

Optimally tackling covariate shift in RKHS-based nonparametric regression

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Abstract

We study the covariate shift problem in the context of nonparametric regression over a reproducing kernel Hilbert space (RKHS). We focus on two natural families of covariate shift problems defined using the likelihood ratios between the source and target distributions. When the likelihood ratios are uniformly bounded, we prove that the kernel ridge regression (KRR) estimator with a carefully chosen regularization parameter is minimax rate-optimal (up to a log factor) for a large family of RKHSs with regular kernel eigenvalues. Interestingly, KRR does not require full knowledge of the likelihood ratio apart from an upper bound on it. In striking contrast to the standard statistical setting without covariate shift, we also demonstrate that a naïve estimator, which minimizes the empirical risk over the function class, is strictly suboptimal under covariate shift as compared to KRR. We then address the larger class of covariate shift problems where likelihood ratio is possibly unbounded yet has a finite second moment. Here, we show via careful simulations that KRR fails to attain the optimal rate. Instead, we propose a reweighted KRR estimator that weights samples based on a careful truncation of the likelihood ratios. Again, we are able to show that this estimator is minimax optimal, up to logarithmic factors.

1 Introduction

A widely adopted assumption in supervised learning [20, 5] is that the training and test data are sampled from the same distribution. Such a no-distribution-shift assumption, however, is frequently violated in practice. For instance, in medical image analysis [4, 8], distribution mismatch is widespread across the hospitals due to inconsistency in medical equipment, scanning protocols, subject populations, etc. As another example, in natural language processing [6], the training data are often collected from domains with abundant labels (e.g., Wall Street Journal), while the test data may well arise from a different domain (e.g., arXiv which is mainly composed of scientific articles).

In this paper, we focus on a special and important case of distribution mismatch, known as *covariate shift*. In this version, the marginal distributions over the input covariates may vary from the training (source) to test (target) data¹, while the conditional distribution of the output label given the input covariates is shared across training and testing. Motivating applications include image, text, and speech classification in which the input covariates determine the output labels [19]. Despite its importance in practice, the covariate shift problem is underexplored in theory, when compared to supervised learning without distribution mismatch—a subject that has been well studied in the past decades.

This paper aims to bridge this gap by addressing several fundamental theoretical questions regarding covariate shift. First, what is the statistical limit of estimation in the presence of covariate shift? And how does this limit depend on the “amount” of covariate shift between the source and target distributions? Second, does non-parametric least-squares estimation—a dominant (and often optimal) approach in the no-distribution-shift case—achieve the optimal rate of estimation with covariate shift? If not, what is the optimal way of tackling covariate shift?

1.1 Contributions and overview

We address the aforementioned theoretical questions regarding covariate shift in the context of nonparametric regression over reproducing kernel Hilbert spaces (RKHSs) [17]. That is, we assume that under both the

¹Hereafter, we use source (resp. target) and training (resp. testing) interchangeably.

source and target distributions, the regression function (i.e., the conditional mean function of the output label given the input covariates) belongs to the an RKHS. In this paper, we focus on two broad families of source-target pairs depending on the configuration of the likelihood ratios between them.

We first consider the uniformly B -bounded family in which the likelihood ratios are uniformly bounded by a quantity B . In this case, we present general performance upper bounds for the kernel ridge regression (KRR) estimator in Theorem 1. Instantiations of this general bound on various RKHSs with regular eigenvalues are provided in Corollary 1. It is also shown in Theorem 2 that KRR—with optimally chosen regularization parameter that depends on the largest likelihood ratio B —achieves the minimax lower bound for covariate shift over this uniformly B -bounded family. It is worth noting that the optimal regularization parameter shrinks as the likelihood ratio bound increases.

We further show—via a constructive argument—that the nonparametric least-squares estimator, which minimizes the empirical risk on the training data over the specified RKHS, falls short of achieving the lower bound; see Theorem 3. This marks a departure from the classical no-covariate-shift setting, where the constrained estimator (i.e., the nonparametric least-squares estimator) and the regularized estimator (i.e., the KRR estimator) can both attain optimal rates of estimation [21]. In essence, the failure arises from the misalignment between the projections under the source and target covariate distributions. Loosely speaking, nonparametric least-squares estimation projects the data onto an RKHS according to the geometry induced by the *source* distribution. Under covariate shift, the resulting projection can be extremely far away from the projection under the *target* covariate distributions.

In the second part of the paper, we turn to a more general setting, where the likelihood ratios between the target and source distributions may not be bounded. Instead, we only require the target and source covariate distributions to have a likelihood ratio with bounded second moment. We demonstrate via careful simulations that under these conditions, the KRR estimator can perform poorly and fail to attain optimal rates of estimation. To remedy this deficiency, we propose a variant of KRR that weights samples based on a careful truncation of the likelihood ratios. We are able to show in Theorem 4 that this estimator is rate-optimal over this larger class of covariate shift problems.

1.2 Related work

There is a large body of work on distribution mismatch and, in particular, on covariate shift. Below we review the work that is directly relevant to ours, and refer the interested reader to the book [19] and the survey [12] for additional references.

Shimodaira [18] first studied the covariate shift problem from a statistical perspective, and established the asymptotic consistency of the importance-reweighted maximum likelihood estimator (without truncation). Similar to our work, Cortes and coauthors [3] analyzed the importance-reweighted estimator when the density ratio is either bounded or has a finite second moment. However, their analysis applies to the function class with finite pseudodimension (cf. the book [14]), while the RKHS considered herein does not necessarily obey this assumption. Recently, Kpotufe and Martinet [9] investigated covariate shift under nonparametric classification. They proposed a novel notion called transfer exponent to measure the amount of covariate shift between the source and target distributions. An estimator based on k nearest neighbors was shown to be minimax optimal over the class of covariate shift problems with bounded transfer exponent. Inspired by the work of Kpotufe and Martinet, the current authors [13] proposed a more fine-grained similarity measure for covariate shift and applied to nonparametric regression over the class of Hölder continuous functions. It is worth pointing out that both the transfer exponent and the new fine-grained similarity measure are different and incomparable notions from the moment conditions we impose on the likelihood ratios in this work. Schmidt-Hieber and Zolotarev [16] recently established the local convergence of the non-parametric least-squares estimator for the specific class of 1-Lipschitz functions over the unit interval $[0, 1]$ and applied it to the covariate shift setting.

