}(\mathbf{A}_{\mathbf{b}^*,\mathbf{\Sigma}}^{-1})$ for optimal $\mathbf{b}^* \in \Delta(\mathcal{A})$ and co-variance matrix $\mathbf{\Sigma}$ in Proposition 4.

Proposition 4. ***(Kiefer-Wolfowitz for PE-Optimal)*** *Define the heteroscedastic design matrix as* $\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}} = \sum_{a=1}^{A} \mathbf{b}(a)\widetilde{\mathbf{x}}(a)\widetilde{\mathbf{x}}(a)^\top$. *Assume that* $\mathcal{A} \subset \mathbb{R}^d$ *is compact and* $\mathrm{span}(\mathcal{A}) = \mathbb{R}^d$. *Then the following are equivalent:*

(a) $\mathbf{b}^*$ *is a minimiser of* $\widetilde{g}(\mathbf{b},\mathbf{\Sigma}) = \mathbf{Tr}\left(\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}\right)$.

(b) $\mathbf{b}^*$ *is a maximiser of* $f(\mathbf{b},\mathbf{\Sigma}) = \log\det\left(\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}\right)$.

(c) $\widetilde{g}\left(\mathbf{b}^*,\mathbf{\Sigma}\right) = d$.

Furthermore, there exists a minimiser $\mathbf{b}^*$ *of* $\widetilde{g}(\mathbf{b},\mathbf{\Sigma})$ *such that* $|\mathrm{Supp}\left(\mathbf{b}^*\right)| \leq d(d+1)/2$.

Proof. We follow the proof technique of Lattimore and Szepesvári (2020b). Let $\mathbf{b} : \mathcal{A} \to [0,1]$ be a distribution on $\mathcal{A}$ so that $\sum_{a\in\mathcal{A}} \mathbf{b}(a) = 1$ and $\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}} \in \mathbb{R}^{d\times d}$ and $g(\mathbf{b}) \in \mathbb{R}$ be given by

$$\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}} = \sum_{a=1}^{A} \mathbf{b}(a)\pi^2(a)\sigma^{-2}(a)\ \mathbf{x}(a)\mathbf{x}(a)^\top = \sum_{a=1}^{A} \mathbf{b}(a)\frac{\pi(a)\mathbf{x}(a)}{\sigma(a)}\left(\frac{\pi(a)\mathbf{x}(a)}{\sigma(a)}\right)^\top$$

where, (a) follows by setting $\widetilde{\mathbf{x}}(a) = \mathbf{x}(a)/\sigma(a)$. First recall that for a square matrix $\mathbf{A}$ let adj $(\mathbf{A})$ be the transpose of the cofactor matrix of $\mathbf{A}$. Use the facts that the inverse of a matrix $\mathbf{A}$ is $\mathbf{A}^{-1} = \mathrm{adj}(\mathbf{A})^\top/\det(\mathbf{A})$ and that if $\mathbf{A} : \mathbb{R} \to \mathbb{R}^{d\times d}$, then

$$\frac{d}{dt}\det(\mathbf{A}(t)) = \mathbf{Tr}\left(\mathrm{adj}(\mathbf{A})\frac{d}{dt}\mathbf{A}(t)\right).$$

It follows then that

$$\begin{aligned}\nabla f(\mathbf{b},\mathbf{\Sigma})_{b(a)} &\overset{(a)}{=} \frac{\mathbf{Tr}\left(\mathrm{adj}(\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}})\widetilde{\mathbf{x}}(a)\widetilde{\mathbf{x}}(a')^\top\right)}{\det(\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}})} \\ &= \frac{\widetilde{\mathbf{x}}(a)^\top\,\mathrm{adj}(\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}})\widetilde{\mathbf{x}}(a')}{\det(\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}})} \overset{(b)}{=} \widetilde{\mathbf{x}}(a)^\top\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}\widetilde{\mathbf{x}}(a') = \widetilde{g}(\mathbf{b})\end{aligned}$$

where, in (a) we show the a-th component of $f(\mathbf{b})$ when we differentiate w.r.t to $\mathbf{b}(a)$, and (b) follows as $\frac{\mathrm{adj}(\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}})}{\det(\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}})} = \mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}$. Also observe that

$$\left(\sum_{a=1}^{A}\mathbf{b}(a)\|\widetilde{\mathbf{x}}(a)\|^2_{\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}}\right) = \mathbf{Tr}\left(\sum_{a=1}^{A}\mathbf{b}(a)\widetilde{\mathbf{x}}(a)\widetilde{\mathbf{x}}(a')^\top\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}\right) = d. \tag{9}$$

Hence, $\max_{\mathbf{b}}\log\det\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}$ is lower bounded by d as in average we have that $\left(\sum_{a=1}^{A}\mathbf{b}(a)\|\widetilde{\mathbf{x}}(a)\|^2_{\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1}}\right) = d$.

(b) $\Rightarrow$ (a): Suppose that $\mathbf{b}^*$ is a maximiser of f. By the first-order optimality criterion, for any $\mathbf{b}$ distribution on $\mathcal{A}$,

$$\begin{aligned}0 &\geq \left\langle\nabla f\left(\mathbf{b}^*,\mathbf{\Sigma}\right),\mathbf{b}-\mathbf{b}^*\right\rangle \\ &\geq \left(\sum_{a=1}^{A}\mathbf{b}(a)\|\widetilde{\mathbf{x}}(a)\|^2_{\mathbf{A}_{\mathbf{b}^*,\mathbf{\Sigma}}^{-1}} - \sum_{a=1}^{A}\mathbf{b}^*(a)\|\widetilde{\mathbf{x}}(a)\|^2_{\mathbf{A}_{\mathbf{b}^*,\mathbf{\Sigma}}^{-1}}\right) \\ &\geq \left(\sum_{a=1}^{A}\mathbf{b}(a)\|\widetilde{\mathbf{x}}(a)\|^2_{\mathbf{A}_{\mathbf{b}^*,\mathbf{\Sigma}}^{-1}} - d\right).\end{aligned}$$

For an arbitrary $a \in \mathcal{A}$, choosing $\mathbf{b}$ to be the Dirac at $a \in \mathcal{A}$ proves that $\sum_{a=1}^{A}\|\widetilde{\mathbf{x}}(a)\|^2_{\mathbf{A}_{\mathbf{b}^*,\mathbf{\Sigma}}^{-1}} \leq d$. Since $\widetilde{g}(\mathbf{b}) \geq d$ for all $\mathbf{b}$ by (9), it follows that $\mathbf{b}^*$ is a minimiser of $\widetilde{g}$ and that $\min_{\mathbf{b}}\widetilde{g}(\mathbf{b}) = d$.

(c) $\implies$ (b): Suppose that $\widetilde{g}(\mathbf{b}^*) = d$. Then, for any $\mathbf{b}$,

$$\langle \nabla f(\mathbf{b}^*, \mathbf{\Sigma}), \mathbf{b} - \mathbf{b}^* \rangle = \left(\sum_{a=1}^{A} \mathbf{b}(a) \|\widetilde{\mathbf{x}}(a)\|^2_{\mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}}} - d \right) \leq 0.$$

And it follows that $\mathbf{b}^*$ is a maximiser of f by the first-order optimality conditions and the concavity of f. This can be shown as follows:

Let $\mathbf{b}$ be a Dirac at a and $\mathbf{b}(t) = \mathbf{b}^* + t(\mathbf{b}^* - \mathbf{b})$. Since $\mathbf{b}^*(a) > 0$ it follows for sufficiently small $t > 0$ that $\mathbf{b}(t)$ is a distribution over $\mathcal{A}$. Because $\mathbf{b}^*$ is a minimiser of f,

$$0 \geq \frac{d}{dt} f(\mathbf{b}(t), \mathbf{\Sigma}) \bigg|_{t=0} = \langle \nabla f(\mathbf{b}^*, \mathbf{\Sigma}), \mathbf{b}^* - \mathbf{b} \rangle = d - \sum_{a=1}^{A} \|\widetilde{\mathbf{x}}(a)\|^2_{\mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}}}.$$

We now show (a) $\implies$ (c). To prove the second part of the theorem, let $\mathbf{b}^*$ be a minimiser of $\widetilde{g}$, which by the previous part is a maximiser of f. Let $S = \mathrm{Supp}(\mathbf{b}^*)$, and suppose that $|S| > d(d+1)/2$. Since the dimension of the subspace of $d \times d$ symmetric matrices is $d(d+1)/2$, there must be a non-zero function $v : \mathcal{A} \to \mathbb{R}$ with $\mathrm{Supp}(v) \subseteq S$ such that

$$\sum_{a \in S} v(a) \widetilde{\mathbf{x}}(a) \widetilde{\mathbf{x}}(a)^\top = \mathbf{0}. \tag{10}$$

Notice that for any $\widetilde{\mathbf{x}}(a) \in S$, the first-order optimality conditions ensure that $\sum_{a=1}^{A} \|\widetilde{\mathbf{x}}(a)\|^2_{\mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}}} = d$. Hence

$$d \sum_{a \in S} v(a) = \sum_{a \in S} v(a) \|\widetilde{\mathbf{x}}(a)\|^2_{\mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}}} = 0,$$

where the last equality follows from (10). Let $\mathbf{b}(t) = \mathbf{b}^* + tv$ and let $\tau = \max\{t > 0 : \mathbf{b}(t) \in \mathcal{P}_{\mathcal{A}}\}$, which exists since $v \neq 0$ and $\sum_{a \in S} v(a) = 0$ and $\mathrm{Supp}(v) \subseteq S$. By (10), $\mathbf{A}_{\mathbf{b}(t),\mathbf{\Sigma}} = \mathbf{A}_{\mathbf{b}^*,\mathbf{\Sigma}}$, and hence $f(\mathbf{b}(\tau), \mathbf{\Sigma}) = f(\mathbf{b}^*, \mathbf{\Sigma})$, which means that $\mathbf{b}(\tau)$ also maximises f. The claim follows by checking that $|\mathrm{Supp}(\mathbf{b}(T))| < |\mathrm{Supp}(\mathbf{b}^*)|$ and then using induction. □

Corollary 1. *From Proposition 4 we know that $\mathbf{b}^*$ is a minimizer for $\mathbf{Tr}(\mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}})$ and $\mathbf{Tr}(\mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}}) = d$. This implies that the loss is bounded at $\mathbf{b}^*$ as $\frac{\lambda_d(\mathbf{V})d}{n} \leq \mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}) \leq \frac{\lambda_1(\mathbf{V})d}{n}$ where $\mathbf{V} = \sum_{a,a'} \mathbf{w}(a)\mathbf{w}(a')^\top$.*

Proof. First recall that we can rewrite the loss for any arbitrary proportion $\mathbf{b}$ and co-variance $\mathbf{\Sigma}$ as

$$\mathcal{L}_n(\pi, \mathbf{b}, \mathbf{\Sigma}) = \frac{1}{n} \left(\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}} \mathbf{w}(a') \right) = \frac{1}{n} \left(\mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}} \sum_{a,a'} \mathbf{w}(a)\mathbf{w}(a')^\top \right) = \frac{1}{n} \left(\mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}} \mathbf{V} \right).$$

From (Fang et al., 1994) we know that for any positive semi-definite matrices $\mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}}$ and $\mathbf{V}$ we have that

$$\lambda_d(\mathbf{V}) \mathbf{Tr}(\mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}}) \leq \mathbf{Tr}(\mathbf{V}\mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}}) \leq \lambda_1(\mathbf{V}) \mathbf{Tr}(\mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}})$$

where $\lambda_i(\mathbf{V})$ is the i th largest eigenvalue of $\mathbf{V}$. Now from Proposition 4 we know that for $\mathbf{b}^*$ is a minimizer for $\mathbf{Tr}(\mathbf{A}^{-1}_{\mathbf{b},\mathbf{\Sigma}})$ and $\mathbf{Tr}(\mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}}) = d$. This implies that the loss is bounded at $\mathbf{b}^*$ as

$$\lambda_d(\mathbf{V}) \mathbf{Tr}(\mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}}) \leq \mathbf{Tr}(\mathbf{V}\mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}}) \leq \lambda_1(\mathbf{V}) \mathbf{Tr}(\mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}}) \implies \frac{\lambda_d(\mathbf{V})d}{n} \leq \mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}) \leq \frac{\lambda_1(\mathbf{V})d}{n}.$$

The claim of the corollary follows. □

C.6. Weighted Least Square Estimator that Minimizes MSE

Proposition 5. ***(Weighted Least Square)*** *Let* $\mathbf{A}_{\mathbf{b},\mathbf{\Sigma}} = \sum_{a,a'} \lceil \mathbf{b}(a)n \rceil \widetilde{\mathbf{x}}(a)\widetilde{\mathbf{x}}(a')^\top$ *be the design matrix such that each action is sampled according to* $\mathbf{b} \in \triangle(A)$*. Define the weighted least square estimate* $\widehat{\boldsymbol{\theta}}_n$ *by* (8)*. Then the weighted least square in* (8) *estimate minimizes* $\mathbb{E}_{\mathcal{D}}\left[\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2\right]$ *by minimizing the quantity* $\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}_{\mathbf{b},\mathbf{\Sigma}}^{-1} \mathbf{w}(a')$*.*

Proof. Recall from Appendix B that the *Weighted* least square estimate is

$$\widehat{\boldsymbol{\theta}}_n \overset{(a)}{=} \arg\min_{\boldsymbol{\theta}} \sum_{t=1}^{n} \frac{1}{\sigma^2(I_t)}(R(I_t) - \mathbf{x}(I_t)^\top \boldsymbol{\theta})^2 \overset{(b)}{=} \left(\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \widetilde{\mathbf{X}}_n\right)^{-1} \mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{R}_n$$
$$= \left(\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{X}_n\right)^{-1} \mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \left(\mathbf{X}_n \boldsymbol{\theta}_* + \eta\right)$$

where, in (a) the I_t is the action sampled at timestep t, and in (b) we define the matrix $\mathbf{\Sigma}_n \in \mathbb{R}^{n \times n}$. The $\mathbf{diag}(\mathbf{\Sigma}_n) = [\sigma^2(I_1), \sigma^2(I_2), \ldots, \sigma^2(I_n)]$. It follows then the value estimate

$$Y_n = \sum_{a=1}^{A} \mathbf{w}(a)^\top \widehat{\boldsymbol{\theta}}_n = \sum_{a=1}^{A} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{R}_n = \sum_{a=1}^{A} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \left(\mathbf{X}_n \boldsymbol{\theta}_* + \eta\right)$$
$$= \sum_{a=1}^{A} \mathbf{w}(a)^\top \boldsymbol{\theta}_* + \sum_{a=1}^{A} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \eta.$$

This means that

$$\sum_{a=1}^{A} \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*) = \sum_{a=1}^{A} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \eta$$
$$= \sum_{a=1}^{A} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1/2} \mathbf{\Sigma}_n^{-1/2} \mathbf{X}_n)^{-1} \mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \eta$$

Again, as η is bounded so we have $\eta \sim \mathcal{SG}(0, \mathbf{\Sigma}_n)$ where $\mathcal{SG}$ denote the sub-Gaussian distribution. Then we can show that

$$\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2 \sim \mathcal{SE}\left(0, \sum_{a=1}^{A} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbb{E}[\eta\eta^\top] \mathbf{\Sigma}_n^{-1} \mathbf{X}_n^\top (\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \sum_{a=1}^{A} \mathbf{w}(a)\right)$$
$$\overset{(a)}{\sim} \mathcal{SE}\left(0, \sum_{a=1}^{A} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{\Sigma}_n \mathbf{\Sigma}_n^{-1} \mathbf{X}_n^\top (\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \sum_{a=1}^{A} \mathbf{w}(a)\right)$$
$$\sim \mathcal{SE}\left(0, \sum_{a,a'} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{w}(a')\right)$$

where, (a) follows as $\eta \sim \mathcal{SG}(0, \mathbf{\Sigma}_n)$ and $\mathcal{SE}$ denotes sub-exponential distribution. Now using sub-exponential concentration inequality in Lemma C.2, setting

$$\nu^2 = \sum_{a,a'} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \mathbf{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{w}(a'),$$

and $\alpha = \nu$, we can show that

$$\mathbb{P}\left(\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2 > t\right) \leq \delta, \qquad \text{if } t \in (0, 1]$$
$$\mathbb{P}\left(\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2 > t^2\right) \leq \delta, \qquad \text{if } t > 1.$$

Combining the above two we can show that

$$\mathbb{P}\left(\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_n-\boldsymbol{\theta}_*)\right)^2>\min\{t,t^2\}\right)\leq\delta,\forall t>0.$$