Apart from covariate shift, other forms of distribution mismatch have been analyzed from a statistical perspective. Cai et al. [1] analyzed posterior shift and proposed an optimal k -nearest-neighbor estimator. Maity et al. [10] conducted the minimax analysis for the label shift problem. Recently, Reeve et al. [15] studied the general distribution match problem (also known as transfer learning) which allows both covariate shift and posterior shift.

Notation. Throughout the paper, we use c, c', c_1, c_2 to denote universal constants, which may vary from line to line.

2 Background and problem formulation

In this section, we formulate and provide background on the problem of covariate shift in non-parametric regression.

2.1 Non-parametric regression under covariate shift

The goal of non-parametric regression is to predict a real-valued response Y based on a vector of covariates $X \in \mathcal{X}$. For each fixed x , the optimal estimator in a mean-squared sense is given by the regression function $f^*(x) := \mathbb{E}[Y \mid X = x]$. In a typical setting, we assume observations of n i.i.d. pairs $\{(x_i, y_i)\}_{i=1}^n$, where each x_i is drawn according to some distribution P over \mathcal{X} , and then y_i is drawn according to the law $(Y \mid X = x_i)$. We assume throughout that for each i , the residual $w_i := y_i - f^*(x_i)$ is a sub-Gaussian random variable with variance proxy σ^2 .

We refer to the distribution P over the covariate space as the *source distribution*. In the standard set-up, the performance of an estimator \hat{f} is measured according to its $L^2(P)$ -error

$$\|\hat{f} - f^*\|_P^2 := \mathbb{E}_{X \sim P}(\hat{f}(X) - f^*(X))^2 = \int_{\mathcal{X}} (\hat{f}(x) - f^*(x))^2 p(x) dx, \quad (1a)$$

where p is the density of P .

In the covariate shift version of this problem, we have a different goal—that is, we wish to construct an estimate \hat{f} whose $L^2(Q)$ -error is small. Here the *target distribution* Q is different from the source distribution P . In analytical terms, letting q be the density of Q , our goal is to find estimators \hat{f} such that

$$\|\hat{f} - f^*\|_Q^2 = \mathbb{E}_{X \sim Q}(\hat{f}(X) - f^*(X))^2 = \int_{\mathcal{X}} (\hat{f}(x) - f^*(x))^2 q(x) dx \quad (1b)$$

is as small as possible. Clearly, the difficulty of this problem should depend on some notion of discrepancy between the source and target distributions.

2.2 Conditions on source-target likelihood ratios

The discrepancy between the $L^2(P)$ and $L^2(Q)$ norms is controlled by the *likelihood ratio*

$$\rho(x) := \frac{q(x)}{p(x)}, \quad (2)$$

which we assume exists for any $x \in \mathcal{X}$. By imposing different conditions on the likelihood ratio, we can define different families of source-target pairs (P, Q) . In this paper, we focus on two broad families of such pairs.

Uniformly B -bounded families: For a constant $B \geq 1$, we say that the likelihood ratio is *B -bounded* if

$$\sup_{x \in \mathcal{X}} \rho(x) \leq B. \quad (3)$$

It is worth noting that $B = 1$ recovers the case without covariate shift, i.e., $P = Q$. Our analysis in Section 3 works under this condition.

χ^2 -bounded families: A uniform bound on the likelihood ratio is a stringent condition, so that it is natural to relax it. One relaxation is to instead bound the second moment: in particular, for a scalar $V^2 \geq 1$, we say that the likelihood ratio is *V^2 -moment bounded* if

$$\mathbb{E}_{X \sim P}[\rho^2(X)] \leq V^2. \quad (4)$$

Note that when the uniform bound (3) holds, the moment bound (4) holds with $V^2 = B$. To see this, we can write $\mathbb{E}_{X \sim P}[\rho^2(X)] = \mathbb{E}_{X \sim Q}[\rho(X)] \leq B$. However, the moment bound (4) is much weaker in general. It is also worth noting that the χ^2 -divergence between Q and P takes the form

$$\chi^2(Q||P) := \mathbb{E}_{X \sim P}[\rho^2(X)] - 1.$$

Therefore, one can understand the quantity $V^2 - 1$ as an upper bound on the χ^2 -divergence between Q and P . Our analysis in Section 4 applies under this weaker condition on the likelihood ratio.

2.3 Unweighted versus likelihood-reweighted estimators

In this paper, we focus on methods for non-parametric regression that are based on optimizing over a Hilbert space \mathcal{H} defined by a reproducing kernel. The Hilbert norm $\|f\|_{\mathcal{H}}$ is used as a means of enforcing “smoothness” on the solution, either by adding a penalty to the objective function or via an explicit constraint.

In the absence of any knowledge of the likelihood ratio, a naïve approach is to simply compute the *unweighted regularized estimate*

$$\hat{f}_{\lambda} := \arg \min_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^n (f(x_i) - y_i)^2 + \lambda \|f\|_{\mathcal{H}}^2 \right\}, \quad (5)$$

where $\lambda > 0$ is a user-defined regularization parameter. When \mathcal{H} is a reproducing kernel Hilbert space (RKHS), then this estimate is known as the *kernel ridge regression* (KRR) estimate. This is a form of empirical risk minimization, but in the presence of covariate shift, the objective involves an empirical approximation to $\mathbb{E}_P[(Y - f(X))^2]$, as opposed to $\mathbb{E}_Q[(Y - f(X))^2]$.

If the likelihood ratio were known, then a natural proposal is to instead compute the *likelihood-reweighted regularized estimate*

$$\tilde{f}_{\lambda}^{\text{rw}} := \arg \min_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^n \rho(x_i) (f(x_i) - y_i)^2 + \lambda \|f\|_{\mathcal{H}}^2 \right\}, \quad (6)$$

The introduction of the likelihood ratio ensures that the objective now provides an unbiased estimate of the expectation $\mathbb{E}_Q[(Y - f(X))^2]$. However, reweighting by the likelihood ratio also increases variance, especially in the case of unbounded likelihood ratios. Accordingly, in Section 4, we study a suitably truncated form of the estimator (6).

2.4 Kernels and their eigenvalues

Any reproducing kernel Hilbert space is associated with a positive semidefinite kernel function $\mathcal{K} : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$. Under mild regularity conditions, Mercer’s theorem guarantees that this kernel has an eigen-expansion of the form

$$\mathcal{K}(x, x') := \sum_{j=1}^{\infty} \mu_j \phi_j(x) \phi_j(x'). \quad (7)$$

for a sequence of non-negative eigenvalues $\{\mu_j\}_{j \geq 1}$, and eigenfunctions $\{\phi_j\}_{j \geq 1}$ taken to be orthonormal in $L^2(Q)$. Given our goal of deriving bounds in the $L^2(Q)$ -norm, it is appropriate to expand the kernel in $L^2(Q)$, as we have done here (7), in order to assess the richness of the function class.

Given the Mercer expansion, the squared norm in the reproducing kernel Hilbert space takes the form

$$\|f\|_{\mathcal{H}}^2 = \sum_{j=1}^{\infty} \frac{\theta_j^2}{\mu_j}, \quad \text{where } \theta_j := \int_{\mathcal{X}} f(x) \phi_j(x) q(x) dx.$$

Consequently, the Hilbert space itself can be written in the form

$$\mathcal{H} := \left\{ f = \sum_{j=1}^{\infty} \theta_j \phi_j \mid \sum_{j=1}^{\infty} \frac{\theta_j^2}{\mu_j} < \infty \right\}. \quad (8)$$

Our goal is to understand the performance of non-parametric regression under covariate shift when the regression function lies in \mathcal{H} .

Throughout this paper, we impose a standard boundedness condition on the kernel function—namely, there exists some finite $\kappa > 0$ such that

$$\sup_{x \in \mathcal{X}} \mathcal{K}(x, x) \leq \kappa^2. \quad (9)$$

Note that any continuous kernel over a compact domain satisfies this condition. Moreover, a variety of commonly used kernels, including the Gaussian and Laplacian kernels, satisfy this condition over any domain.

3 Analysis for bounded likelihood ratios

We begin our analysis in the case of bounded likelihood ratios. Our first main result is to prove an upper bound on the performance of the unweighted KRR estimate (5). First, we prove a family of upper bounds (Theorem 1) depending on the regularization parameter λ . By choosing λ so as to minimize this family of upper bounds, we obtain concrete results for different classes of kernels (Corollary 1). We then turn to the complementary question of lower bounds: in Theorem 2, we prove a family of lower bounds that establish that for covariate shift with B -bounded likelihood ratios, the KRR estimator is minimax-optimal up to logarithmic factors in the sample size. This optimality guarantee is notable since it applies to the unweighted estimator that does not involve full knowledge of the likelihood ratio (apart from an upper bound).

In the absence of covariate shift, it is well-known that performing empirical risk minimization with an explicit constraint on the function also leads to minimax-optimal results. Indeed, without covariate shift, projecting an estimate onto a convex constraint set containing the true function can never lead to a worse result. In Theorem 3, we show that this natural property is no longer true under covariate shift: performing empirical risk minimization over the smallest Hilbert ball containing f^* can be sub-optimal. Optimal procedures—such as the regularized KRR estimate—are actually operating over Hilbert balls with radius substantially larger than the true norm $\|f^*\|_{\mathcal{H}}$.

3.1 Unweighted kernel ridge regression is near-optimal

We begin by deriving a family of upper bounds on the kernel ridge regression estimator (5) under covariate shift. In conjunction with our later analysis, these bounds will establish that the KRR estimate is minimax-optimal up to logarithmic factors for covariate shift with bounded likelihood ratios.

Theorem 1. *Consider a covariate-shifted regression problem with likelihood ratio that is B -bounded (3) over a Hilbert space with a κ -uniformly bounded kernel (9). Then for any $\lambda \geq 10\kappa^2/n$, the KRR estimate \hat{f}_λ satisfies the bound*

$$\|\hat{f}_\lambda - f^*\|_Q^2 \leq \underbrace{4\lambda B \|f^*\|_{\mathcal{H}}^2}_{\mathbf{b}_\lambda^2(B)} + \underbrace{80\sigma^2 B \frac{\log n}{n} \sum_{j=1}^{\infty} \frac{\mu_j}{\mu_j + \lambda B}}_{\mathbf{v}_\lambda(B)} \quad (10)$$

with probability at least $1 - 28 \frac{\kappa^2}{\lambda} e^{-\frac{n\lambda}{16\kappa^2}} - \frac{1}{n^{10}}$.

See Section 5.1 for the proof of this theorem.

Note that the upper bound (10) involves two terms. The first term $\mathbf{b}_\lambda^2(B)$ corresponds to the squared bias of the KRR estimate, and it grows proportionally with the regularization parameter λ and the likelihood

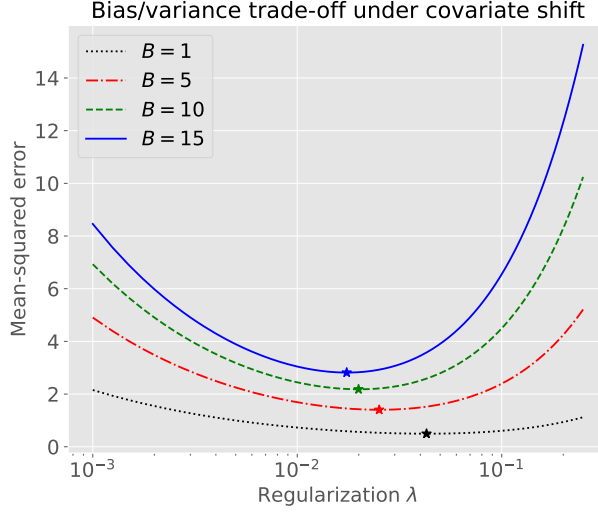


Figure 1. Plot of the upper bound (10) on the mean-squared error versus the log regularization parameter $\log \lambda$ for four different choices of the likelihood ratio bound B , in all cases with eigenvalues $\mu_j = (1/j)^2$, noise variance $\sigma^2 = 1$ and sample size $n = 8000$. The points marked with \star on each curve corresponds to the choice of $\lambda^*(B)$ that minimizes the upper bound. Note how this minimizing value shifts to the left as B increases above the standard problem without covariate shift ($B = 1$).