Further define matrix $\overline{\boldsymbol{\Sigma}}_n\in\mathbb{R}^{d\times d}$ as $\overline{\boldsymbol{\Sigma}}_n^{-1}:=(\mathbf{X}_n^\top\boldsymbol{\Sigma}_n^{-1}\mathbf{X}_n)^{-1}$. Hence using sub-exponential concentration inequality we can show that

$$\mathbb{P}\left(\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_n-\boldsymbol{\theta}_*)\right)^2>\min\left\{\sqrt{2\sum_{a,a'}\mathbf{w}(a)^\top\overline{\boldsymbol{\Sigma}}_n^{-1}\mathbf{w}(a')\log(1/\delta)},2\sum_{a,a'}\mathbf{w}(a)^\top\overline{\boldsymbol{\Sigma}}_n^{-1}\mathbf{w}(a')\log(1/\delta)\right\}\right)\leq\delta.$$

This means that we have with probability $(1-\delta)$ that

$$\begin{aligned}\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_n-\boldsymbol{\theta}_*)\right)^2&\leq\min\left\{\sqrt{2\sum_{a,a'}\mathbf{w}(a)^\top\overline{\boldsymbol{\Sigma}}^{-1}\mathbf{w}(a')\log(1/\delta)},2\sum_{a,a'}\mathbf{w}(a)^\top\overline{\boldsymbol{\Sigma}}_n^{-1}\mathbf{w}(a')\log(1/\delta)\right\}\\&=2\sum_{a,a'}\mathbf{w}(a)^\top\overline{\boldsymbol{\Sigma}}_n^{-1}\mathbf{w}(a')\log(1/\delta).\end{aligned}$$

Recall that we have sampled each action till n in some proportion $\mathbf{b}\in\triangle(\mathcal{A})$. Then we have that

$$\begin{aligned}\overline{\boldsymbol{\Sigma}}_n=\mathbf{X}_n^\top\boldsymbol{\Sigma}_n^{-1}\mathbf{X}_n&=\sum_{a=1}^{A}\lceil\mathbf{b}(a)n\rceil\pi^2(a)\sigma^{-2}(a)\mathbf{x}(a)\mathbf{x}(a)^\top\\&=\sum_{a=1}^{A}\lceil\mathbf{b}(a)n\rceil\widetilde{\mathbf{x}}(a)\widetilde{\mathbf{x}}(a')^\top=n\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}}.\end{aligned}$$

It follows then that

$$\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_n-\boldsymbol{\theta}_*)\right)^2\leq\frac{2}{n}\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}}^{-1}\mathbf{w}(a')\log(1/\delta).$$

Hence, using the weighted least square estimate we can show that it minimizes $\mathbb{E}_{\mathcal{D}}\left[\left(\sum_{a=1}^{A}\mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_n-\boldsymbol{\theta}_*)\right)^2\right]$, by minimizing the quantity $\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}}^{-1}\mathbf{w}(a')$ where $\mathbf{A}_{\mathbf{b},\boldsymbol{\Sigma}}=\sum_{a,a'}\lceil\mathbf{b}(a)n\rceil\widetilde{\mathbf{x}}(a)\widetilde{\mathbf{x}}(a')^\top$. □

Remark C.5. Note that the estimator $\widehat{\boldsymbol{\theta}}_n$ is an unbiased estimator of $\boldsymbol{\theta}_*$. This can be shown as follows

$$\begin{aligned}\mathbb{E}\left[\widehat{\boldsymbol{\theta}}_n\right]-\boldsymbol{\theta}_*&=\mathbb{E}\left[\left(\mathbf{X}_n^\top\boldsymbol{\Sigma}_n^{-1}\mathbf{X}_n\right)^{-1}\mathbf{X}_n^\top\boldsymbol{\Sigma}_n^{-1}\mathbf{R}_n\right]-\boldsymbol{\theta}_*\\&=\mathbb{E}\left[\left(\mathbf{X}_n^\top\boldsymbol{\Sigma}_n^{-1}\mathbf{X}_n\right)^{-1}\mathbf{X}_n^\top\boldsymbol{\Sigma}_n^{-1}\left(\mathbf{X}_n\boldsymbol{\theta}^*+\eta\right)\right]-\boldsymbol{\theta}_*\\&=\mathbb{E}\left[\left(\mathbf{X}_n^\top\boldsymbol{\Sigma}_n^{-1}\mathbf{X}_n\right)^{-1}\mathbf{X}_n^\top\boldsymbol{\Sigma}_n^{-1}\mathbf{X}_n\boldsymbol{\theta}^*\right]+\mathbb{E}\left[\left(\mathbf{X}_n^\top\boldsymbol{\Sigma}_n^{-1}\mathbf{X}_n\right)^{-1}\mathbf{X}_n^\top\boldsymbol{\Sigma}_n^{-1}\eta\right]-\boldsymbol{\theta}_*\\&=\boldsymbol{\theta}_*+\left(\mathbf{X}_n^\top\boldsymbol{\Sigma}_n^{-1}\mathbf{X}_n\right)^{-1}\mathbf{X}_n^\top\boldsymbol{\Sigma}_n^{-1}\mathbb{E}\left[\eta\right]-\boldsymbol{\theta}_*\overset{(a)}{=}0\end{aligned}$$

where, (a) follows as noise is zero mean.

D. Bandit Regret Proofs

D.1. Loss of Bandit Oracle

Proposition 6. ***(Bandit Oracle MSE)*** *Let the oracle sample each action a for $\lceil n\mathbf{b}^*(a)\rceil$ times, where $\mathbf{b}^*$ is the solution to (2). Then the MSE is given by*

$$\mathcal{L}_n^*(\pi,\mathbf{b}^*,\boldsymbol{\Sigma}_*)\leq O\left(\frac{d\lambda_1(V)\log n}{n}\right)+O\left(\frac{1}{n}\right).$$

Proof. Recall the matrix $\mathbf{X}_n = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n]^\top \in \mathbb{R}^{n\times d}$ are the observed features for the n samples taken. Let $\mathbf{R}_n = [R_1, R_2, \ldots, R_n]^\top \in \mathbb{R}^{n\times 1}$ be the n rewards observed and $\eta \in \mathbb{R}^{n\times 1}$ and η is the bounded noise vectors. Then using weighted least square estimates we have

$$\widehat{\boldsymbol{\theta}}_n \overset{(a)}{=} \arg\min_{\boldsymbol{\theta}} \sum_{t=1}^{n} \frac{1}{\sigma^2(I_t)} (R(I_t) - \mathbf{x}(I_t)\boldsymbol{\theta})^2$$

where, in (a) we I_t is the action sampled at timestep t, Recall that the $\mathbf{diag}(\boldsymbol{\Sigma}_n) = [\sigma^2(I_1), \sigma^2(I_2), \ldots, \sigma^2(I_n)]$, where $I_1, I_2, \ldots, I_n$ are the actions pulled at time $t = 1, 2, \ldots, n$. We have that:

$$\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_* = (\mathbf{X}_n^\top \boldsymbol{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{X}_n^\top \boldsymbol{\Sigma}_n^{-1} \eta$$

where the noise vector $\eta \sim \mathcal{SG}(0, \boldsymbol{\Sigma}_n)$ where $\boldsymbol{\Sigma}_n \in \mathbb{R}^{n\times n}$. For any $\mathbf{z} \in \mathbb{R}^d$ we have

$$\mathbf{z}^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*) = \mathbf{z}^\top (\mathbf{X}_n^\top \boldsymbol{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{X}_n^\top \boldsymbol{\Sigma}_n^{-1} \eta$$

Let $\mathbf{b}^*$ be the PE-Optimal design for $\mathcal{A}$ defined in (2). Then the oracle pulls action $a \in \mathcal{A}$ exactly $\lceil n\mathbf{b}^* \rceil$ times for some $n > d(d+1)/2$ and computes the least square estimator $\widehat{\boldsymbol{\theta}}_n$. Observe that

$$\sum_{a=1}^{A} \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*) \sim \mathcal{SG}\left(0, \sum_{a,a'} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \boldsymbol{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{w}(a')\right).$$

So $\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2 \sim \mathcal{SE}\left(0, \sum_{a,a'} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \boldsymbol{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{w}(a')\right)$ where $\mathcal{SE}$ denotes the sub-exponential distribution. Denote the quantity,

$$t := \sqrt{2 \sum_{a,a'} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \boldsymbol{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{w}(a') \log(1/\delta)}.$$

Now using sub-exponential concentration inequality in Lemma C.2, setting

$$\nu^2 = \sum_{a,a'} \mathbf{w}(a)^\top (\mathbf{X}_n^\top \boldsymbol{\Sigma}_n^{-1} \mathbf{X}_n)^{-1} \mathbf{w}(a'),$$

and $\alpha = \nu$, we can show that

$$\mathbb{P}\left(\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2 > t\right) \le \delta, \qquad \text{if } t \in (0, 1]$$

$$\mathbb{P}\left(\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2 > t^2\right) \le \delta, \qquad \text{if } t > 1.$$

Combining the above two we can show that

$$\mathbb{P}\left(\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2 > \min\{t, t^2\}\right) \le \delta, \forall t > 0.$$

Further define matrix $\overline{\boldsymbol{\Sigma}}_n \in \mathbb{R}^{d\times d}$ as $\overline{\boldsymbol{\Sigma}}_n^{-1} := (\mathbf{X}_n^\top \boldsymbol{\Sigma}_n^{-1} \mathbf{X}_n)^{-1}$. This means that we have with probability $(1-\delta)$ that

$$\begin{aligned}
\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top (\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2 &\le \min\left\{\sqrt{2 \sum_{a,a'} \mathbf{w}(a)^\top \overline{\boldsymbol{\Sigma}}_n^{-1} \mathbf{w}(a') \log(1/\delta)}, 2 \sum_{a,a'} \mathbf{w}(a)^\top \overline{\boldsymbol{\Sigma}}_n^{-1} \mathbf{w}(a') \log(1/\delta)\right\} \\
&\overset{(a)}{=} \min\left\{\sqrt{\frac{2}{n} \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}_{\mathbf{b}^*,\boldsymbol{\Sigma}_*}^{-1} \mathbf{w}(a') \log(1/\delta)}, \frac{2}{n} \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}_{\mathbf{b}^*,\boldsymbol{\Sigma}_*}^{-1} \mathbf{w}(a') \log(1/\delta)\right\} \\
&\overset{(b)}{\le} \min\left\{\sqrt{\frac{8d\lambda_1(\mathbf{V}) \log(1/\delta)}{n}}, \frac{8d\lambda_1(\mathbf{V}) \log(1/\delta)}{n}\right\}
\end{aligned}$$

and we have taken at most n pulls such that $n > \frac{d(d+1)}{2}$ pulls. Here (a) follows as $n\mathbf{A}_{\mathbf{b}^*,\mathbf{\Sigma}_*} = \overline{\mathbf{\Sigma}}_n$ and observing that oracle has access to $\mathbf{\Sigma}_*$, and optimal proportion $\mathbf{b}^*$. The (b) follows from applying Corollary 1 such that $\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}_*} \mathbf{w}(a') \leq d\lambda_1(\mathbf{V})$ where $\mathbf{V} = \sum_{a,a'} \mathbf{w}(a)\mathbf{w}(a')^\top$. Thus, for any $\delta \in (0,1)$ we have

$$\mathbb{P}\left(\left\{\left(\sum_{a=1}^{A} \widetilde{\mathbf{x}}(a)^\top(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2 > \min\left\{\sqrt{\frac{8d\lambda_1(\mathbf{V})\log(1/\delta)}{n}}, \frac{8d\lambda_1(\mathbf{V})\log(1/\delta)}{n}\right\}\right\}\right) \leq \delta. \tag{11}$$

Define the good event $\xi_\delta(n)$ as follows:

$$\xi_\delta(n) := \left\{\left(\sum_{a=1}^{A} \widetilde{\mathbf{x}}(a)^\top(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2 \leq \min\left\{\sqrt{\frac{8d\lambda_1(\mathbf{V})\log(1/\delta)}{n}}, \frac{8d\lambda_1(\mathbf{V})\log(1/\delta)}{n}\right\}\right\}.$$

Then the loss of the oracle following PE-Optimal $\mathbf{b}^*$ is given by

$$\begin{aligned}
\mathcal{L}_n^*(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*) &= \mathbb{E}_{\mathcal{D}}\left[\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top\left(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*\right)\right)^2\right] \\
&\leq \mathbb{E}_{\mathcal{D}}\left[\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top\left(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*\right)\right)^2 \xi_\delta(n)\right] + \mathbb{E}_{\mathcal{D}}\left[\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top\left(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*\right)\right)^2 \xi_\delta^c(n)\right] \\
&\overset{(a)}{\leq} \mathbb{E}_{\mathcal{D}}\left[\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top\left(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*\right)\right)^2 \xi_\delta(n)\right] + \sum_{t=1}^{n} AM^2B^2\mathbb{P}(\xi_\delta^c(n)) \\
&\overset{(b)}{\leq} \min\left\{\sqrt{\frac{8d\lambda_1(\mathbf{V})\log(1/\delta)}{n}}, \frac{8d\lambda_1(\mathbf{V})\log(1/\delta)}{n}\right\} + \sum_{t=1}^{n} AH_U^2B^2\mathbb{P}(\xi_\delta^c(n)) \\
&\overset{(c)}{\leq} \min\left\{\sqrt{\frac{16d\lambda_1(\mathbf{V})\log n}{n}}, \frac{16d\lambda_1(\mathbf{V})\log n}{n}\right\} + O\left(\frac{1}{n}\right) \\
&\leq \frac{48d\lambda_1(\mathbf{V})\log n}{n} + O\left(\frac{1}{n}\right)
\end{aligned}$$

where, (a) follows as the noise $\eta^2 \leq B^2$ and $\sum_a \|\mathbf{x}(a)\|^2 \leq AH_U^2$ which implies

$$\mathbb{E}_{\mathcal{D}}\left[\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top\left(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*\right)\right)^2\right] \leq nAH_U^2B^2.$$

The (b) follows from (11), and (c) follows by setting $\delta = 1/n^3$, and noting that $n > A$. □

D.2. OLS-WLS Concentration Lemma

Lemma D.1. ***(Concentration Lemma)*** *After Γ samples of exploration, we can show that $\mathbb{P}\left(\xi_\delta^{var}(\Gamma)\right) \geq 1 - 8\delta$ where, $C > 0$ is a constant.*

Proof. We observed $(\mathbf{x}_t, r_t) \in \mathbb{R}^d \times \mathbb{R}, i = 1, \ldots, \Gamma$ from the model

$$r_t = \mathbf{x}_t^\top \boldsymbol{\theta}_* + \eta_t, \tag{12}$$

$$\eta_t \sim \mathcal{SG}(0, \mathbf{x}_t^\top \mathbf{\Sigma}_* \mathbf{x}_t), \tag{13}$$

where $\boldsymbol{\theta}_* \in \mathbb{R}^d$ and $\mathbf{\Sigma}_* \in \mathbb{R}^{d\times d}$ are unknown.

Given an initial estimate $\widehat{\boldsymbol{\theta}}_\Gamma$ of $\boldsymbol{\theta}_*$, we first compute the squared residual $y_t := \left(\mathbf{x}_t^\top \widehat{\boldsymbol{\theta}}_\Gamma - r_t\right)^2$, and then obtain an estimate of $\boldsymbol{\Sigma}_*$ via

$$\min_{\mathbf{S}\in\mathbb{R}^{d\times d}} \sum_{t=1}^{\Gamma} \left(\left\langle \mathbf{x}_t\mathbf{x}_t^\top, \mathbf{S}\right\rangle - y_t\right)^2. \tag{14}$$

Observe that if $\widehat{\boldsymbol{\theta}}_\Gamma = \boldsymbol{\theta}_*$, then the expectation of the squared residual y_t is

$$\mathbb{E}\left[y_t\right] = \mathbb{E}\left[\left(\mathbf{x}_t^\top \boldsymbol{\theta}_* - r_t\right)^2\right] = \mathbb{E}\left[\eta_t^2\right] = \mathbf{x}_t^\top \boldsymbol{\Sigma}_* \mathbf{x}_t = \left\langle \mathbf{x}_t\mathbf{x}_t^\top, \boldsymbol{\Sigma}_*\right\rangle,$$

which is a linear function of $\boldsymbol{\Sigma}_*$. The program (14) is thus a least square formulation for estimating $\boldsymbol{\Sigma}_*$.