ratio bound B . The second term $\mathbf{v}_\lambda(B)$ represents the variance of the KRR estimator, and it shrinks as λ increases, so that λ controls the bias-variance trade-off. This type of trade-off is standard in non-parametric regression; what is novel of interest to us here is how the shapes of these trade-off curves change as a function of the likelihood ratio bound B .

Figure 3.1 plots the right-hand side of the upper bound (10) as a function of λ for several different choices $B \in \{1, 5, 10, 15\}$. (In all cases, we fixed a kernel with eigenvalues decaying as $\mu_j = j^{-2}$, sample size $n = 8000$, and noise variance $\sigma^2 = 1$.) Of interest to us is the choice $\lambda^*(B)$ that minimizes this upper bound; note how this optimizing $\lambda^*(B)$ shifts leftwards to smaller values as B is increased.

We would like to understand the balancing procedure that leads to an optimal $\lambda^*(B)$ in analytical terms. This balancing procedure is most easily understood for kernels with *regular eigenvalues*, a notion introduced in past work [22] on kernel ridge regression. For a given targeted error level $\delta > 0$, it is natural to consider the first index $d(\delta)$ for which the associated eigenvalue drops below δ^2 —that is, $d(\delta) := \min\{j \geq 1 \mid \mu_j \leq \delta^2\}$. The eigenvalue sequence is said to be regular if²

$$\sum_{j=d(\delta)+1}^{\infty} \mu_j \leq c d(\delta) \delta^2 \quad (11)$$

holds for some universal constant $c > 0$. The class of kernels with regular eigenvalues includes kernels of finite-rank and those with various forms of polynomial or exponential decay in their eigenvalues; all are widely used in practice. For the class of regular eigenvalues, the bound (10) implies that there is a universal constant c' such that

$$\|\hat{f}_\lambda - f^*\|_Q^2 \leq c' \left\{ \delta^2 \|f^*\|_{\mathcal{H}}^2 + \sigma^2 B \frac{d(\delta) \log n}{n} \right\} \quad \text{where } \delta^2 = \lambda B. \quad (12)$$

We verify this claim as part of proving Corollary 1 below.

This bound (12) enables to make (near)-optimal choices of δ —and hence $\lambda = \delta^2/B$. Let us summarize the outcome of this procedure for a few kernels of interest. In particular, we say that a kernel has *finite rank* D if the eigenvalues $\mu_j = 0$ for all $j > D$. The kernels that underlie linear regression and polynomial regression more generally are of this type. A richer family of kernels has eigenvalues that

²In fact, we can relax this to only require the minimizing δ in equation (12) to obey the tail bound.

exhibit α -polynomial decay $\mu_j \leq c j^{-2\alpha}$ for some $\alpha > 1/2$. This kind of eigenvalue decay is seen in various types of spline and Sobolev kernels, as well as the Laplacian kernel. It is easy to verify that both of these families have regular eigenvalues. To simplify the presentation, we assume $\|f^*\|_{\mathcal{H}} = 1$.

Corollary 1 (Bounds for specific kernels). *(a) For a kernel with rank D , as long as $\sigma^2 D \log n \geq 10\kappa^2$, the choice $\lambda = \frac{\sigma^2 D \log n}{n}$ yields an estimate \hat{f}_λ such that*

$$\|\hat{f}_\lambda - f^*\|_Q^2 \leq c\sigma^2 B \frac{D \log n}{n}. \quad (13a)$$

with high probability.

(b) For a kernel with α -decaying eigenvalues, suppose that σ^2 is sufficiently large so that $\lambda = B^{-\frac{1}{2\alpha+1}} \left(\frac{\sigma^2 \log n}{n}\right)^{\frac{2\alpha}{2\alpha+1}} \geq 10\kappa^2/n$. Then the estimate \hat{f}_λ obeys

$$\|\hat{f}_\lambda - f^*\|_Q^2 \leq c \left(\frac{\sigma^2 B \log n}{n}\right)^{\frac{2\alpha}{2\alpha+1}} \quad (13b)$$

with high probability.

Proof. We begin by proving the upper bound (12). With the shorthand $\delta^2 = \lambda B$, the variance term in our bound (10) can be bounded as

$$\frac{1}{80} \mathbf{v}_\lambda(B) \leq \sigma^2 B \frac{\log n}{n} \sum_{j=1}^{\infty} \frac{\mu_j}{\mu_j + \delta^2} \leq \sigma^2 B \frac{\log n}{n} \left\{ \sum_{j=1}^{d(\delta)} 1 + \sum_{j>d(\delta)} \frac{\mu_j}{\mu_j + \delta^2} \right\}$$

where, by the definition of $d(\delta)$, we have split the eigenvalues into those that are larger than δ^2 , and those that are smaller than δ^2 . By the definition of a regular kernel, the second term can be upper bounded

$$\sum_{j>d(\delta)} \frac{\mu_j}{\mu_j + \delta^2} \leq \frac{1}{\delta^2} c' d(\delta) \delta^2 = c' d(\delta).$$

Putting together the pieces yields $\frac{1}{80} \mathbf{v}_\lambda(B) \leq c_2 \sigma^2 B \frac{\log n}{n} d(\delta)$, for some universal constant c_2 . Combining with the bias term yields the claim (12).

We now prove claims (13a) and (13b). For a finite-rank kernel, using the fact that $d(\delta) \leq D$ for any $\delta > 0$, we can set $\lambda = \frac{\sigma^2 D \log n}{n}$ to obtain the claimed bound (13a). Now suppose that the kernel has α -polynomial decay—that is, $\mu_j \leq c j^{-2\alpha}$ for some $c > 0$. For any $\delta > 0$, we then have $d(\delta) \leq c' (1/\delta)^{1/\alpha}$, and hence

$$\delta^2 + \sigma^2 B \frac{d(\delta) \log n}{n} \leq \delta^2 + c' \sigma^2 B \frac{\log n}{n} \left(\frac{1}{\delta}\right)^{1/\alpha}.$$

By equating the two terms, we can solve for near-optimal δ : in particular, we set $\delta^2 = \left(\frac{\sigma^2 B \log n}{n}\right)^{\frac{2\alpha}{2\alpha+1}}$ to obtain the claimed result. Notice that this choice of δ^2 corresponds to

$$\lambda = \delta^2 / B = B^{-\frac{1}{2\alpha+1}} \left(\frac{\sigma^2 \log n}{n}\right)^{\frac{2\alpha}{2\alpha+1}},$$

as claimed in the corollary. \square

3.2 Lower bounds with covariate shift

Thus far, we have established a family of upper bounds on the unweighted KRR estimate, and derived concrete results for various classes of regular kernels. We now establish that, for the class of regular eigenvalues, the bounds achieved by the unweighted KRR estimator are minimax-optimal. Recall the definition $d(\delta) := \min\{j \geq 1 \mid \mu_j \leq \delta^2\}$, and the notion of regular eigenvalues (11). For a Hilbert space \mathcal{H} , we let $\mathcal{B}_{\mathcal{H}}(1)$ denote the Hilbert norm ball of radius one.

Theorem 2. For any $B \geq 1$, there exists a pair (P, Q) with B -bounded likelihood ratio (3) and an orthonormal basis $\{\phi_j\}_{j \geq 1}$ of $L^2(Q)$ such that for any regular sequence of kernel eigenvalues $\{\mu_j\}_{j \geq 1}$, we have

$$\inf_{\hat{f}} \sup_{f^* \in \mathcal{B}_{\mathcal{H}}(1)} \mathbb{E}[\|\hat{f} - f^*\|_Q^2] \geq c \min_{\delta > 0} \left\{ \delta^2 + \sigma^2 B \frac{d(\delta)}{n} \right\}. \quad (14)$$

See Appendix A for the proof of this claim.

Comparing the lower bound (14) to our achievable result (12) for the unweighted KRR estimate, we see that—with an appropriate choice of the regularization parameter λ —the KRR estimator is minimax optimal up to a $\log n$ term. In particular, it is straightforward to derive the following consequences of Theorem 2, which parallel the guarantees in Corollary 1:

- For a finite-rank kernel, the minimax risk for B -bounded covariate shift satisfies the lower bound

$$\inf_{\hat{f}} \sup_{f^* \in \mathcal{B}_{\mathcal{H}}(1)} \mathbb{E}[\|\hat{f} - f^*\|_Q^2] \geq c \sigma^2 B \frac{D}{n}.$$

- For a kernel with α -polynomial eigenvalues, the minimax risk for B -bounded covariate shift satisfies the lower bound

$$\inf_{\hat{f}} \sup_{f^* \in \mathcal{B}_{\mathcal{H}}(1)} \mathbb{E}[\|\hat{f} - f^*\|_Q^2] \geq c \left(\frac{\sigma^2 B}{n} \right)^{\frac{2\alpha}{2\alpha+1}}.$$

Note that both of these minimax lower bounds reduce to the known lower bounds [22] in the case of no covariate shift ($B = 1$).

3.3 Constrained kernel regression is sub-optimal

In the absence of covariate shift, procedures based on empirical risk minimization with explicit constraints are also known to be minimax-optimal. In the current setting, one such estimator is the constrained kernel regression estimate

$$\hat{f}_{\text{erm}} := \arg \min_{f \in \mathcal{B}_{\mathcal{H}}(1)} \left\{ \frac{1}{n} \sum_{i=1}^n (f(x_i) - y_i)^2 \right\}. \quad (15)$$

Without covariate shift and for any regular kernel, this constrained empirical risk minimization procedure is minimax-optimal over all functions f^* with $\|f^*\|_{\mathcal{H}} \leq 1$.

In the presence of covariate shift, this minimax-optimality turns out to be false. In particular, suppose that the eigenvalues decay as $\mu_j = (1/j)^2$, so that our previous results show that the minimax risk for B -bounded likelihood ratios scales as $(\frac{B\sigma^2}{n})^{2/3}$. It turns out that there exists B -bounded pair (P, Q) and an associated kernel class with the prescribed eigendecay for which the constrained estimator (15) is sub-optimal for a broad range of (B, n) pairs. In the following statement, we use c_1, c_2 to denote universal constants.

Theorem 3. Assume that $\|f^*\|_{\mathcal{H}} = 1$, and that $\sigma^2 = 1$. For any $B \in [c_1(\log n)^2, c_2 n^{2/3}]$, there exists a B -bounded pair (P, Q) and RKHS with eigenvalues $\mu_j \leq (1/j^2)$ such that

$$\sup_{f^* \in \mathcal{B}_{\mathcal{H}}(1)} \mathbb{E}[\|\hat{f}_{\text{erm}} - f^*\|_Q^2] \geq c_3 \frac{B^3}{n^2}. \quad (16)$$

See Appendix B for the proof of this negative result.