Let $\mathbf{X}_t := \mathbf{x}_t\mathbf{x}_t^\top$. Below we abuse notation and view $\boldsymbol{\Sigma}_*, \widehat{\boldsymbol{\Sigma}}_*, \mathbf{X}_t, \mathbf{S}$ as vectors in $\mathbb{R}^{d^2}$ endowed with the trace inner product $\langle\cdot,\cdot\rangle$. Let $\mathbf{X} \in \mathbb{R}^{\Gamma\times d^2}$ have rows $\{\mathbf{X}_t\}$, and $y = (y_1, \ldots, y_\Gamma)^\top \in \mathbb{R}^\Gamma$. Suppose $\mathbf{x}_t$ can only take on M possible values from $\{\phi_1, \ldots, \phi_M\}$, so $\mathbf{X}_t \in \{\Phi_1, \ldots, \Phi_M\}$, where $\Phi_m := \phi_m\phi_m^\top$. Note that for the forced exploration setting we have $M = d < A$. Moreover, each value appears exactly Γ/M times. Then (14) can be rewritten as

$$\min_{\mathbf{S}\in\mathbb{R}^{d^2}} \sum_{m=1}^{M} \sum_{t:\mathbf{X}_t=\Phi_m} \left(\langle\Phi_m, \mathbf{S}\rangle - y_t\right)^2 = \min_{\mathbf{S}\in\mathbb{R}^{d^2}} \sum_{m=1}^{M} \left(\langle\Phi_m, \mathbf{S}\rangle - \frac{1}{\Gamma/M}\sum_{t:\mathbf{X}_t=\Phi_m} y_t\right)^2.$$

Let $z_m := \frac{1}{\Gamma/M}\sum_{t:\mathbf{X}_t=\Phi_m} y_t$. Then it becomes

$$\min_{\mathbf{S}\in\mathbb{R}^{d^2}} \sum_{m=1}^{M} \left(\langle\Phi_m, \mathbf{S}\rangle - z_m\right)^2 = \min_{\mathbf{S}\in\mathbb{R}^{d^2}} \left\|\Phi\mathbf{S} - z\right\|_2^2,$$

where $\Phi \in \mathbb{R}^{m\times d^2}$ has rows $\{\Phi_m\}$, and $z := (z_1, \ldots, z_m)^\top \in \mathbb{R}/M$. Note that $\{\Phi_m\}$ may or may not span $\mathbb{R}^{d^2}$. Observe that $\widehat{\boldsymbol{\Sigma}}_\Gamma$ be an optimal solution to the above problem. Then

$$\begin{aligned}\left\|\Phi(\widehat{\boldsymbol{\Sigma}}_\Gamma - \boldsymbol{\Sigma}_*)\right\|_2^2 + \left\|\Phi\boldsymbol{\Sigma}_* - z\right\|_2^2 + 2\left\langle \Phi(\widehat{\boldsymbol{\Sigma}}_\Gamma - \boldsymbol{\Sigma}_*), \Phi\boldsymbol{\Sigma}_* - z\right\rangle &= \left\|\Phi\widehat{\boldsymbol{\Sigma}}_\Gamma - \Phi\boldsymbol{\Sigma}_* + \Phi\boldsymbol{\Sigma}_* - z\right\|_2^2 \\ &= \left\|\Phi\widehat{\boldsymbol{\Sigma}}_\Gamma - z\right\|_2^2 \le \left\|\Phi\boldsymbol{\Sigma}_* - z\right\|_2^2.\end{aligned}$$

Hence, we can show that

$$\begin{aligned}\left\|\Phi(\widehat{\boldsymbol{\Sigma}}_\Gamma - \boldsymbol{\Sigma}_*)\right\|_2^2 &\le -2\left\langle \Phi(\widehat{\boldsymbol{\Sigma}}_\Gamma - \boldsymbol{\Sigma}_*), \Phi\boldsymbol{\Sigma}_* - z\right\rangle \\ &\overset{(a)}{\le} 2\left\|\Phi(\widehat{\boldsymbol{\Sigma}}_\Gamma - \boldsymbol{\Sigma}_*)\right\|_2 \left\|\Phi\boldsymbol{\Sigma}_* - z\right\|_2.\end{aligned}$$

where, (a) follows from Cauchy Schwarz inequality. So

$$\left\|\Phi(\widehat{\boldsymbol{\Sigma}}_\Gamma - \boldsymbol{\Sigma}_*)\right\|_2 \le 2\left\|\Phi\boldsymbol{\Sigma}_* - z\right\|_2.$$

Observe that the RHS does not contain the $\widehat{\boldsymbol{\Sigma}}_\Gamma$ anymore. Note that the m-th entry of $\Phi\boldsymbol{\Sigma}_* - z$ is

$$\langle\Phi_m, \boldsymbol{\Sigma}_*\rangle - z_m = \phi_m^\top\boldsymbol{\Sigma}_*\phi_m - \frac{1}{\Gamma/M}\sum_{t:\mathbf{X}_t=\Phi_m} y_t.$$

But let $\zeta_\Gamma := \widehat{\boldsymbol{\theta}}_\Gamma - \boldsymbol{\theta}_*$, then

$$\begin{aligned}y_t &= \left(\mathbf{x}_t^\top\widehat{\boldsymbol{\theta}}_t - r_t\right)^2 \\ &= (\eta_t + \mathbf{x}_t^\top\zeta_\Gamma)^2 \\ &= \eta_t^2 + 2\eta_t\mathbf{x}_t^\top\zeta_\Gamma + \left(\mathbf{x}_t^\top\zeta_\Gamma\right)^2 \\ &= \mathbf{x}_t^\top\boldsymbol{\Sigma}_*\mathbf{x}_t + \epsilon_t.\end{aligned}$$

Then we can show that

$$\epsilon_t := y_t - \mathbf{x}_t^\top \mathbf{\Sigma}_* \mathbf{x}_t = \eta_t^2 - \mathbb{E}\left[\eta_t^2\right] + 2\eta_t \mathbf{x}_t^\top \zeta_\Gamma + \left(\mathbf{x}_t^\top \zeta_\Gamma\right)^2 \overset{(a)}{\leq} \underbrace{2(\eta_t^2 - \mathbb{E}\left[\eta_t^2\right])}_{\textbf{Part A}} + \underbrace{2\left(\mathbf{x}_t^\top \zeta_\Gamma\right)^2}_{\textbf{Part B}}.$$

where, (a) follows as $(a+b)^2 \leq 2a^2 + 2b^2$. So

$$\langle \Phi_m, \mathbf{\Sigma}_* \rangle - z_m \leq -\frac{1}{\Gamma/M} \sum_{t:\mathbf{X}_t = \Phi_m} \epsilon_t.$$

We can divide the ϵ_t into two parts. Looking into the first part A, observe that η_t^2 is a sub-exponential random variable as $\eta_t \sim \mathcal{SG}(0, \mathbf{x}_t^\top \mathbf{\Sigma}_* \mathbf{x}_t)$. Also let $\nu = \mathbf{x}_t^\top \mathbf{\Sigma}_* \mathbf{x}_t = O(M^2 B^2 d^2) = c' d^2$ for some constant $c' > 0$. From Lemma C.2, we have that

$$\begin{aligned}
&\mathbb{P}\left(\left\{\eta_t^2 - \mathbb{E}\left[\eta_t^2\right] > \min\left\{\sqrt{\frac{2\nu \log(A/\delta)}{\tau}}, \frac{2\nu^2 \log(A/\delta)}{\tau}\right\}\right\}\right) \\
&\overset{(a)}{\leq} \mathbb{P}\left(\left\{\eta_t^2 - \mathbb{E}\left[\eta_t^2\right] > \min\left\{\sqrt{\frac{2c' d^2 \log(A/\delta)}{\tau}}, \frac{2c' d^2 \log(A/\delta)}{\tau}\right\}\right\}\right) \\
&\leq \exp\left(-\min\left\{\sqrt{\frac{2c' d^2 \log(A/\delta)}{\tau}}, \frac{2c' d^2 \log(A/\delta)}{\tau}\right\}\right) \\
&\overset{(b)}{\leq} \exp\left(-\min\left\{\sqrt{\frac{2c' d^2 \log(A/\delta)}{2c' d^2}}, \frac{2c' d^2 \log(A/\delta)}{2c' d^2}\right\}\right) \leq \delta.
\end{aligned}$$

where, (a) follows for some $c' > 0$ we have that $\nu = \mathbf{x}^\top \mathbf{\Sigma}_* \mathbf{x} \leq c' d^2$, and observing that

$$\min\left\{\sqrt{\frac{2\nu \log(1/\delta)}{\tau}}, \frac{2\nu^2 \log(A/\delta)}{\tau}\right\} > \min\left\{\sqrt{\frac{2c' d^2 \log(1/\delta)}{\tau}}, \frac{2c' d^2 \log(A/\delta)}{\tau}\right\}$$

and (b) follows for $\tau > c' d^2 (c' d^2 + 1)/2$.

Now for the second part B first recall that $\zeta_\Gamma := \widehat{\boldsymbol{\theta}}_\Gamma - \boldsymbol{\theta}_*$. Then using Lemma C.3 we can show that

$$\begin{aligned}
\mathbb{P}\left((\mathbf{x}^\top \zeta_\Gamma)^2 > \sigma^2 \frac{r + \log(A/\delta)}{\Gamma}\right) &\overset{(a)}{=} \mathbb{P}\left((\mathbf{x}^\top \zeta_\Gamma)^2 > \frac{d^2 A + d^2 \log(A/\delta)}{\Gamma}\right) \\
&\overset{(b)}{\leq} \mathbb{P}\left(\left(\mathbf{x}^\top \left(\widehat{\boldsymbol{\theta}}_\Gamma - \boldsymbol{\theta}_*\right)\right)^2 > \frac{2c'' A d^2 \log(A/\delta)}{\Gamma}\right) \leq \delta
\end{aligned}$$

where, in (a) we have $\sigma^2 \leq \max_a \sigma^2(a) \leq \max_a \mathbf{x}^\top(a) \mathbf{\Sigma}_* \mathbf{x}(a) \leq c_1 d^2$ for some $c_1 > 0$. Note that r is the rank of $\mathbf{X}^\top \mathbf{X}$ which is equal to A. In (a) we have for some $c'' > 0$ we have $d^2(r+1) > 2c'' A d^2$. Hence we can show that

$$\mathbb{P}\left(\left(\eta_t \mathbf{x}^\top \zeta_\Gamma\right)^2 > \left(\frac{2c'' A d^2 \log(A/\delta)}{\Gamma}\right)\right) \leq \delta.$$

Combining all of the steps above we can show that

$$\begin{aligned}
&\mathbb{P}\left(\langle \Phi_m, \mathbf{\Sigma}_* \rangle - z_m > -\frac{M}{\Gamma} \sum_{t:\mathbf{X}_t = \Phi_m} \left(\frac{2c'' A d^2 \log(A/\delta)}{\Gamma} + \frac{2c' d^2 \log(A/\delta)}{\Gamma}\right)\right) \\
&\overset{(a)}{\leq} \mathbb{P}\left(\langle \Phi_m, \mathbf{\Sigma}_* \rangle - z_m > -\frac{d}{\sqrt{n}} \sum_{t:\mathbf{X}_t = \Phi_m} \left(\frac{2C d^2 \log(A/\delta)}{\Gamma}\right)\right) \\
&\overset{(b)}{=} \mathbb{P}\left(\langle \Phi_m, \mathbf{\Sigma}_* \rangle - z_m > -\left(\frac{2C d^2 \log(A/\delta)}{\Gamma}\right)\right) \leq 4\delta/A,
\end{aligned}$$

where, (a) follows for some constant $C > 0$, and (b) follows by setting $\Gamma = \sqrt{n}$ and $M = d < A$ and noting that the m-th row consist of $\sqrt{n}/d$ entries. Hence the above implies that

$$\mathbb{P}\left(\mathbf{x}(a)^\top \widehat{\mathbf{\Sigma}}_\Gamma \mathbf{x}(a) - \mathbf{x}(a)^\top \mathbf{\Sigma}_* \mathbf{x}(a) \geq \frac{2Cd^2 \log(A/\delta)}{\Gamma}\right) \leq 4\delta/A.$$

Also note that $\eta_t \sim \mathcal{SG}(0, \mathbf{x}_t^\top \mathbf{\Sigma}_* \mathbf{x}_t)$. So we can have a two tail concentration inequality. It then follows that

$$\mathbb{P}\left(\mathbf{x}(a)^\top \widehat{\mathbf{\Sigma}}_\Gamma \mathbf{x}(a) - \mathbf{x}(a)^\top \mathbf{\Sigma}_* \mathbf{x}(a) \leq -\frac{2Cd^2 \log(A/\delta)}{\Gamma}\right) \leq 4\delta/A.$$

Hence we can show by union bounding over all actions $A > d$ that

$$\mathbb{P}\left(\forall a, \left|\mathbf{x}(a)^\top \left(\widehat{\mathbf{\Sigma}}_\Gamma - \mathbf{\Sigma}_*\right) \mathbf{x}(a)\right| \geq \frac{2Cd^2 \log(A/\delta)}{\Gamma}\right) \leq 2A\frac{4\delta}{A} = 8\delta.$$

The claim of the lemma follows. □

Lemma D.2. ***(Operator Norm Concentration Lemma)*** *We have that*

$$\mathbb{P}\left(\|\widehat{\mathbf{\Sigma}}_\Gamma - \mathbf{\Sigma}_*\| \geq \frac{2Cd^2 \lambda_{\min}^{-1}(\mathbf{Y}) \log(A/\delta)}{\Gamma}\right) \leq 8\delta$$

for a constant $C > 0$.

Proof. Define the set of actions $\mathcal{Z}$ such that it has a span over $\mathbf{X}$ and $\mathbf{X}\mathbf{X}^\top$. Define the vector $\mathbf{y}(a) = \mathbf{x}(a)\mathbf{x}(a)^\top \in \mathbb{R}^{d^2}$. Also observe that $|\mathcal{Z}| = d^2$. Without loss of generosity, we assume that $\mathcal{Z} = \{1, 2, \ldots, d^2\}$. Now define the matrix $\mathbf{Y} \in \mathbb{R}^{d^2 \times d^2}$ such that

$$\mathbf{Y} = [\mathbf{y}(1), \mathbf{y}(2), \ldots, \mathbf{y}(|\mathcal{Z}|)]$$

We further assume that the $\lambda_{\min}(\mathbf{Y}) > 0$. We already have from Lemma 4.1 that

$$\begin{aligned}
&\mathbb{P}\left(\forall a \in \mathcal{A}, \left|\mathbf{x}(a)^\top (\widehat{\mathbf{\Sigma}}_\Gamma - \mathbf{\Sigma}_*)\mathbf{x}(a)\right| \leq \frac{2Cd^2 \log(A/\delta)}{\Gamma}\right) \geq 1 - 8\delta \\
\overset{(a)}{\implies} &\mathbb{P}\left(\forall a \in \mathcal{Z}, \left|\langle \widehat{\mathbf{\Sigma}}_\Gamma, \mathbf{y}(a)\rangle - \langle \mathbf{\Sigma}_*, \mathbf{y}(a)\rangle\right| \leq \frac{2Cd^2 \log(A/\delta)}{\Gamma}\right) \geq 1 - 8\delta.
\end{aligned}$$

where, (a) follows by the fact that $\mathcal{Z} \subset \mathcal{A}$. Now take an arbitrary vector $\mathbf{x}$ in unit ball such that $\|\mathbf{x}\|_2 \leq 1$. Now we define the vector $\mathbf{y} = \mathbf{x}\mathbf{x}^\top$ such that $\mathbf{y} \in \mathbb{R}^{d^2}$. Then following Assumption 3.1 we have that

$$\mathbf{x}\mathbf{x}^\top = \mathbf{y} = \sum_{a \in \mathcal{Z}} \alpha(a)\mathbf{y}(a) = \alpha \mathbf{Y} \overset{(a)}{\implies} \alpha = \mathbf{Y}^{-1}\mathbf{y}$$

where, in (a) we can take the inverse because $\lambda_{\min}(\mathbf{Y}) > 0$. Now we want to bound

$$\begin{aligned}
\|\widehat{\mathbf{\Sigma}}_\Gamma - \mathbf{\Sigma}_*\| = \left|\mathbf{x}^\top \left(\widehat{\mathbf{\Sigma}}_\Gamma - \mathbf{\Sigma}_*\right)\mathbf{x}\right| = \left|\langle \widehat{\mathbf{\Sigma}}_\Gamma - \mathbf{\Sigma}_*, \mathbf{y}\rangle\right| &\leq \frac{2Cd^2 \log(A/\delta)}{\Gamma} \left\|\underbrace{\sum_a \alpha(a)}_{\alpha}\right\| \\
&= \frac{2Cd^2 \log(A/\delta)}{\Gamma} \|\mathbf{Y}^{-1}\mathbf{y}\| \\
&\leq \frac{2Cd^2 \log(A/\delta)}{\Gamma} \|\mathbf{Y}^{-1}\| \|\mathbf{x}\|^2 \\
&\leq \frac{2Cd^2 \lambda_{\min}^{-1}(\mathbf{Y}) \log(A/\delta)}{\Gamma}.
\end{aligned}$$