In order to appreciate some implications of this theorem, suppose that we use it to construct ensembles with $B_n \asymp n^{2/3}$. The lower bound (16) then implies that over this sequence of problems, say with $\sigma^2 = 1$, the minimax risk is bounded below by a universal constant. On the other hand, if we apply the unweighted KRR procedure, then we obtain consistent estimates, in particular with $L^2(Q)$ -error that decays as

$$\left(\frac{B_n}{n} \right)^{2/3} = \left(\frac{n^{2/3}}{n} \right)^{2/3} = n^{-2/9}.$$

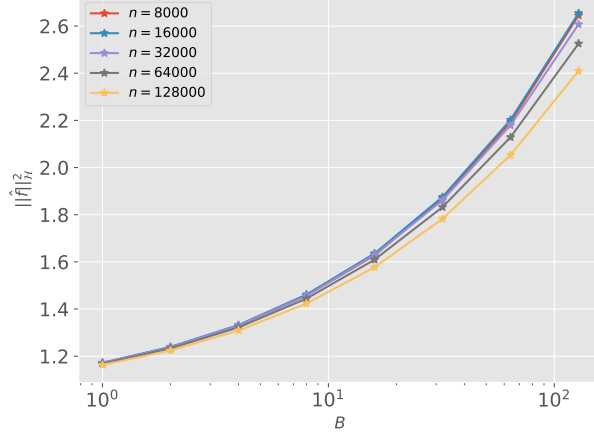


Figure 2. Results based on computing the regularized KRR estimate for the “bad” problems, indexed by the pair (n, B) , that underlie the proof of Theorem 3. Each curve shows the squared Hilbert norm of the regularized KRR estimate $\|\hat{f}_\lambda\|_{\mathcal{H}}^2$, computed with $\lambda = 4^{2/3}n^{-2/3}B^{-1/3}$, versus the likelihood ratio bound B . Each curve corresponds to a different choice of sample size n as indicated in the legend.

It is worth understanding why the constrained form of KRR is sub-optimal, while the regularized form is minimax-optimal. Recall from Corollary 1 that achieving minimax-optimal rates with KRR requires particular choices of the regularization parameter $\lambda^*(B)$, ones that decrease as B increases (see Figure 3.1). This behavior suggests that the Hilbert norm $\|\hat{f}_\lambda\|_{\mathcal{H}}$ of the regularized KRR estimate with optimal choice of λ should grow significantly above $\|f^*\|_{\mathcal{H}} = 1$ when we apply this method.

In order to confirm this intuition, we performed some illustrative simulations over the ensembles, indexed by the pair (B, n) , that underlie the proof of Theorem 3; see Appendix B for the details. With $\sigma^2 = 1$ remaining fixed, for each given pair (B, n) , we simulated regularized kernel ridge regression with the choice $\lambda = 4^{2/3}n^{-2/3}B^{-1/3}$, as suggested by Corollary 1. In Figure 2, for each fixed n , we plot the squared Hilbert norm $\|\hat{f}_\lambda\|_{\mathcal{H}}^2$ of the regularized KRR estimate versus the parameter B . We vary the choice of sample size $n \in \{8000, 16000, 32000, 64000, 128000\}$, as indicated in the figure legend. In all of these curves, we see that the squared Hilbert norm is increasing as a polynomial function of B . This behavior is to be expected, given the sub-optimality of the constrained KRR estimate with a fixed radius.

4 Unbounded likelihood ratios

Thus far, our analysis imposed the B -bound (3) on the likelihood ratio. In practice, however, it is often the case that the likelihood ratio is unbounded. As a simple univariate example, suppose that the target distribution Q is standard normal $\mathcal{N}(0, 1)$, whereas the source distribution P takes the form $\mathcal{N}(0, 0.9)$. It is easy to see that the likelihood ratio $\rho(x)$ tends to ∞ as $|x| \rightarrow \infty$. On the other hand, the second moment of the likelihood ratio under P remains bounded, so that χ^2 -condition (4) applies.

4.1 Unweighted KRR is no longer optimal

A natural question arises as to whether the unweighted KRR estimate (5)—which we have seen is minimax-optimal up to logarithmic factors for bounded likelihood ratios—continues to perform optimally in the more general setting of bounded χ^2 -divergence. In order to motivate the analysis to follow, we begin with some numerical evidence for its sub-optimality.

Sub-optimality of the unweighted estimate: Consider first-order Sobolev space defined on the unit interval:

$$\mathcal{H}^1[0, 1] := \{f: [0, 1] \rightarrow \mathbb{R} \mid f(0) = 0, \text{ and } f \text{ is absolutely continuous with } f' \in L^2[0, 1]\}.$$

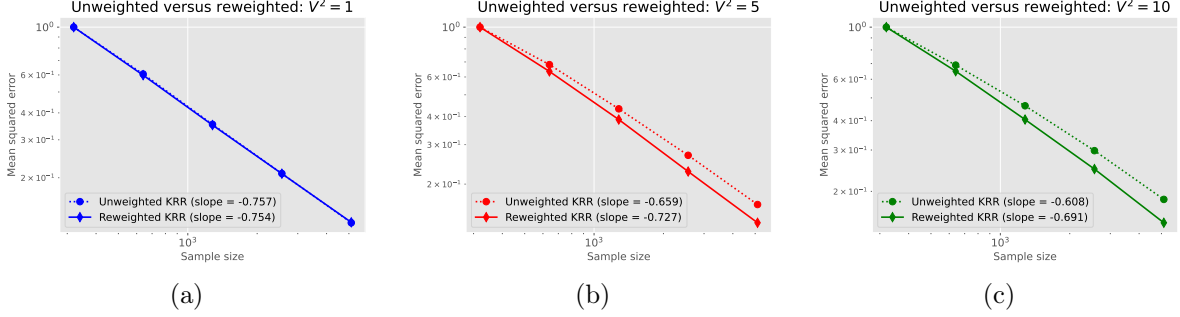


Figure 3. Comparison of the performance of the unweighted KRR estimate (5) with the likelihood-reweighted version (18) over the first-order Sobolev class. The three panels correspond to source-target pairs with second moment bound $V^2 = 1$ in panel (a) (equivalent to covariate shift), and $V^2 = 5$ and $V^2 = 10$ in panels (b) and (c) respectively. Each panel gives plots for each estimator of the mean-squared error versus the sample size n , along with the reported slopes of linear regressions in the log-log domain. The divergence in slopes between the two procedures as we shift from no covariate shift (panel (a)) to covariate shift (panels (b) and (c)) show that the reweighted estimate (18) achieves faster error rates than the unweighted KRR estimate (5).