The claim of the lemma follows. □

Corollary D.3. *For, $n \geq 4C^2d^2\log^2(A/\delta)/\sigma^2_{\min}$, we have that with probability at least $1-8\delta$, the following holds: for all action a, $\frac{\sigma^2(a)}{\widehat{\sigma}^2_\Gamma(a)} \leq 1 + \frac{4Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma}$.*

Proof. From the Lemma 4.1, we know that $\left|\mathbf{x}(a)^\top(\widehat{\mathbf{\Sigma}}_\Gamma - \mathbf{\Sigma}_*)\mathbf{x}(a)\right| \leq \frac{2Cd^2\log(A/\delta)}{\Gamma}$ with probability at least $1-8\delta$. Hence we can show that

$$
\begin{aligned}
|\widehat{\sigma}^2_\Gamma(a) - \sigma^2(a)| \leq \frac{2Cd^2\log(A/\delta)}{\Gamma} &\implies \sigma^2(a) - \frac{2Cd^2\log(A/\delta)}{\Gamma} \leq \widehat{\sigma}^2_\Gamma(a) \leq \sigma^2(a) + \frac{2Cd^2\log(A/\delta)}{\Gamma} \\
&\implies 1 - \frac{2Cd^2\log(A/\delta)}{\sigma^2(a)\Gamma} \leq \frac{\widehat{\sigma}^2_\Gamma(a)}{\sigma^2(a)} \leq 1 + \frac{2Cd^2\log(A/\delta)}{\sigma^2(a)\Gamma} \\
&\implies 1 - \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma} \leq \frac{\widehat{\sigma}^2_\Gamma(a)}{\sigma^2(a)} \leq 1 + \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma} \\
&\implies \frac{1}{1 + \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma}} \leq \frac{\sigma^2(a)}{\widehat{\sigma}^2_\Gamma(a)} \leq \frac{1}{1 - \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma}}.
\end{aligned}
$$

It follows then that

$$
\frac{\sigma^2(a)}{\widehat{\sigma}^2_\Gamma(a)} \leq \frac{1}{1 - \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma}} \overset{(a)}{\leq} 1 + \frac{4Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma}
$$

where, (a) follows for $x = \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma}$ and

$$
\frac{1}{1-x} \leq 1 + 2x \implies 1 \leq 1 + x - 2x^2 \implies x(1-2x) \geq 0
$$

which holds for $x = \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma} \leq \frac{1}{2}$. For $n \geq 4C^2d^2\log^2(A/\delta)/\sigma^2_{\min}$ we can show that $x \leq \frac{1}{2}$. The claim of the corollary follows. □

D.3. (Bonus) Loss of Algorithm 1

Proposition 7. ***(Loss of Algorithm 1, formal)*** *Let $\widehat{\mathbf{b}}$ be the empirical PE-Optimal design followed by Algorithm 1 and it samples each action a as $\lceil n\widehat{\mathbf{b}}(a)\rceil$ times. Then the MSE of Algorithm 1 for for $n \geq \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma}$ is given by*

$$
\mathcal{L}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) \leq \underbrace{O\left(\frac{d^3\lambda_1(\mathbf{V})\log n}{n}\right)}_{\substack{\textit{PE-Optimal MSE} \\ \textit{and exploration error}}} + \underbrace{O\left(\frac{d^2\lambda_1(\mathbf{V})\log n}{n^{3/2}}\right)}_{\textit{Approximation error}} + \underbrace{O\left(\frac{1}{n}\right)}_{\textit{Failure event MSE}}.
$$

Proof. Recall that the $\widehat{\mathbf{\Sigma}}_\Gamma$ be the empirical co-variance after Γ timesteps. Then Algorithm 1 pulls each action $a \in \mathcal{A}$ exactly $\left\lceil (n-\Gamma)\widehat{\mathbf{b}}(a)\right\rceil$ times for some $\sqrt{n} > A$ and computes the least squares estimator $\widehat{\boldsymbol{\theta}}_n$. Recall that the estimate $\widehat{\boldsymbol{\theta}}_n$ only uses the $(n-\Gamma)$ data sampled under $\widehat{\mathbf{b}}$. Also recall we actually use $\widehat{\mathbf{\Sigma}}_\Gamma$ as input for optimization problem (2), where $\Gamma = \sqrt{n}$. We first define the good event $\xi_\delta(n-\Gamma)$ as follows:

$$
\xi_\delta(n-\Gamma) := \left\{ \left(\sum_{a=1}^{A} \mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*)\right)^2 \leq \min\left\{\sqrt{\frac{(8d\lambda_1(\mathbf{V}) + \alpha_0 + \alpha)\log(1/\delta)}{n-\Gamma}}, \frac{(8d\lambda_1(\mathbf{V}) + \alpha_0 + \alpha)\log(1/\delta)}{n-\Gamma}\right\}\right\}
$$

where, α_0, and α will be defined later. Also, define the good variance event as follows:

$$
\xi^{var}_\delta(\Gamma) := \left\{\forall a, \left|\mathbf{x}(a)^\top\left(\widehat{\mathbf{\Sigma}}_\Gamma - \mathbf{\Sigma}_*\right)\mathbf{x}(a)\right| < \frac{2Cd^2\log(A/\delta)}{\Gamma}\right\}. \tag{15}
$$

Then we can bound the loss of the SPEED as follows:

$$\overline{\mathcal{L}}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) = \mathbb{E}_{\mathcal{D}}\left[\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top \left(\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*\right)\right)^2\right]$$
$$= \mathbb{E}_{\mathcal{D}}\left[\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top \left(\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*\right)\right)^2 \mathbb{I}\{\xi_\delta(n-\Gamma)\}\mathbb{I}\{\xi_\delta^{var}(\Gamma)\}\right] + \mathbb{E}_{\mathcal{D}}\left[\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top \left(\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*\right)\right)^2 \mathbb{I}\{\xi_\delta^{c}(n-\Gamma)\}\right]$$
$$+ \mathbb{E}_{\mathcal{D}}\left[\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top \left(\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*\right)\right)^2 \mathbb{I}\{(\xi_\delta^{var}(\Gamma))^c\}\right]. \tag{16}$$

Now we bound the first term of the (16). Note that using weighted least square estimates we have

$$\widehat{\boldsymbol{\theta}}_{n-\Gamma} \overset{(a)}{=} \arg\min_{\boldsymbol{\theta}} \sum_{t=1}^{n} \frac{1}{\widehat{\sigma}_\Gamma^2(I_t)} (R(I_t) - \mathbf{x}(I_t)^\top \boldsymbol{\theta})^2$$

where, in (a) we I_t is the action sampled at timestep t. Recall that the $\mathbf{diag}(\widehat{\mathbf{\Sigma}}_\Gamma) = [\widehat{\sigma}_\Gamma^2(I_1), \widehat{\sigma}_\Gamma^2(I_2), \ldots, \widehat{\sigma}_\Gamma^2(I_n)]$, where $I_1, I_2, \ldots, I_{n-\Gamma}$ are the actions pulled at time $t = 1, 2, \ldots, n$. We have that:

$$\widehat{\boldsymbol{\theta}}_{n-\Gamma} = (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{R}_n = (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} (\mathbf{X}_{n-\Gamma} \boldsymbol{\theta}_* + \eta)$$
$$\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_* = (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \eta$$

where the noise vector $\eta \sim \mathcal{SG}(0, \mathbf{\Sigma}_{n-\Gamma})$ where $\mathbf{diag}(\mathbf{\Sigma}_n) = [\sigma^2(I_1), \sigma^2(I_2), \ldots, \sigma^2(I_{n-\Gamma})]$. For any $\mathbf{z} := \sum_a \mathbf{w}(a) \in \mathbb{R}^d$ we have

$$\mathbf{z}^\top (\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*) = \mathbf{z}^\top (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \eta. \tag{17}$$

It implies from (17) that

$$\left(\mathbf{z}^\top (\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*)\right)^2 \sim \mathcal{SE}\left(0, \mathbf{z}^\top (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbb{E}\left[\eta\eta^\top\right] \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma} (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{z}\right) \tag{18}$$

where $\mathcal{SE}$ denotes the sub-exponential distribution. Hence to bound the quantity $\left(\mathbf{z}^\top (\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*)\right)^2$ we need to bound the variance. We first begin by rewriting the loss function for $n \geq \frac{2Cd^2 \log(A/\delta)}{\sigma_{\min}^2 \Gamma}$ as follows

$$\mathbb{E}\left[\left(\mathbf{z}^\top (\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*)\right)^2\right] = \mathbf{z}^\top (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbb{E}\left[\eta\eta^\top\right] \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma} (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{z}$$
$$\overset{(a)}{=} \mathbf{z}^\top (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{\Sigma}_n \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma} (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{z}$$
$$= \mathbf{z}^\top (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-\frac{1}{2}} \widehat{\mathbf{\Sigma}}_\Gamma^{-\frac{1}{2}} \mathbf{\Sigma}_n \widehat{\mathbf{\Sigma}}_\Gamma^{-\frac{1}{2}} \widehat{\mathbf{\Sigma}}_\Gamma^{-\frac{1}{2}} \mathbf{X}_{n-\Gamma} (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{z}$$
$$\overset{(b)}{=} \underbrace{\mathbf{z}^\top (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-\frac{1}{2}}}_{\mathbf{m}^\top \in \mathbb{R}^{n-\Gamma}} \widehat{\mathbf{\Sigma}}_\Gamma^{-\frac{1}{2}} \mathbf{\Sigma}_n \widehat{\mathbf{\Sigma}}_\Gamma^{-\frac{1}{2}} \underbrace{\widehat{\mathbf{\Sigma}}_\Gamma^{-\frac{1}{2}} \mathbf{X}_{n-\Gamma} (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{z}}_{\mathbf{m} \in \mathbb{R}^{n-\Gamma}}$$
$$\overset{(c)}{\leq} \mathbf{z}^\top (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1/2} \left((1 + 2C_\Gamma(\delta)) \mathbf{I}_n\right) \widehat{\mathbf{\Sigma}}_\Gamma^{-1/2} \mathbf{X}_{n-\Gamma} (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{z}$$
$$\overset{(d)}{=} (1 + 2C_\Gamma(\delta)) \mathbf{z}^\top (\mathbf{X}_{n-\Gamma}^\top \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{X}_{n-\Gamma})^{-1} \mathbf{z} \tag{19}$$

where, (a) follows as $\mathbb{E}\left[\eta\eta^\top\right] = \mathbf{\Sigma}_n$, in (b) $\mathbf{m}$ is a vector in $\mathbb{R}^{n-\Gamma}$. The (c) follows by first observing that

$$\widehat{\mathbf{\Sigma}}_\Gamma^{-\frac{1}{2}} \mathbf{\Sigma}_n \widehat{\mathbf{\Sigma}}_\Gamma^{-\frac{1}{2}} = \widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{\Sigma}_n = \mathbf{diag}(\widehat{\mathbf{\Sigma}}_\Gamma^{-1} \mathbf{\Sigma}_n) = \left[\frac{\sigma^2(I_1)}{\widehat{\sigma}_\Gamma^2(I_1)}, \frac{\sigma^2(I_2)}{\widehat{\sigma}_\Gamma^2(I_2)}, \ldots, \frac{\sigma^2(I_n)}{\widehat{\sigma}_\Gamma^2(I_n)}\right].$$

Then note that using Corollary D.3 we have

$$\frac{\sigma^2(I_t)}{\widehat{\sigma}^2_\Gamma(I_t)} \leq 1 + 2 \cdot \underbrace{\frac{2Cd^2 \log(A/\delta)}{\sigma^2_{\min}\Gamma}}_{C_\Gamma(\delta)}$$

for each $t \in [n]$, and (d) follows as $1 + 2C_\Gamma(\delta)$ is not a random variable. Let $\widehat{\mathbf{b}}^*$ be the empirical PE-Optimal design returned by the approximator after it is supplied with $\widehat{\mathbf{\Sigma}}_\Gamma$. Now observe that the quantity of the samples collected (following $\widehat{\mathbf{b}}^*$) after exploration is as follows:

$$\left(\widetilde{\mathbf{X}}^\top_{n-\Gamma}\widehat{\mathbf{\Sigma}}^{-1}_\Gamma\widetilde{\mathbf{X}}_{n-\Gamma}\right)^{-1} = \left(\sum_a \left[(n-\Gamma)\widehat{\mathbf{b}}^*(a)\widehat{\sigma}^{-2}_\Gamma(a)\right]\mathbf{w}(a)\mathbf{w}(a)^\top\right)^{-1} = \frac{1}{n-\Gamma}\mathbf{A}^{-1}_{\widehat{\mathbf{b}}^*,\widehat{\mathbf{\Sigma}}_\Gamma}.$$

Hence we use the loss function

$$\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) := (1 + 2C_\Gamma(\delta))\,\mathbf{z}^\top(\widetilde{\mathbf{X}}^\top_{n-\Gamma}\widehat{\mathbf{\Sigma}}^{-1}_\Gamma\widetilde{\mathbf{X}}_{n-\Gamma})^{-1}\mathbf{z} = \frac{(1+2C_\Gamma(\delta))}{n-\Gamma}\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}^{-1}_{\widehat{\mathbf{b}}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a'). \tag{20}$$

Also recall that we define

$$\mathcal{L}_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma) = \frac{1}{n}\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a').$$

So to minimize the quantity $\mathbb{E}\left[\left(\sum_a \mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*)\right)^2\right]$ is minimizing the quantity $\frac{(1+2C_\Gamma(\delta))}{n-\Gamma}\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}^{-1}_{\widehat{\mathbf{b}}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a')$. Further recall that we can show that from Assumption 3.2 (approximation oracle) and Kiefer-Wolfowitz theorem in Corollary 1 that for the proportion $\mathbf{b}^*$ and any arbitrary positive semi-definite matrix $\widehat{\mathbf{\Sigma}}_\Gamma$ the following holds

$$\begin{aligned}\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a') = \mathbf{Tr}\left(\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a')\right) &= \mathbf{Tr}\Bigg(\mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\underbrace{\sum_{a,a'}\mathbf{w}(a)\mathbf{w}(a')^\top}_{\mathbf{V}}\Bigg)\\ &= \mathbf{Tr}\left(\mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{V}\right) \leq d\lambda_1(\mathbf{V}).\end{aligned} \tag{21}$$

Then we can decompose the loss as follows:

$$\begin{aligned}\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) &= \mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma) + \mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma)\\ &= \underbrace{\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma)}_{\textbf{Approximation error}} + \underbrace{\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma)}_{\textbf{Comparing two diff loss}} + \mathcal{L}_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma).\end{aligned} \tag{22}$$

For the approximation error we need access to an oracle (see Assumption 3.2) that gives ϵ approximation error. Then setting $\epsilon = \frac{1}{\sqrt{n}}$ we have that

$$\begin{aligned}\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma) &= \frac{(1+2C_\Gamma(\delta))}{n-\Gamma}\underbrace{\mathbf{Tr}\left(\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}^{-1}_{\widehat{\mathbf{b}},\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a') - \sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}^{-1}_{\widehat{\mathbf{b}}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a')\right)}_{\epsilon}\\ &\overset{(a)}{\leq} O\left(\frac{d^2\log(A/\delta)}{n^{3/2}}\right)\end{aligned} \tag{23}$$

where, (a) follows by setting $\Gamma = \sqrt{n}$, $\epsilon = 1/\sqrt{n}$ and $C_\Gamma(\delta) = \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma} = \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\sqrt{n}}$. Let us define $\mathbf{K}_1 := \mathbf{Tr}(\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}^{-1}_{\widehat{\mathbf{b}}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a'))$, and $\mathbf{K}_2 := \mathbf{Tr}(\mathbf{w}(a)^\top\mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a'))$. For the second part of comparing the two losses we can show that

$$
\begin{aligned}
\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma) &= \frac{1}{(n-\Gamma)}\mathbf{Tr}\left((1+2C_\Gamma(\delta))\, K_1\right) - \frac{1}{n}K_2 \\
&= \frac{(1+2C_\Gamma(\delta))\mathbf{K}_1}{n-\Gamma} - \frac{(1+2C_\Gamma(\delta))\mathbf{K}_2}{n-\Gamma} + \frac{(1+2C_\Gamma(\delta))\mathbf{K}_2}{n-\Gamma} - \frac{1}{n}\mathbf{K}_2 \\
&= \frac{(1+2C_\Gamma(\delta))}{n-\Gamma}\left(\mathbf{K}_1 - \mathbf{K}_2\right) + \frac{2C_\Gamma(\delta)\mathbf{K}_2}{n-\Gamma} + \frac{1}{n-\Gamma}\mathbf{K}_2 - \frac{1}{n}\mathbf{K}_2 \\
&\overset{(a)}{=} \frac{\Gamma}{n(n-\Gamma)} \underbrace{\mathbf{Tr}\left(\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a') - \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a')\right)}_{\leq 0} \\
&\quad + \frac{2C_\Gamma(\delta)}{n-\Gamma}\mathbf{Tr}\left(\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a')\right) + \frac{\Gamma}{n(n-\Gamma)}\mathbf{Tr}\left(\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a')\right) \\
&\overset{(b)}{\leq} O\left(\frac{d^3\lambda_1(\mathbf{V})\log(A/\delta)}{n^{3/2}}\right)
\end{aligned} \tag{24}
$$

where, (a) follows by substituting the definition of $\mathbf{K}_1$ and $\mathbf{K}_2$. The (b) follows by setting $\Gamma = \sqrt{n}$, $C_\Gamma(\delta) = \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma} = \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\sqrt{n}}$, and $\mathbf{Tr}\left(\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a')\right) \leq d\lambda_1(\mathbf{V})$.

Now we combine all parts together in (22) using (21), (23) and (24). First we define the quantity

$$
\alpha := 2C_\Gamma(\delta)\mathbf{Tr}\left(\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a')\right) + \frac{\Gamma}{n}\mathbf{Tr}\left(\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a')\right).
$$

It follows then that (22) can be written as

$$
\begin{aligned}
\frac{1+2C_\Gamma(\delta)}{n-\Gamma}\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a') &\leq \underbrace{\frac{(1+2C_\Gamma(\delta))\epsilon}{(n-\Gamma)}}_{\textbf{Approximation error}} + \frac{\alpha}{n-\Gamma} + \frac{1}{n}\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a') \\
\implies (1+2C_\Gamma(\delta))\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a') &\leq \underbrace{(1+2C_\Gamma(\delta))\epsilon}_{\alpha_0} + \alpha + \frac{n-\Gamma}{n}\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a') \\
&\overset{(a)}{\leq} \alpha_0 + \alpha + d\lambda_1(\mathbf{V})
\end{aligned} \tag{25}
$$

where, (a) follows from Assumption 3.2, Corollary 1 and (21). Also observe that from (18) we have that $\left(\sum_{a=1}^A \mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2$ is a sub-exponential random variable. Then using the sub-exponential concentration inequality we have with probability at least $1-\delta$

$$
\begin{aligned}
\left(\sum_{a=1}^A \mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*)\right)^2 &\leq \min\Bigg\{\sqrt{(1+2C_\Gamma(\delta))\sum_{a,a'} \mathbf{w}(a)\left(\mathbf{X}^\top_{n-\Gamma}\widehat{\mathbf{\Sigma}}^{-1}_\Gamma\mathbf{X}_{n-\Gamma}\right)^{-1}\mathbf{w}(a')2\log(1/\delta)}, \\
&\qquad (1+2C_\Gamma(\delta))\sum_{a,a'} \mathbf{w}(a)^\top\left(\mathbf{X}^\top_{n-\Gamma}\widehat{\mathbf{\Sigma}}^{-1}_\Gamma\mathbf{X}_{n-\Gamma}\right)^{-1}\mathbf{w}(a')2\log(1/\delta)\Bigg\} \\
&= \min\Bigg\{\frac{1}{\sqrt{n-\Gamma}}\sqrt{(1+2C_\Gamma(\delta))\sum_{a,a'} \mathbf{w}(a)^\top\mathbf{A}^{-1}_{\mathbf{b}, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a')2\log(1/\delta)}, \\
&\qquad \frac{(1+2C_\Gamma(\delta))}{n-\Gamma}\sum_{a,a'} \mathbf{w}(a)^\top\mathbf{A}^{-1}_{\mathbf{b}, \widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a')2\log(1/\delta)\Bigg\} \\
&\overset{(a)}{\leq} \min\left\{\sqrt{\frac{(8d\lambda_1(\mathbf{V}) + \alpha_0 + \alpha)\log(1/\delta)}{n-\Gamma}}, \frac{(8d\lambda_1(\mathbf{V}) + \alpha_0 + \alpha)\log(1/\delta)}{n-\Gamma}\right\}
\end{aligned}
$$

where, (a) follows from (25), and we have taken at most $n-\Gamma$ pulls to estimate $\widehat{\boldsymbol{\theta}}_n$ after forced exploration and $\sqrt{n} > d$. Thus, for any $\delta \in (0,1)$ we have

$$\mathbb{P}\left(\left\{\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\right)^2 > \min\left\{\sqrt{\frac{(8d\lambda_1(\mathbf{V})+\alpha_0+\alpha)\log(1/\delta)}{n-\Gamma}}, \frac{(8d\lambda_1(\mathbf{V})+\alpha_0+\alpha)\log(1/\delta)}{n-\Gamma}\right\}\right\}\right) \leq \delta. \tag{26}$$

This gives us a bound on the first term of (16). Combining everything in (16) we can bound the loss of the SPEED as follows:

$$\begin{aligned}
\overline{\mathcal{L}}_n(\pi, \widehat{\mathbf{b}}, \widehat{\boldsymbol{\Sigma}}_\Gamma) &\leq \mathbb{E}_{\mathcal{D}}\left[\left(\sum_{a=1}^{A} \mathbf{w}(a)^\top\left(\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*\right)\right)^2 \mathbb{I}\{\xi_\delta(n-\Gamma)\}\mathbb{I}\{\xi_\delta^{var}(\Gamma)\}\right] + \sum_{t=1}^{n} AH_U^2B^2\mathbb{P}(\xi_\delta^c(n-\Gamma)) \\
&\quad + \sum_{t=1}^{n} AH_U^2B^2\mathbb{P}\left((\xi_\delta^{var}(\Gamma))^c\right) \\
&\leq \min\left\{\frac{2Cd^2\log(A/\delta)}{\Gamma}, \sqrt{\frac{(8d\lambda_1(\mathbf{V})+\alpha_0+\alpha)\log(A/\delta)}{n-\Gamma}}, \frac{(8d\lambda_1(\mathbf{V})+\alpha_0+\alpha)\log(A/\delta)}{n-\Gamma}\right\} \\
&\quad + \sum_{t=1}^{n} AH_U^2B^2\mathbb{P}(\xi_\delta^c(n-\Gamma)) + \sum_{t=1}^{n} AH_U^2B^2\mathbb{P}\left((\xi_\delta^{var}(\Gamma))^c\right)
\end{aligned}$$

$$\begin{aligned}
&\overset{(a)}{\leq} \min\left\{\frac{8Cd^2\log(nA)}{\sqrt{n}}, \sqrt{\frac{48(d\lambda_1(\mathbf{V})+\alpha_0+\alpha)\log(nA)}{n}}, \frac{48(d\lambda_1(\mathbf{V})+\alpha_0+\alpha)\log(nA)}{n}\right\} + O\left(\frac{1}{n}\right) \\
&\leq \frac{48d^2\lambda_1(\mathbf{V})\log(nA)}{n} + \frac{48\alpha\log(nA)}{n} + \frac{48\alpha_0\log(nA)}{n} + O\left(\frac{1}{n}\right) \\
&\overset{(b)}{\leq} \frac{48d^2\lambda_1(\mathbf{V})\log(nA)}{n} + \frac{144d\lambda_1(\mathbf{V})C_\Gamma(\delta)\log(nA)}{n} + \frac{48d\lambda_1(\mathbf{V})\Gamma\log(nA)}{n^{3/2}} + \frac{48\epsilon\log(nA)}{n} + O\left(\frac{1}{n}\right)
\end{aligned}$$

where (a) follows as Proposition 7 and setting $\delta = 1/n^3$ and noting that $\sqrt{n} > d$. The (b) follows by setting $(1+2C_\Gamma(\delta))\epsilon$ and the definition of α. Recall that for $\Gamma = \sqrt{n}$ we have that $C_\Gamma(\delta) = \frac{2Cd^2\log(A/\delta)}{\sigma_{\min}^2\Gamma} = \frac{2Cd^2\log(A/\delta)}{\sigma_{\min}^2\sqrt{n}}$. Then setting $\epsilon = 1/\sqrt{n}$ we can bound the loss of the following PE-Optimal $\widehat{\mathbf{b}}$ as

$$\overline{\mathcal{L}}_n(\pi, \widehat{\mathbf{b}}, \widehat{\boldsymbol{\Sigma}}_\Gamma) \leq O\left(\frac{d^3\lambda_1(\mathbf{V})\log(nA)}{n}\right) + O\left(\frac{d^2\lambda_1(\mathbf{V})\log(nA)}{n^{3/2}}\right) + O\left(\frac{1}{n}\right).$$

The claim of the proposition follows. □

Remark D.4. **(Discussion on loss)** Observe that from Proposition 7 that the MSE for policy evaluation setting scales as $O(\frac{d^3\log(n)}{n})$. We contrast this result with Chaudhuri et al. (2017) who obtain a bound on the MSE $\mathbb{E}_{\mathcal{D}}[\|\boldsymbol{\theta}_* - \widehat{\boldsymbol{\theta}}_n\|^2] \leq O(\frac{d\log(n)}{n})$ in a related setting. Note that Chaudhuri et al. (2017) only considers the setting when $\boldsymbol{\Sigma}_*$ is rank 1. We make no such assumption and get an additional factor of d in our result due to exploration in d^2 dimension to estimate $\boldsymbol{\Sigma}_*$. Finally we get the scaling as d^3 due to $\sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\boldsymbol{\Sigma}}_\Gamma}\mathbf{w}(a') \leq d\lambda_1(\mathbf{V})$ from Corollary 1. Also observe that we estimate $\mathbb{E}_{\mathcal{D}}[\sum_a \mathbf{w}(a)^\top(\boldsymbol{\theta}_* - \widehat{\boldsymbol{\theta}}_n)^2]$ as opposed to $\mathbb{E}_{\mathcal{D}}[\|\boldsymbol{\theta}_* - \widehat{\boldsymbol{\theta}}_n\|^2]$ in Chaudhuri et al. (2017).

D.4. Regret of Algorithm 1

Corollary D.5. *For, $n \geq 16C^2d^4\log^2(A/\delta)/\sigma_{\min}^4$ we have that for all action a, $|\widehat{\sigma}_\Gamma^2(a) - \sigma^2(a)| \leq \sigma_{\min}^2/2$.*

Proof. From the Lemma 4.1, we know that $\left|\mathbf{x}(a)^\top(\widehat{\mathbf{\Sigma}}_\Gamma - \mathbf{\Sigma}_*)\mathbf{x}(a)\right| \leq \frac{2Cd^2\log(A/\delta)}{\Gamma}$ with probability $1-8\delta$. Hence we can show that

$$|\widehat{\sigma}^2_\Gamma(a) - \sigma^2(a)| \leq \frac{2Cd^2\log(A/\delta)}{\Gamma} = \frac{2Cd^2\log(A/\delta)}{\sqrt{n}} \overset{(a)}{\leq} \frac{2Cd^2\log(A/\delta)}{\sqrt{16C^2d^4\log^2(A/\delta)/\sigma^4_{\min}}} = \frac{\sigma^2_{\min}}{2},$$

where (a) follows for $n \geq 16C^2d^4\log^2(A/\delta)/\sigma^4_{\min}$. The claim of the corollary follows. □

Lemma D.6. ***(Loss Concentration of design matrix)*** *Let $\widehat{\mathbf{\Sigma}}_\Gamma$ be the empirical estimate of $\mathbf{\Sigma}_*$. Define $\mathbf{V} = \sum_{a,a'}\mathbf{w}(a)\mathbf{w}(a')^\top$. We have that for any arbitrary proportion $\mathbf{b}$ the following*

$$\mathbb{P}\left(\left|\sum_{a,a'}\mathbf{w}(a)^\top(\mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma} - \mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}_*})\mathbf{w}(a')\right| \leq \frac{2CB^*d^3\log(A/\delta)}{\Gamma}\right) \geq 1-\delta$$

where B^* is a problem-dependent quantity such that

$$B^* = \left(\left\|\mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}_*}\mathbf{w}\right\|^2 \left\|\sum_{a=1}^{A}\mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top H_U^2\right\| \left\|\left(\sum_{a=1}^{A}\frac{\mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top}{\sigma^2(a) + \frac{2Cd^2\log(9H_U^2/\delta)}{\sqrt{n}}}\right)^{-1}\mathbf{w}\right\|\right)$$

and $C > 0$ is a universal constant.

Proof. We have the following

$$\begin{aligned}
&\left|\sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a') - \sum_{a,a'}\mathbf{w}(a)^\top\mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}_*}\mathbf{w}(a')\right| = \left|\underbrace{\sum_{a}\mathbf{w}(a)^\top}_{\mathbf{w}}\left(\mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma} - \mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}_*}\right)\underbrace{\sum_{a}\mathbf{w}(a)}_{\mathbf{w}}\right| \\
&= \left|\mathbf{w}^\top\left(\mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}_*}\left(\mathbf{A}_{\mathbf{b}^*,\mathbf{\Sigma}_*} - \mathbf{A}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\right)\mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\right)\mathbf{w}\right| = \left|\underbrace{\mathbf{w}^\top(\,\mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}_*}}_{\mathbf{u}}\left(\mathbf{A}_{\mathbf{b}^*,\mathbf{\Sigma}_*} - \mathbf{A}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\right)\underbrace{\mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\,)\,\mathbf{w}}_{\mathbf{v}}\right| \\
&= \left|\mathbf{u}\left(\mathbf{A}_{\mathbf{b}^*,\mathbf{\Sigma}_*} - \mathbf{A}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\right)\mathbf{v}\right| \overset{(a)}{\leq} \|\mathbf{u}\|\underbrace{\left\|\mathbf{A}_{\mathbf{b}^*,\mathbf{\Sigma}_*} - \mathbf{A}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\right\|}_{\Delta}\|\mathbf{v}\| \qquad (27)
\end{aligned}$$

where, (a) follows by Cauchy-Schwarz inequality. Now observe that the vector $\mathbf{u} \in \mathbb{R}^d$ is a problem dependent quantity.

We now bound the Δ in (27) as follows

$$
\begin{aligned}
\Delta &= \left\| \sum_{a=1}^{A} \frac{\mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top}{\mathbf{x}(a)^\top \boldsymbol{\Sigma}_* \mathbf{x}(a)} - \sum_{a=1}^{A} \frac{\mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top}{\mathbf{x}(a)^\top \widehat{\boldsymbol{\Sigma}}_\Gamma \mathbf{x}(a)} \right\| \\
&\overset{(a)}{=} \left\| \sum_{a} \frac{\mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top}{\sigma^2(a)} - \sum_{a} \frac{\mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top}{\widehat{\sigma}^2_\Gamma(a)} \right\| \\
&= \left\| \sum_{a} \mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top \left(\frac{1}{\sigma^2(a)} - \frac{1}{\widehat{\sigma}^2_\Gamma(a)} \right) \right\| \\
&= \left\| \sum_{a} \mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top \left(\frac{\widehat{\sigma}^2_\Gamma(a) - \sigma^2(a)}{\widehat{\sigma}^2_\Gamma(a)\sigma^2(a)} \right) \right\| \\
&\overset{(b)}{\leq} \left\| \sum_{a} \mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top \left(\frac{\widehat{\sigma}^2_\Gamma(a) - \sigma^2(a)}{\sigma^4_{\min}} \right) \right\| \\
&= \left\| \frac{1}{\sigma^4_{\min}} \sum_{a} \mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top \left(\mathbf{x}(a)^\top \widehat{\boldsymbol{\Sigma}}_\Gamma \mathbf{x}(a) - \mathbf{x}(a)^\top \boldsymbol{\Sigma}_* \mathbf{x}(a) \right) \right\| \\
&= \frac{1}{\sigma^4_{\min}} \left\| \sum_{a=1}^{A} \underbrace{\mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top}_{\textbf{Problem dependent quantity}} \underbrace{\left(\mathbf{x}(a)^\top \left(\widehat{\boldsymbol{\Sigma}}_\Gamma - \boldsymbol{\Sigma}_* \right) \mathbf{x}(a) \right)}_{\textbf{Random Quantity}} \right\|
\end{aligned}
$$

where, (a) follows $\widehat{\sigma}^2_\Gamma(a) = \mathbf{x}(a)^\top \widehat{\boldsymbol{\Sigma}}_\Gamma \mathbf{x}(a)$ and $\sigma^2(a) = \mathbf{x}(a)^\top \boldsymbol{\Sigma}_* \mathbf{x}(a)$, ad (b) follows from Corollary D.5. Now observe that we can bound the quantity

$$
\|\widehat{\boldsymbol{\Sigma}}_\Gamma - \boldsymbol{\Sigma}_*\| \leq \frac{2Cd^2 \lambda^{-1}_{\min}(\mathbf{Y}) \log(A/\delta)}{\Gamma}
$$

then we also have that the spread of maximum eigenvalue of $\|\widehat{\boldsymbol{\Sigma}}_\Gamma - \boldsymbol{\Sigma}_*\|_2$ is controlled which implies

$$
\begin{aligned}
&\frac{1}{\sigma^4_{\min}} \left\| \sum_{a=1}^{A} \underbrace{\mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top}_{\textbf{Problem dependent quantity}} \underbrace{\left(\mathbf{x}(a)^\top \left(\widehat{\boldsymbol{\Sigma}}_\Gamma - \boldsymbol{\Sigma}_* \right) \mathbf{x}(a) \right)}_{\textbf{Random Quantity}} \right\| \\
&\qquad \overset{(a)}{\leq} \left\| \sum_{a=1}^{A} \mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top (\mathbf{x}(a)^\top \mathbf{x}(a)) \right\| \frac{2Cd^2 \lambda^{-1}_{\min}(\mathbf{Y}) \log(A/\delta)}{\Gamma}
\end{aligned}
$$

where, (a) follows by Lemma D.2. Next for the third quantity in (27) we can bound as follows

$$
\|\mathbf{v}\| = \|\mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\boldsymbol{\Sigma}}_\Gamma} \mathbf{w}\| = \left\| \left(\sum_{a=1}^{A} \frac{\mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top}{\widehat{\sigma}^2_\Gamma(a)} \right)^{-1} \mathbf{w} \right\| \overset{(a)}{\leq} \left\| \left(\sum_{a=1}^{A} \frac{\mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top}{\sigma^2(a) + \frac{2Cd^2 \log(A/\delta)}{\sqrt{n}}} \right)^{-1} \mathbf{w} \right\|
$$

where, (a) follows as

$$
\widehat{\sigma}^2(a) \leq \sigma^2(a) + \frac{2Cd^2 \log(A/\delta)}{\Gamma}
$$

from Lemma 4.1. Finally observe that the first part of (27) we have that $\mathbf{w}^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \boldsymbol{\Sigma}_*}$ is a problem dependent parameter.