It is generated by the kernel $\mathcal{K}(x, z) = \min\{x, z\}$, and when Q is uniform on $[0, 1]$, this kernel is known to have polynomially decaying eigenvalues of the form $\mu_j \asymp j^{-2}$ (e.g., see Chapter 14 of the book [21]). As a corollary of Theorem 4 to follow, for this family and any choice of $V^2 \geq 1$, there is an estimator that achieves MSE decaying at least as fast as $(\frac{V^2}{n})^{2/3}$, up to logarithmic factors in n .

We performed some simulations in order to assess whether the unweighted estimate (5) remains optimal, at least when implemented using the choice of regularization λ suggested by our analysis in the bounded case. With the target distribution Q uniform on $[0, 1]$, we performed simulations with $f^*(x) = |x - \frac{1}{2}| - \frac{1}{2}$, and the source distribution $P = \text{Beta}(1 - \sqrt{1 - \frac{1}{V^2}}, 1)$. These choices ensure that the pair (P, Q) has V^2 -bounded likelihood ratio.

For each choice of sample size n and $V^2 \in \{1, 5, 10\}$, we implemented the unweighted KRR estimate (5) with $\lambda \asymp (nV)^{-2/3}$, in analogy with the choice from Corollary 1(b) in the bounded case. We then perform a linear regression of the log MSE versus the log sample size; note that our theory predicts that for an optimal procedure, this slope should be $-2/3 \approx -0.66$ or smaller.

The results of these simulations are shown in Figure 3. In the case of no covariate shift ($V^2 = 1$ in panel (a)), there is no difference between the two estimators, and they both achieve a MSE decaying with exponent roughly $-0.75 < -2/3$, showing that this particular instance is not the most difficulty in the class. As V^2 increases to 5 (panel (b)) and 10 (panel (c)), we start to see a divergence between the error rates of the two estimators. In panel (c), the unweighted KRR estimate has slope approximately $-0.61 > -2/3$, so that it is decaying more slowly than the minimax rate in this case. On the other hand, the likelihood ratio-reweighted estimator exhibits a rate of convergence at least as fast as $n^{-2/3}$, in all three simulations above.

4.2 Importance-reweighted estimator

Given that the unweighted KRR estimator (5) does not appear to achieve optimality with unbounded likelihood ratios, it is natural to consider the likelihood-reweighted estimate (6), as previously introduced in Section 2.3. In contrast to the unweighted KRR estimator, it requires knowledge of the likelihood ratio, but we will see that—when combined with a suitable form of truncation—it achieves minimax-optimal rates (up to logarithmic factors) over the much larger classes of χ^2 -bounded source-target pairs.

As noted before, one concern with likelihood-reweighted estimators is that they can lead to substantial inflation of the variance, in particular due to the multiplication by the potentially unbounded quantity $\rho(x)$. For this reason, it is natural to consider truncation: more precisely, for a given $\tau_n > 0$, we define the *truncated likelihood ratio*

$$\rho_{\tau_n}(x) := \rho(x) \mathbb{1}[\rho(x) \leq \tau_n] = \begin{cases} \rho(x), & \text{if } \rho(x) \leq \tau_n, \\ 0, & \text{otherwise.} \end{cases} \quad (17)$$

We then consider the family of estimators

$$\hat{f}_\lambda^{\text{rw}} := \arg \min_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^n \rho_{\tau_n}(x_i) (f(x_i) - y_i)^2 + \lambda \|f\|_{\mathcal{H}}^2 \right\}, \quad (18)$$

where $\lambda > 0$, along with the truncation level τ_n , are parameters to be specified.

We analyze the behavior of this estimator for kernels whose eigenfunctions are 1-uniformly bounded in sup-norm, meaning that

$$\|\phi_j\|_\infty := \sup_{x \in \mathcal{X}} |\phi_j(x)| \leq 1 \quad \text{for all } j = 1, 2, \dots \quad (19)$$

Our choice of the constant 1 is for notational simplicity. Although there exist kernels whose eigenfunctions are not uniformly bounded, there are many kernels for which this condition does hold. Whenever the domain \mathcal{X} is compact and the eigenfunctions are continuous, this condition will hold. Another class of examples is given by convolutional kernels (i.e., of the form $\mathcal{K}(x, z) = \Psi(x - z)$ for some $\Psi : \mathcal{X} \rightarrow \mathbb{R}$), which have sinusoids as their eigenfunctions, and so satisfy this condition. The numerical example used to showcase the failure of the unweighted KRR estimate also obeys this condition.

Our theorem on the truncated-reweighted KRR estimate (18) involves the kernel complexity function $\Psi(\delta, \mu) := \sum_{j=1}^\infty \min\{\delta^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}$, and works for any solution $\delta_n > 0$ to the inequality $\mathcal{M}(\delta) \leq \delta^2/2$, where

$$\mathcal{M}(\delta) := c_0 \sqrt{\frac{\sigma^2 V^2 \log^3(n)}{n}} \Psi(\delta, \mu). \quad (20)$$

Here c_0 is a universal constant, whose value is specified via the proof.

Below, we present the performance guarantee of $\hat{f}_\lambda^{\text{rw}}$ in the large noise regime (i.e., when $\sigma^2 \geq \kappa^2 \|f^*\|_{\mathcal{H}}^2$) to simplify the statement. Theoretical guarantees for all ranges of σ^2 can be found in Appendix D.

Theorem 4. *Consider a kernel with sup-norm bounded eigenfunctions (19), and a source-target pair with $\mathbb{E}_P[\rho^2(X)] \leq V^2$. Further assume that the noise level obeys $\sigma^2 \geq \kappa^2 \|f^*\|_{\mathcal{H}}^2$. Then the estimate $\hat{f}_\lambda^{\text{rw}}$ with truncation $\tau_n = \sqrt{n}V^2$ and regularization $\lambda \|f^*\|_{\mathcal{H}}^2 \geq \delta_n^2/3$ satisfies the bound*

$$\|\hat{f}_\lambda^{\text{rw}} - f^*\|_Q^2 \leq \delta_n^2 + 3\lambda \|f^*\|_{\mathcal{H}}^2 \quad (21)$$

with probability at least $1 - c n^{-10}$.