Finally, plugging back everything in (27) we get

$$
\begin{aligned}
&\|\mathbf{u}\| \left\| \mathbf{A}_{\mathbf{b}^*,\mathbf{\Sigma}_*} - \mathbf{A}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma} \right\| \|\mathbf{v}\| \\
&\leq \left\| \mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}_*} \mathbf{w} \right\| \left\| \sum_{a=1}^{A} \mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top (\mathbf{x}(a)^\top \mathbf{x}(a)) \right\| \frac{2Cd^2\log(A/\delta)}{\sigma^4_{\min}\Gamma} \left\| \left(\sum_{a=1}^{A} \frac{\mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top}{\sigma^2(a) + \frac{2Cd^3\log(A/\delta)}{\Gamma}} \right)^{-1} \mathbf{w} \right\| \\
&\leq \underbrace{\left(\left\| \mathbf{A}^{-1}_{\mathbf{b}^*,\mathbf{\Sigma}_*} \mathbf{w} \right\|^2 \left\| \sum_{a=1}^{A} \mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top H_U^2 \right\| \left\| \left(\sum_{a=1}^{A} \frac{\mathbf{b}^*(a)\mathbf{w}(a)\mathbf{w}(a)^\top}{\sigma^2(a) + \frac{2Cd^2\log(A/\delta)}{\Gamma}} \right)^{-1} \mathbf{w} \right\| \right)}_{B^*} \frac{2Cd^3\log(A/\delta)}{\Gamma} \\
&\overset{(a)}{=} \frac{2CB^*d^3\lambda^{-1}_{\min}(\mathbf{Y})\log(A/\delta)}{\Gamma}
\end{aligned}
$$

where, (a) follows by substituting the value of B^*. □

D.5. Regret Bound of SPEED

Theorem 1. ***(formal)*** *The regret of Algorithm 1 for $n \geq 16C^2d^4\log^2(A/\delta)/\sigma^4_{\min}$ running PE-Optimal design in Equation (4) is given by*

$$
\mathcal{R}_n \leq \frac{1}{n^{3/2}} + O\left(\frac{d^2\log(n)}{n^{3/2}}\right) + \frac{2B^*Cd^3\log(n)}{n^{3/2}} + \frac{d^2}{n^2}\mathbf{Tr}\left(\sum_{a,a'} \mathbf{w}(a)\mathbf{w}(a')^\top\right) + \frac{2AH_U^2B^2}{n^2} = O\left(\frac{B^*d^3\log(n)}{n^{3/2}}\right).
$$

Proof. We follow the same steps as in Proposition 7. Observe that $\frac{16C^2d^4\log^2(A/\delta)}{\sigma^4_{\min}} > \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma}$. Hence for $\mathbf{z} = \sum_a \mathbf{w}(a)$ the loss function for $n \geq \frac{2Cd^2\log(A/\delta)}{\sigma^2_{\min}\Gamma}$ as follows

$$
\overline{\mathcal{L}}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) := \mathbb{E}\left[\left(\mathbf{z}^\top(\widehat{\boldsymbol{\theta}}_{n-\Gamma} - \boldsymbol{\theta}_*)\right)^2\right] \overset{(a)}{\leq} (1 + 2C_\Gamma(\delta))\, \mathbf{z}^\top(\widetilde{\mathbf{X}}^\top_{n-\Gamma}\widehat{\mathbf{\Sigma}}^{-1}_\Gamma\widetilde{\mathbf{X}}_{n-\Gamma})^{-1}\mathbf{z}.
$$

where, (a) follows from (19). Recall that the quantity of the samples collected (following $\widehat{\mathbf{b}}^*$) after exploration is as follows:

$$
\left(\widetilde{\mathbf{X}}^\top_{n-\Gamma}\widehat{\mathbf{\Sigma}}^{-1}_\Gamma\widetilde{\mathbf{X}}_{n-\Gamma}\right)^{-1} = \left(\sum_a \left[(n-\Gamma)\widehat{\mathbf{b}}^*(a)\widehat{\sigma}^{-2}_\Gamma(a)\right] \mathbf{w}(a)\mathbf{w}(a)^\top\right)^{-1} = \frac{1}{n-\Gamma}\mathbf{A}^{-1}_{\widehat{\mathbf{b}}^*,\widehat{\mathbf{\Sigma}}_\Gamma}.
$$

Hence we use the loss function

$$
\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) := (1 + 2C_\Gamma(\delta))\, \mathbf{z}^\top(\widetilde{\mathbf{X}}^\top_{n-\Gamma}\widehat{\mathbf{\Sigma}}^{-1}_\Gamma\widetilde{\mathbf{X}}_{n-\Gamma})^{-1}\mathbf{z} = \frac{(1 + 2C_\Gamma(\delta))}{n-\Gamma}\sum_{a,a'} \mathbf{w}(a)^\top\mathbf{A}^{-1}_{\widehat{\mathbf{b}}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a').
$$

Also recall that we define

$$
\mathcal{L}_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma) = \frac{1}{n}\sum_{a,a'} \mathbf{w}(a)^\top\mathbf{A}^{-1}_{\mathbf{b}^*,\widehat{\mathbf{\Sigma}}_\Gamma}\mathbf{w}(a').
$$

Then we can decompose the regret as follows:

$$
\begin{aligned}
\mathcal{R}_n &= \overline{\mathcal{L}}_n(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*) \\
&\leq \mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma) + \mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*) \\
&= \underbrace{\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma)}_{\textbf{Approximation error}} + \underbrace{\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}^*_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma)}_{\textbf{Comparing two diff loss}} + \underbrace{\mathcal{L}^*_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}^*_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*)}_{\textbf{Estimation error of } \mathbf{\Sigma}_*}
\end{aligned}
$$

First recall that the good variance event as follows:

$$\xi_\delta^{var}(\Gamma) := \left\{ \forall a, \left| \mathbf{x}(a)^\top \left(\widehat{\mathbf{\Sigma}}_\Gamma - \mathbf{\Sigma}_* \right) \mathbf{x}(a) \right| < \frac{2Cd^2 \log(A/\delta)}{\Gamma} \right\}.$$

Under the good variance event, following the same steps as Proposition 7 we can bound the approximation error setting $\delta = 1/n^3$ as follows

$$\begin{aligned}
\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma) &\leq O\left(\frac{d^2 \log(A/\delta)}{n^{3/2}} \right) \mathbb{I}\{\xi_\delta^{var}(\Gamma)\} + \sum_{t=1}^n AH_U^2 B^2 \mathbb{P}\left((\xi_\delta^{var}(\Gamma))^c \right) \\
&\leq O\left(\frac{d^2 \log(A/\delta)}{n^{3/2}} \right) + \frac{AH_U^2 B^2}{n^2}
\end{aligned}$$

and the second part of comparing the two losses as

$$\begin{aligned}
\mathcal{L}'_{n-\Gamma}(\pi, \widehat{\mathbf{b}}^*, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma) &\leq O\left(\frac{d^2 \log(A/\delta)}{n^{3/2}} \right) \mathbb{I}\{\xi_\delta^{var}(\Gamma)\} + \sum_{t=1}^n AH_U^2 B^2 \mathbb{P}\left((\xi_\delta^{var}(\Gamma))^c \right) \\
&\leq O\left(\frac{d^2 \log(A/\delta)}{n^{3/2}} \right) + \frac{AH_U^2 B^2}{n^2}
\end{aligned}$$

We define the good estimation event as follows:

$$\xi_\delta^{est}(\Gamma) := \left\{ \left| \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma} \mathbf{w}(a') - \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \mathbf{\Sigma}_*} \mathbf{w}(a') \right| \leq \frac{2CB^* d^3 \log(9H_U^2/\delta)}{\sigma_{\min}^4 \Gamma} \right\}$$

Under the good estimation event $\xi^{est}(\Gamma)$ and using Lemma 4.2 we can show that the estimation error is given by

$$\begin{aligned}
\mathcal{L}_n(\pi, \mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma) - \mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*) &\leq \left(\frac{1}{n} \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma} \mathbf{w}(a') - \frac{1}{n} \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \mathbf{\Sigma}_*} \mathbf{w}(a') \right) \mathbb{I}\{\xi_\delta^{est}(\Gamma)\} \\
&\quad + \left(\frac{1}{n} \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma} \mathbf{w}(a') - \frac{1}{n} \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \mathbf{\Sigma}_*} \mathbf{w}(a') \right) \mathbb{I}\{\xi_\delta^{est}(\Gamma)^C\} \\
&= \left(\frac{1}{n} \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma} \mathbf{w}(a') - \frac{1}{n} \sum_{a,a'} \mathbf{w}(a)^\top \mathbf{A}^{-1}_{\mathbf{b}^*, \mathbf{\Sigma}_*} \mathbf{w}(a') \right) \mathbb{I}\{\xi_\delta^{est}(\Gamma)\} \\
&\quad + \frac{1}{n} \mathbf{Tr}\left(\left(\mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma} - \mathbf{A}^{-1}_{\mathbf{b}^*, \mathbf{\Sigma}_*} \right) \left(\sum_{a,a'} \mathbf{w}(a) \mathbf{w}(a')^\top \right) \right) \mathbb{I}\{\xi_\delta^{est}(\Gamma)^C\} \\
&\overset{(a)}{\leq} \frac{1}{n} 2B^* \frac{Cd^3 \log(1/\delta)}{\Gamma} + \frac{1}{n} \mathbf{Tr}\left(\mathbf{A}^{-1}_{\mathbf{b}^*, \mathbf{\Sigma}_*} \right) \mathbf{Tr}\left(\mathbf{A}^{-1}_{\mathbf{b}^*, \widehat{\mathbf{\Sigma}}_\Gamma} \right) \mathbf{Tr}\left(\sum_{a,a'} \mathbf{w}(a) \mathbf{w}(a')^\top \right) \delta \\
&\overset{(b)}{\leq} \frac{1}{n} 2B^* \frac{Cd^3 \log(n)}{\sqrt{n}} + \frac{d^2}{n^2} \mathbf{Tr}\left(\sum_{a,a'} \mathbf{w}(a) \mathbf{w}(a')^\top \right) = \frac{2B^* Cd^3 \log(n)}{n^{3/2}} + \frac{d^2}{n^2} \mathbf{Tr}\left(\sum_{a,a'} \mathbf{w}(a) \mathbf{w}(a')^\top \right)
\end{aligned}$$

where, (a) follows from Lemma 4.2, (b) follows as $\Gamma = \sqrt{n}$ and setting $\delta = \frac{1}{n^3}$. Combining everything we have the following regret as

$$\mathcal{R}_n \leq \frac{1}{n^{3/2}} + O\left(\frac{d^2 \log(n)}{n^{3/2}} \right) + \frac{2B^* Cd^3 \log(n)}{n^{3/2}} + \frac{d^2}{n^2} \mathbf{Tr}\left(\sum_{a,a'} \mathbf{w}(a) \mathbf{w}(a')^\top \right) + \frac{2AH_U^2 B^2}{n^2} = O\left(\frac{B^* d^3 \log(n)}{n^{3/2}} \right)$$

where, $B^* = \left(\left\| \mathbf{A}^{-1}_{\mathbf{b}^*, \mathbf{\Sigma}_*} \mathbf{w} \right\|^2 \left\| \sum_{a=1}^{A} \mathbf{b}^*(a) \mathbf{w}(a) \mathbf{w}(a)^\top H_U^2 \right\| \left\| \left(\sum_{a=1}^{A} \frac{\mathbf{b}^*(a) \mathbf{w}(a) \mathbf{w}(a)^\top}{\sigma^2(a) + \frac{2Cd^3 \log(9H_U^2/\delta)}{\sqrt{n}}} \right)^{-1} \mathbf{w} \right\| \right)$. The claim of the theorem follows. □

E. Regret Lower Bound

Theorem 2. ***(Lower Bound)*** *Let $|\mathbf{\Theta}| = 2^d$ and $\boldsymbol{\theta}_* \in \mathbf{\Theta}$. Then any δ-PAC policy π satisfies $\mathcal{R}'_n = \mathcal{L}_n(\pi, \widehat{\mathbf{b}}, \mathbf{\Sigma}_*) - \mathcal{L}_n(\pi, \mathbf{b}^*, \mathbf{\Sigma}_*) \geq \Omega\left(\frac{d^2 \lambda_d(\mathbf{V}) \log(n)}{n^{3/2}} \right)$ for the environment in (28).*

Proof. **Step 1 (Define Environment):** We define an environment model B_j consisting of A actions and J hypotheses with true hypothesis $\boldsymbol{\theta}_* = \boldsymbol{\theta}_j$ (j-th column) as follows:

$$
\begin{array}{ccccccc}
\boldsymbol{\theta} & = & \boldsymbol{\theta}_1 & \boldsymbol{\theta}_2 & \boldsymbol{\theta}_3 & \dots & \boldsymbol{\theta}_J \\
\hline
\mu_1(\boldsymbol{\theta}) & = & \beta & \beta - \frac{\beta}{J} & \beta - \frac{2\beta}{J} & \dots & \beta - \frac{(J-1)\beta}{J} \\
\mu_2(\boldsymbol{\theta}) & = & \iota_{21} & \iota_{22} & \iota_{23} & \dots & \iota_{2J} \\
 & \vdots & & & \vdots & & \\
\mu_A(\boldsymbol{\theta}) & = & \iota_{A1} & \iota_{A2} & \iota_{A3} & \dots & \iota_{AJ}
\end{array}
\tag{28}
$$

where, each ι_{ij} is distinct and satisfies $\iota_{ij} < \beta/4J$. $\boldsymbol{\theta}_1$ is the optimal hypothesis in B_1, $\boldsymbol{\theta}_2$ is the optimal hypothesis in B_2 and so on such that for each B_j and $j \in [J]$ we have column j as the optimal hypothesis. Finally assume that $\mathbf{\Sigma}_* = \boldsymbol{\theta}_* \boldsymbol{\theta}_*^\top$ is a rank one matrix. Hence for any algorithm, identifying the co-variance matrix $\mathbf{\Sigma}_*$ is same as identifying the $\boldsymbol{\theta}_*$. Also assume that $\pi(a) = \frac{1}{A}$. Hence each action is equally weighted by the target policy.

This is a general hypothesis testing setting where the functions $\mu_a(\boldsymbol{\theta})$ can be thought of as linear functions of $\boldsymbol{\theta}$ such that $\mu_a(\boldsymbol{\theta}) = \mathbf{x}(a)^\top \boldsymbol{\theta}$. Assume that $0 < \mu_a(\boldsymbol{\theta}) \leq 1$, and $\log(\mu_a(\boldsymbol{\theta})/\mu_a(\boldsymbol{\theta}')) > 1/4$. Here the learning proceeds as we defined before: the learner selects an action $I_t \in [A]$ and observes a reward $Y_t = \mu_{I_t}(\boldsymbol{\theta}_*) + \epsilon_t$ where, $\epsilon_t \sim \mathcal{N}(\mu_{I_t}(\boldsymbol{\theta}_*), \sigma^2(I_t))$ and $\sigma^2(I_t) = \mathbf{x}_{I_t}^\top \mathbf{\Sigma}_* \mathbf{x}_{I_t} = (\mathbf{x}_{I_t}^\top \boldsymbol{\theta}_*)^2$ as $\mathbf{\Sigma}_* = \boldsymbol{\theta}_* \boldsymbol{\theta}_*^\top$. Also, observe that

$$
\mathrm{KL}(\mu_i(\boldsymbol{\theta}) || \mu_i(\boldsymbol{\theta}')) = 2 \log(\frac{\mu_i(\boldsymbol{\theta}')}{\mu_i(\boldsymbol{\theta})}) + \frac{\mu_i^2(\boldsymbol{\theta}) + (\mu_i(\boldsymbol{\theta}) - \mu_i(\boldsymbol{\theta}'))^2}{2\mu_i^2(\boldsymbol{\theta}')} - \frac{1}{2} \overset{(a)}{\geq} \frac{(\mu_i(\boldsymbol{\theta}) - \mu_i(\boldsymbol{\theta}'))^2}{8}
\tag{29}
$$

where, (a) follows from the condition that $0 < \mu_a(\boldsymbol{\theta}) \leq 1$, and $\log(\mu_a(\boldsymbol{\theta})/\mu_a(\boldsymbol{\theta}')) > 1/4$.

Step 2 (Minimum samples to verify $\boldsymbol{\theta}_*$): Let, Λ_1 be the set of alternate models having a different optimal hypothesis than $\boldsymbol{\theta}^* = \boldsymbol{\theta}_1$ such that all models having different optimal hypothesis than $\boldsymbol{\theta}_1$ such as $B_2, B_3, \dots B_J$ are in Λ_1. Let τ_δ be the stopping time for any δ-PAC policy $\mathbf{b}$. That is τ_δ is the time that any algorithm stops and outputs its estimate $\widehat{\boldsymbol{\theta}}_{\tau_\delta}$. Let $T_t(a)$ denote the number of times the action a has been sampled till round t. Let $\widehat{\boldsymbol{\theta}}_{\tau_\delta}$ be the predicted optimal hypothesis at round τ_δ. We first consider the model B_1. Define the event $\xi = \{\widehat{\boldsymbol{\theta}}_{\tau_\delta} \neq \boldsymbol{\theta}_*\}$ as the error event in model B_1. Let the event $\xi' = \{\widehat{\boldsymbol{\theta}}_{\tau_\delta} \neq \boldsymbol{\theta}'^*\}$ be the corresponding error event in model B_2. Note that $\xi^\complement \subset \xi'$. Now since $\mathbf{b}$ is δ-PAC policy we have $\mathbb{P}_{B_1, \mathbf{b}}(\xi) \leq \delta$ and $\mathbb{P}_{B_2, \mathbf{b}}(\xi^\complement) \leq \delta$. Hence we can show that,

$$
\begin{aligned}
2\delta \geq \mathbb{P}_{B_1,\mathbf{b}}(\xi) + \mathbb{P}_{B_2,\mathbf{b}}(\xi^{\complement}) &\overset{(a)}{\geq} \frac{1}{2}\exp\left(-\mathrm{KL}\left(P_{B_1,\mathbf{b}}||P_{B_2,\mathbf{b}}\right)\right) \\
\mathrm{KL}\left(P_{B_1,\mathbf{b}}||P_{B_2,\mathbf{b}}\right) &\geq \log\left(\frac{1}{4\delta}\right) \\
\frac{1}{8}\sum_{i=1}^{A}\mathbb{E}_{B_1,\mathbf{b}}[T_{\tau_\delta}(i)]\cdot\left(\mu_i(\boldsymbol{\theta}_*) - \mu_i(\boldsymbol{\theta}^{'*})\right)^2 &\overset{(b)}{\geq} \log\left(\frac{1}{4\delta}\right) \\
\frac{1}{8}\left(\beta - \beta + \frac{\beta}{J}\right)^2\mathbb{E}_{B_1,\mathbf{b}}[T_{\tau_\delta}(1)] + \frac{1}{8}\sum_{i=2}^{A}(\iota_{i1}-\iota_{i2})^2\mathbb{E}_{B_1,\mathbf{b}}[T_{\tau_\delta}(i)] &\overset{(c)}{\geq} \log\left(\frac{1}{4\delta}\right) \\
\frac{1}{8}\left(\frac{1}{J}\right)^2\beta^2\mathbb{E}_{B_1,\mathbf{b}}[T_{\tau_\delta}(1)] + \frac{1}{8}\sum_{i=2}^{A}(\iota_{i1}-\iota_{i2})^2\mathbb{E}_{B_1,\mathbf{b}}[T_{\tau_\delta}(i)] &\geq \log\left(\frac{1}{4\delta}\right) \\
\frac{1}{8}\left(\frac{1}{J}\right)^2\beta^2\mathbb{E}_{B_1,\mathbf{b}}[T_{\tau_\delta}(1)] + \frac{1}{8}\sum_{i=2}^{A}\frac{\beta^2}{4J^2}\mathbb{E}_{B_1,\mathbf{b}}[T_{\tau_\delta}(i)] &\overset{(d)}{\geq} \log\left(\frac{1}{4\delta}\right) \qquad (30)
\end{aligned}
$$

where, (a) follows from Lemma E.2, (b) follows from Lemma E.1, (c) follows from the construction of the bandit environments and (29), and (d) follows as $(\iota_{ij} - \iota_{ij'})^2 \leq \frac{\beta^2}{4J^2}$ for any i-th action and j-th hypothesis.

Now, we consider the alternate model B_3. Again define the event $\xi = \{\widehat{\boldsymbol{\theta}}_{\tau_\delta} \neq \boldsymbol{\theta}_*\}$ as the error event in model B_1 and the event $\xi' = \{\widehat{\boldsymbol{\theta}}_{\tau_\delta} \neq \boldsymbol{\theta}^{''*}\}$ be the corresponding error event in model B_3. Note that $\xi^{\complement} \subset \xi'$. Now since $\mathbf{b}$ is δ-PAC policy we have $\mathbb{P}_{B_1,\mathbf{b}}(\xi) \leq \delta$ and $\mathbb{P}_{B_3,\mathbf{b}}(\xi^{\complement}) \leq \delta$. Following the same way as before we can show that,

$$
\frac{1}{8}\left(\frac{2}{J}\right)^2\beta^2\mathbb{E}_{B_3,\mathbf{b}}[T_{\tau_\delta}(1)] + \frac{1}{8}\sum_{i=2}^{A}\frac{\beta^2}{4J^2}\mathbb{E}_{B_3,\mathbf{b}}[T_{\tau_\delta}(i)] \overset{(d)}{\geq} \log\left(\frac{1}{4\delta}\right). \qquad (31)
$$

Similarly, we get the equations for all the other $(J-2)$ alternate models in Λ_1. Now consider an optimization problem (ignoring the constant factor of $\frac{1}{8}$ across all the constraints)

$$
\begin{aligned}
&\min_{t_i : i\in[A]} \sum t_i \\
s.t. \quad &\left(\frac{1}{J}\right)^2\beta^2 t_1 + \frac{\beta^2}{4J^2}\sum_{i=2}^{A} t_i \geq \log(1/4\delta) \\
&\left(\frac{2}{J}\right)^2\beta^2 t_1 + \frac{\beta^2}{4J^2}\sum_{i=2}^{A} t_i \geq \log(1/4\delta) \\
&\vdots \\
&\left(\frac{J-1}{J}\right)^2\beta^2 t_1 + \frac{\beta^2}{4J^2}\sum_{i=2}^{A} t_i \geq \log(1/4\delta) \\
&t_i \geq 0, \forall i \in [A]
\end{aligned}
$$

where the optimization variables are t_i. It can be seen that the optimum objective value is $J^2\beta^{-2}\log(1/4\delta)$. Interpreting $t_i = \mathbb{E}_{B_1,\mathbf{b}}[T_{\tau_\delta}(i)]$ for all i, we get that $\mathbb{E}_{B_1,\mathbf{b}}[\tau_\delta] = \sum_i t_i = t_1 \geq J^2\beta^{-2}\log(1/4\delta)$ which gives us the required lower bound to the number of pulls of action 1. Observe that the optimum objective value is reached by substituting $t_1 = J^2\beta^{-2}\log(1/4\delta)$ and $t_2 = \ldots = t_A = 0$. It follows that for verifying any hypothesis $\boldsymbol{\theta}_j \neq \boldsymbol{\theta}_*$ the verification proportion is given by $\mathbf{b}_{\boldsymbol{\theta}_j} = (1, \underbrace{0, 0, \ldots, 0}_{\text{(A-1) zeros}})$. Observe setting $\beta = J\sqrt{\log(1/4\delta)/n}$ recovers $\tau_\delta = n$ which implies that a budget of n samples is required for verifying hypothesis $\boldsymbol{\theta}_j = \boldsymbol{\theta}_*$. For the remaining steps we take $\beta = J\sqrt{\log(1/4\delta)/n}$.

Step 3 (Lower Bounding Regret): Then we can show that the MSE of any hypothesis $\boldsymbol{\theta}_j = \boldsymbol{\theta}_*$

$$\mathbb{E}_{\mathcal{D}}\left[\left(\sum_a \pi(a)\mathbf{x}(a)^\top(\boldsymbol{\theta}_j - \widehat{\boldsymbol{\theta}}_n)\right)^2\right] = \frac{1}{n}\sum_{a,a'}\mathbf{w}(a)\mathbf{A}^{-1}_{\mathbf{b}_{\boldsymbol{\theta}_j},\boldsymbol{\Sigma}_*}\mathbf{w}(a') = \frac{1}{n}\mathbf{Tr}\Bigg(\mathbf{A}^{-1}_{\mathbf{b}_{\boldsymbol{\theta}_j},\boldsymbol{\Sigma}_*}\underbrace{\sum_{a,a'}\mathbf{w}(a)\mathbf{w}(a')}_{\mathbf{V}}\Bigg)$$

where, $\mathbf{b}_{\boldsymbol{\theta}_j}(a)$ is the number of samples allocated to action a. First we will bound the loss of the oracle for this environment given by $\mathcal{L}_n(\pi, \mathbf{b}, \boldsymbol{\Sigma}_*) = \frac{1}{n}\mathbf{Tr}(\mathbf{A}^{-1}_{\mathbf{b}_{\boldsymbol{\theta}_j},\boldsymbol{\Sigma}_*}\mathbf{V})$. Note that the oracle has access to the $\boldsymbol{\Sigma}_*$, so it only need to verify whether $\boldsymbol{\theta}_j = \boldsymbol{\theta}_*$ by following $\mathbf{b}_{\boldsymbol{\theta}_j}$. Then we have that

$$\begin{aligned}
\mathbf{A}_{\mathbf{b}_{\boldsymbol{\theta}_j},\boldsymbol{\Sigma}_*} &= \sum_a \mathbf{b}_{\boldsymbol{\theta}_j}(a)\frac{\mathbf{x}(a)\mathbf{x}(a)^\top}{\sigma^2(a)} = \frac{\mathbf{w}(1)\mathbf{w}(1)^\top}{(\mathbf{x}(1)^\top\boldsymbol{\theta}_j)^2} = \frac{\mathbf{w}(1)\mathbf{w}(1)^\top}{(\beta - \frac{j\beta}{J})^2} \\
\implies \mathbf{Tr}(\mathbf{A}^{-1}_{\mathbf{b}_{\boldsymbol{\theta}_j},\boldsymbol{\Sigma}_*}) &= \frac{(\beta - \frac{j\beta}{J})^2}{\mathbf{Tr}(\mathbf{w}(1)\mathbf{w}(1)^\top)}
\end{aligned}$$

Now we will bound the loss of the algorithm that uses $\widehat{\boldsymbol{\Sigma}}_\beta$ to estimate $\widehat{\mathbf{b}}$. It then collects the $\mathcal{D}$ and uses it to estimate $\boldsymbol{\theta}_*$ following the WLS estimation using $\boldsymbol{\Sigma}_*$.

Denote the number of times the algorithm samples each action i be $T'_n(i)$. Let the algorithm allocate $T'_n(1) = J^2\beta^{-2}\log(1/4\delta) - d$ samples to action 1 and to any other action i' it allocates $T'_n(i') = d$ samples such that $d \geq 1$. WLOG let $i' = 2$. Finally let $T'_n(3) = \ldots = T'_n(A) = 0$. Hence the optimal action 1 is under-allocated and the sub-optimal action 2 is over-allocated. The loss of such an algorithm now is given by

$$\mathcal{L}_n(\pi, \widehat{\mathbf{b}}, \boldsymbol{\Sigma}_*) = \frac{1}{n}\mathbf{Tr}(\mathbf{A}^{-1}_{\widehat{\mathbf{b}},\boldsymbol{\Sigma}_*}\mathbf{V}).$$

Hence it follows by setting $\delta = 1/(nJ)$ that

$$\begin{aligned}
\mathbf{A}_{\widehat{\mathbf{b}},\boldsymbol{\Sigma}_*} = \frac{1}{n}\sum_a n\widehat{\mathbf{b}}(a)\frac{\mathbf{x}(a)\mathbf{x}(a)^\top}{\sigma^2(a)} &= \frac{1}{n}\sum_a T'_n(a)\frac{\mathbf{x}(a)\mathbf{x}(a)^\top}{\sigma^2(a)} \\
&= \frac{1}{n}T'_n(1)\frac{\mathbf{x}(1)\mathbf{x}(1)^\top}{\sigma^2(1)} + \underbrace{\frac{1}{n}T'_n(2)\frac{\mathbf{x}(2)\mathbf{x}(2)^\top}{\sigma^2(2)}}_{\geq 0} \\
&\geq \frac{1}{n}T'_n(1)\frac{\mathbf{w}(1)\mathbf{w}(1)^\top}{(\mathbf{x}(1)^\top\boldsymbol{\theta}_j)^2} \\
&\overset{(a)}{=} \frac{J^2\beta^{-2}\log(nJ) - d}{n}\frac{\mathbf{w}(1)\mathbf{w}(1)^\top}{(\beta - \frac{j\beta}{J})^2}
\end{aligned}$$

where, (a) follows by substituting the value of T'_n. Then we have that

$$\begin{aligned}
\mathbf{Tr}(\mathbf{A}^{-1}_{\widehat{\mathbf{b}},\boldsymbol{\Sigma}_*}) \geq \frac{n}{J^2\beta^{-2}\log(nJ) - d}\frac{(\beta - \frac{j\beta}{J})^2}{\mathbf{Tr}(\mathbf{w}(1)\mathbf{w}(1)^\top)} &= \frac{n}{J^2\beta^{-2}(\log(nJ) - \frac{d}{J^2\beta^{-2}})}\frac{(\beta - \frac{j\beta}{J})^2}{\mathbf{Tr}(\mathbf{w}(1)\mathbf{w}(1)^\top)} \\
&\overset{(a)}{\geq} \frac{\beta^2\log(nJ) + \frac{d}{J^2\beta^{-2}}}{J^2}\frac{(\beta - \frac{j\beta}{J})^2}{\mathbf{Tr}(\mathbf{w}(1)\mathbf{w}(1)^\top)} \\
&\geq \frac{\beta^2\log(nJ)}{J^2}\frac{(\beta - \frac{j\beta}{J})^2}{\mathbf{Tr}(\mathbf{w}(1)\mathbf{w}(1)^\top)}
\end{aligned}$$

where, (a) follows as for $d \geq 1$ we have that

$$n - (\log(nJ))^2 \geq -\frac{d^2}{(J^2\beta^{-2})^2} \implies (\log(nJ) - \frac{d}{J^2\beta^{-2}})^{-1} \geq \log(nJ) + \frac{d}{J^2\beta^{-2}}.$$

Step 4 (Lower Bound regret): Hence we have the regret for verifying any hypothesis $\boldsymbol{\theta}_j = \boldsymbol{\theta}_*$ as follows:

$$
\begin{aligned}
\mathcal{R}'_n &= \mathcal{L}_n(\pi, \widehat{\mathbf{b}}, \boldsymbol{\Sigma}_*) - \mathcal{L}_n(\pi, \mathbf{b}^*, \boldsymbol{\Sigma}_*) \\
&\geq \frac{1}{n}\mathbf{Tr}\left(\mathbf{A}^{-1}_{\widehat{\mathbf{b}},\boldsymbol{\Sigma}_*}\mathbf{V}\right) - \frac{1}{n}\mathbf{Tr}\left(\mathbf{A}^{-1}_{\mathbf{b}_{\boldsymbol{\theta}_j},\boldsymbol{\Sigma}_*}\mathbf{V}\right) = \frac{1}{n}\mathbf{Tr}\left(\left(\mathbf{A}^{-1}_{\widehat{\mathbf{b}},\boldsymbol{\Sigma}_*} - \mathbf{A}^{-1}_{\mathbf{b}_{\boldsymbol{\theta}_j},\boldsymbol{\Sigma}_*}\right)\mathbf{V}\right) \\
&\geq \frac{\lambda_d(\mathbf{V})}{n}\mathbf{Tr}\left(\mathbf{A}^{-1}_{\widehat{\mathbf{b}},\boldsymbol{\Sigma}_*} - \mathbf{A}^{-1}_{\mathbf{b}_{\boldsymbol{\theta}_j},\boldsymbol{\Sigma}_*}\right) \\
&= \frac{\lambda_d(\mathbf{V})}{n}\left[\mathbf{Tr}\left(\mathbf{A}^{-1}_{\widehat{\mathbf{b}},\boldsymbol{\Sigma}_*}\right) - \mathbf{Tr}\left(\mathbf{A}^{-1}_{\mathbf{b}_{\boldsymbol{\theta}_j},\boldsymbol{\Sigma}_*}\right)\right] \\
&= \frac{\lambda_d(\mathbf{V})}{n}\left[\frac{\beta^2\log(nJ)}{J^2}\frac{(\beta - \frac{j\beta}{J})^2}{\mathbf{Tr}(\mathbf{w}(1)\mathbf{w}(1)^\top)} - \frac{(\beta - \frac{j\beta}{J})^2}{\mathbf{Tr}(\mathbf{w}(1)\mathbf{w}(1)^\top)}\right] \\
&= \frac{\lambda_d(\mathbf{V})\beta^2(\beta - \frac{j\beta}{J})^2}{n\mathbf{Tr}(\mathbf{w}(1)\mathbf{w}(1)^\top)}\left[\frac{\log(nJ)}{J^2} - 1\right]
\end{aligned}
$$

$$
\begin{aligned}
&\overset{(a)}{\geq} \frac{\lambda_d(\mathbf{V})\beta^2(\beta - \frac{j\beta}{J})^2}{n\mathbf{Tr}(\mathbf{w}(1)\mathbf{w}(1)^\top)}\left[\frac{\log(nJ)}{2J^2}\right] \\
&\overset{(b)}{\geq} \frac{d\lambda_d(\mathbf{V})\beta^2}{n^{3/2}\mathbf{Tr}(\mathbf{w}(1)\mathbf{w}(1)^\top)}\left[\frac{\log(nJ)}{2J^2}\right] \\
&\overset{(c)}{\geq} \frac{d^2\lambda_d(\mathbf{V})\beta^2}{n^{3/2}\mathbf{Tr}(\mathbf{w}(1)\mathbf{w}(1)^\top)}\log(2n) \\
&= \Omega\left(\frac{d^2\lambda_d(\mathbf{V})\log(n)}{n^{3/2}}\right)
\end{aligned}
$$

where, (a) follows as $\frac{\log(nJ)}{J^2} - 1 \geq \frac{\log(nJ)}{2J^2}$, (b) follows as gap $(\beta - \frac{j\beta}{J})^2 \geq \frac{d}{\sqrt{n}}$ for any $\boldsymbol{\theta}_j$, and (c) follows by substituting $|\boldsymbol{\Theta}| = J = 2^d$. □

Lemma E.1. ***(Restatement of Lemma 15.1 in Lattimore and Szepesvári (2020a), Divergence Decomposition)*** *Let B and B' be two bandit models having different optimal hypothesis $\boldsymbol{\theta}_*$ and $\boldsymbol{\theta}'^*$ respectively. Fix some policy π and round n. Let $\mathbb{P}_{B,\pi}$ and $\mathbb{P}_{B',\pi}$ be two probability measures induced by some n-round interaction of π with B and π with B' respectively. Then*

$$
\mathrm{KL}\left(\mathbb{P}_{B,\pi}||\mathbb{P}_{B',\pi}\right) = \sum_{i=1}^{A}\mathbb{E}_{B,\pi}[T_n(i)]\cdot\mathrm{KL}(\mu_i(\boldsymbol{\theta})||\mu_i(\boldsymbol{\theta}_*))
$$

where, $\mathrm{KL}\left(.||.\right)$ denotes the Kullback-Leibler divergence between two probability measures and $T_n(i)$ denotes the number of times action i has been sampled till round n.

Lemma E.2. ***(Restatement of Lemma 2.6 in Tsybakov (2008))*** *Let $\mathbb{P}, \mathbb{Q}$ be two probability measures on the same measurable space $(\Omega, \mathcal{F})$ and let $\xi \subset \mathcal{F}$ be any arbitrary event then*

$$
\mathbb{P}(\xi) + \mathbb{Q}\left(\xi^{\complement}\right) \geqslant \frac{1}{2}\exp\left(-\mathrm{KL}(\mathbb{P}||\mathbb{Q})\right)
$$

where $\xi^{\complement}$ denotes the complement of event ξ and $\mathrm{KL}(\mathbb{P}||\mathbb{Q})$ denotes the Kullback-Leibler divergence between $\mathbb{P}$ and $\mathbb{Q}$.

Environment $\mathcal{E}$: Consider the environment $\mathcal{E}$ which consist of 3 actions in $\mathbb{R}^2$ such that $\mathbf{x}(1) = [1, 0]$ is along x-axis, $\mathbf{x}(2) = [0, 1]$ is along y-axis and $\mathbf{x}(3) = [1/\sqrt{2}, 1/\sqrt{2}]$. Let $\boldsymbol{\theta}_* = [1, 0]$ and so the optimal action is action 1. Let the target policy $\pi = [0.9, 0.1, 0.0]$. Finally, let the variances be $\sigma^2(1) = 5/100$, $\sigma^2(2) = 1.0$ and $\sigma^2(3) = 5/100$.

Proposition 8. ***(Onpolicy regret)*** *Let the Onpolicy algorithm have access to the variance in environment $\mathcal{E}$. Then the regret of Onpolicy scales as $O\left(\frac{\lambda_1(\mathbf{V})}{n}\right)$.*

Proof. Recall that in $\mathcal{E}$, there are 3 actions in $\mathbb{R}^2$ such that $\mathbf{x}(1) = [1, 0]$ is along x-axis, $\mathbf{x}(2) = [0, 1]$ is along y-axis and $\mathbf{x}(3) = [1/\sqrt{2}, 1/\sqrt{2}]$. The $\boldsymbol{\theta}_* = [1, 0]$ and so the optimal action is action 1. The target policy $\pi = [0.9, 0.1, 0.0]$. Finally, let the variances be $\sigma^2(1) = 1.0$, $\sigma^2(2) = 1.0$ and $\sigma^2(3) = 5/100$. Hence, PE-Optimal design results in $\mathbf{b}^* = [0.5, 0.5, 0.0]$.

$$\mathbf{A}_{\pi,\boldsymbol{\Sigma}_*} = \sum_a \pi(a) \frac{\mathbf{x}(a)\mathbf{x}(a)^\top}{\sigma^2(a)} = \frac{9}{10} \cdot \mathbf{x}(1)\mathbf{x}(1)^\top + \frac{1}{10}\mathbf{x}(2)\mathbf{x}(2)^\top$$

$$\mathbf{A}_{\mathbf{b}_*,\boldsymbol{\Sigma}_*} = \sum_a \mathbf{b}_*(a) \frac{\mathbf{x}(a)\mathbf{x}(a)^\top}{\sigma^2(a)} = \frac{1}{2} \cdot \mathbf{x}(1)\mathbf{x}(1)^\top + \frac{1}{2}\mathbf{x}(2)\mathbf{x}(2)^\top$$

Recall that $\mathbf{V} = \sum_a \mathbf{w}(a)\mathbf{w}(a)^\top$. Hence, the regret scales as

$$\mathcal{R}_n = \mathcal{L}_n(\pi, \pi, \boldsymbol{\Sigma}_*) - \mathcal{L}_n(\pi, \mathbf{b}^*, \boldsymbol{\Sigma}_*) \leq \frac{1}{n}\mathbf{Tr}\left(\mathbf{A}^{-1}_{\pi,\boldsymbol{\Sigma}_*}\mathbf{V}\right) - \frac{1}{n}\mathbf{Tr}\left(\mathbf{A}^{-1}_{\mathbf{b}_*,\boldsymbol{\Sigma}_*}\mathbf{V}\right) = \frac{1}{n}\mathbf{Tr}\left(\left(\mathbf{A}^{-1}_{\pi,\boldsymbol{\Sigma}_*} - \mathbf{A}^{-1}_{\mathbf{b}_*,\boldsymbol{\Sigma}_*}\right)\mathbf{V}\right)$$
$$\overset{(a)}{\leq} O\left(\frac{\lambda_1(\mathbf{V})}{n}\right)$$

where, (a) follows by substituting the value of $\mathbf{A}_{\pi,\boldsymbol{\Sigma}_*}$ and $\mathbf{A}_{\mathbf{b}_*,\boldsymbol{\Sigma}_*}$. □

F. Additional Experiments

In this section, we state additional experimental details.

Unit Ball: This experiment consists of a set of 4 actions that are arranged in a unit ball in $\mathbb{R}^2$, and $\|\mathbf{x}(a)\| = 1$ for all $a \in \mathcal{A}$. We consider three groups of actions: **a)** the reward-maximizing action in the direction of $\boldsymbol{\theta}^*$, **b)** the informative action (orthogonal to optimal action) that maximally reduces the uncertainty of $\widehat{\boldsymbol{\theta}}_t$ and **c)** the less-informative actions as shown in Figure 1 (Top-Left). The variance of the most informative action is chosen to be high (0.35), but the target probability is set as low 0.1, which forces the on-policy algorithm to sample the high variance action less. Figure 1 (Top-Right) shows that SPEED outperforms Onpolicy, G-Optimal , and A-Optimal . Note that we experiment with A-Optimal design (Fontaine et al., 2021) because this criterion results in minimizing the average variance of the estimates of the regression coefficients and is most closely aligned with our goal than G-, or, D-optimal designs (Jamieson and Jain, 2022).

Air Quality: We perform this experiment on real-world dataset Air Quality from UCI datasets. The Air quality dataset consists of 1500 samples each of which consists of 6 features. We first select 400 samples which are the actions in our setting. We then fit a weighted least square estimate to the original dataset and get an estimate of $\boldsymbol{\theta}_*$ and $\boldsymbol{\Sigma}_*$. The reward model is linear and given by $\mathbf{x}_{I_t}^\top \boldsymbol{\theta}_* +$ noise where $\mathbf{x}_{I_t}$ is the observed action at round t, and the noise is a zero-mean additive noise with variance scaling as $\mathbf{x}_{I_t}^\top \boldsymbol{\Sigma}_* \mathbf{x}_{I_t}$. Hence the variance of each action depends on their feature vectors and $\boldsymbol{\Sigma}_*$. Finally, we set a level τ, such that 30 actions having variance crossing τ are set with low target probability, and the remaining probability mass is uniformly distributed among the rest 370 action. Hence, again high variance actions are set with a low target probability, which forces the on-policy algorithm to sample the high-variance action less number of times. We apply SPEED to this problem and compare it to baselines A-Optimal , G-Optimal , and the Onpolicy algorithm.

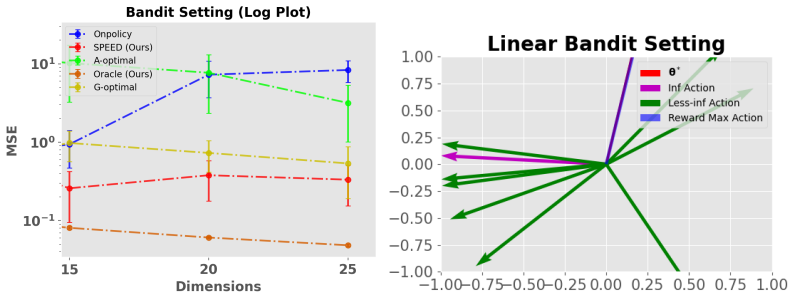

Figure 2. 10 action unit ball environment

Red Wine Quality: The UCI Red Wine Quality dataset consist of 1600 samples of red wine with each sample i having feature $\mathbf{x}_i \in \mathbb{R}^{11}$. We first fit a weighted least square estimate to the original dataset and get an estimate of $\boldsymbol{\theta}^*$ and $\boldsymbol{\Sigma}_*$. The

reward model is linear and given by $\mathbf{x}_{I_t}^T \boldsymbol{\theta}^* +$ noise where $\mathbf{x}_{I_t}$ is the observed action at round t, and the noise is a zero-mean additive noise with variance scaling as $\mathbf{x}_{I_t}^\top \boldsymbol{\Sigma}_* \mathbf{x}_{I_t}$. Note that we consider the 1600 samples as actions. Then we run each of our benchmark algorithms on this dataset and reward model. Finally, we set a level τ, such that 40 actions having variance crossing τ are set with low target probability, and the remaining probability mass is uniformly distributed among the rest 1560 action. Hence, again high variance actions are set with a low target probability, which forces the on-policy algorithm to sample the high-variance action less number of times. We apply SPEED to this problem and compare it to baselines A-Optimal , G-Optimal , and the Onpolicy algorithm.

Movielens: We experiment with a movie recommendation problem on the MovieLens 1M dataset (Lam and Herlocker, 2016). This dataset contains one million ratings given by 6 040 users to 3 952 movies. We first apply a low-rank factorization to the rating matrix to obtain 5-dimensional representations: $\boldsymbol{\theta}_j \in \mathbb{R}^5$ for user $j \in [6\,040]$ and $\mathbf{x}(a) \in \mathbb{R}^5$ for movie $a \in [3\,952]$. In each run, we choose one user $\boldsymbol{\theta}_j$ and 100 movies $\mathbf{x}(a)$ randomly, and they represent the unknown model parameter and known feature vectors of actions, respectively.

Increasing Dimension: We perform this experiment to show how the MSE of SPEED scales with increasing dimensions and number of actions. We choose dimension $d \in \{15, 20, 25\}$. For each dimension $d \in \{15, 20, 25\}$ we choose the number of actions $|\mathcal{A}| = d^2 + 20$. Hence we ensure that the number of actions are greater than d^2 dimensions. We also choose the horizon as $T \in \{13000, 18000, 25000\}$ for each $d \in \{15, 20, 25\}$. We choose the same environment as the unit ball experiment. So the actions arranged in a unit ball in $\mathbb{R}^2$ and $\|\mathbf{x}(a)\| = 1$ for all $a \in \mathcal{A}$. Again we consider three groups of actions: **a)** the reward-maximizing action in the direction of $\boldsymbol{\theta}^*$, **b)** the informative action (orthogonal to optimal action) that maximally reduces the uncertainty of $\widehat{\boldsymbol{\theta}}_t$ and **c)** the less-informative actions as shown in Figure 2 but scaled to a larger set of actions. For each case of dimension $d \in \{15, 20, 25\}$, the variance of the most informative actions along the directions orthogonal to the reward maximizing action are chosen to be high, but the target probability is set as low, which forces the on-policy algorithm to sample the high variance action less. We again show the performance in Figure 1 (Bottom-left). We observe that with increasing dimensions d the SPEED outperforms on-policy. Also, observe that the oracle with knowledge of $\boldsymbol{\Sigma}_*$ performs the best.

G. Table of Notations

Notations	**Definition**
$\pi(a)$	Target policy probability for action a
$\mathbf{b}(a)$	Behavior policy probability for action a
$\mathbf{x}(a)$	Feature of action a
$\boldsymbol{\theta}_*$	Optimal mean parameter
$\widehat{\boldsymbol{\theta}}_n$	Estimate of $\boldsymbol{\theta}_*$
$\mu(a) = \mathbf{x}^\top \boldsymbol{\theta}_*$	Mean of action a
$\widehat{\mu}_t(a) = \mathbf{x}^\top \widehat{\boldsymbol{\theta}}_t$	Empirical mean of action a at time t
$R_t(a)$	Reward for action a at time t
$\boldsymbol{\Sigma}_*$	Optimal co-variance matrix
$\widehat{\boldsymbol{\Sigma}}_t$	Empirical co-variance matrix at time t
$\sigma^2(a) = \mathbf{x}(a)^\top \boldsymbol{\Sigma}_* \mathbf{x}(a)$	Variance of action a
$\widehat{\sigma}_t^2(a) = \mathbf{x}(a)^\top \widehat{\boldsymbol{\Sigma}}_t \mathbf{x}(a)$	Empirical variance of action a at time t
n	Total budget
$T_n(a)$	Total Samples of action a after n timesteps

Table 1. Table of Notations