See Section 5.2 for the proof of this claim.

To appreciate the connection to our previous analysis, in the proof of Corollary 2 below, we show that for any regular sequence of eigenvalues and $\|f^*\|_{\mathcal{H}} = 1$, we have

$$\Psi(\delta, \mu) \leq c' d(\delta) \delta^2 \quad (22)$$

for some universal constant c' . Moreover, the condition $\mathcal{M}(\delta) \leq \delta^2/2$ can be verified by checking the inequality

$$\sqrt{\frac{\sigma^2 V^2 \log^3(n)}{n}} d(\delta) \lesssim \delta. \quad (23)$$

This further allows us to obtain the rates of estimation over specific kernel classes.

Corollary 2. *Consider kernels with sup-norm bounded eigenfunctions (19).*

(a) *For a kernel with rank D , the truncated-reweighted estimator with $\lambda \geq c \frac{DV^2 \log^3(n) \sigma^2}{n}$ achieves*

$$\|\hat{f}_\lambda^{\text{rw}} - f^*\|_Q^2 \leq c' \frac{DV^2 \log^3(n) \sigma^2}{n} \quad (24)$$

with high probability.

(b) For a kernel with α -polynomial eigenvalues, we have with high probability

$$\|\hat{f}_\lambda^{\text{rw}} - f^*\|_Q^2 \leq c' \left(\frac{V^2 \log^3 n}{n} \sigma^2 \right)^{\frac{2\alpha}{2\alpha+1}}, \quad (25)$$

provided that $\lambda \geq c \left(\frac{V^2 \log^3 n}{n} \sigma^2 \right)^{\frac{2\alpha}{2\alpha+1}}$.

Proof. We begin by verifying the claim (22). Recalling the definition of $d(\delta)$ as the smallest integer for which $\mu_j \leq \delta^2$, we can write

$$\Psi(\delta, \mu) = \sum_{j=1}^{d(\delta)} \min\{\delta^2, \mu_j\} + \sum_{j=d(\delta)+1}^{\infty} \min\{\delta^2, \mu_j\} \leq d(\delta)\delta^2 + cd(\delta)\delta^2$$

where the bound on the second sum follows from the regularity condition. This completes the proof of the bound (22).

Given our bound (22), it is straightforward to verify the claim (23).

We now prove the bounds (24) and (25). For the finite rank case, we have $\Psi(\delta, \mu) \leq D\delta^2$, which implies $\delta_n^2 \leq c \frac{DV^2 \log^3(n)\sigma^2}{n}$ for some universal constant c . Apply Theorem 4 to obtain the desired rate. Now we move on to the kernel with α -polynomial eigenvalues. We know from the proof of Corollary 1 that $d(\delta) \leq c(1/\delta)^{1/\alpha}$, and hence $\Psi(\delta, \mu) \leq c'\delta^{2-1/\alpha}$. This implies $\delta_n^2 \leq c \left(\frac{V^2 \log^3 n}{n} \sigma^2 \right)^{\frac{2\alpha}{2\alpha+1}}$, which together with Theorem 4 yields the claim. \square

Corollary 2 showcases that the reweighted KRR estimator is minimax optimal (up to log factors) over this more general χ^2 -bounded family. This can be seen from the lower bound established in Theorem 2 and the fact that the χ^2 -bounded family is a larger family compared to the uniformly bounded family.

5 Proofs

In this section, we provide the proofs of our two sets of upper bounds on different estimators. Section 5.1 is devoted to the proof of Theorem 1 on upper bounds on unweighted KRR for B -bounded likelihood ratios, whereas Section 5.2 is devoted to the proof of Theorem 4 on the performance of LR-reweighted KRR with truncation.

5.1 Proof of Theorem 1

Define the empirical covariance operator³

$$\hat{\Sigma}_P := \frac{1}{n} \sum_{i=1}^n \phi(x_i) \phi(x_i)^\top, \quad (26)$$

the population covariance operator $\Sigma_P := \mathbb{E}_{X \sim P}[\phi(X) \phi(X)^\top]$, and the diagonal operator $\mathbf{M} := \text{diag}(\{\mu_j\}_{j \geq 1})$.

Before we embark on the proof, we single out two important properties regarding Σ_P and $\hat{\Sigma}_P$ that will be useful in later proofs. For a given $\lambda > 0$, we define the event

$$\mathcal{E}(\lambda) := \left\{ \mathbf{M}^{1/2} \hat{\Sigma}_P \mathbf{M}^{1/2} + \lambda \mathbf{I} \succeq \frac{1}{2} (\mathbf{M}^{1/2} \Sigma_P \mathbf{M}^{1/2} + \lambda \mathbf{I}) \right\}, \quad (27)$$

where \mathbf{I} is the identity operator on $\ell^2(\mathbb{N})$.

Lemma 1. *For any B -bounded source-target pair (3), we have the deterministic lower bound*

$$\Sigma_P \succeq \frac{1}{B} \mathbf{I}. \quad (28a)$$

If, in addition, the kernel is κ -uniformly bounded (9), then whenever $n\lambda \geq 10\kappa^2$, the event $\mathcal{E}(\lambda)$ defined in equation (27) satisfies

$$\mathbb{P}[\mathcal{E}(\lambda)] \geq 1 - 28 \frac{\kappa^2}{\lambda} e^{-\frac{n\lambda}{16\kappa^2}}. \quad (28b)$$

³In this proof, all the operators are defined with respect to the space $\ell^2(\mathbb{N})$.

See Section 5.1.3 for the proof of this claim.

Equipped with Lemma 1, we now proceed to the proof of the theorem. In terms of the basis $\{\phi_j\}_{j \geq 1}$, the KRR estimate has the expansion $\hat{f}_\lambda = \sum_{j=1}^\infty \hat{\theta}_j \phi_j$, where $\hat{\theta} = \{\hat{\theta}_j\}_{j \geq 1}$ is a sequence of coefficients in $\ell^2(\mathbb{N})$. By the optimality conditions for the KRR problem, we have

$$\hat{\theta} - \theta^\star = -\lambda(\hat{\Sigma}_P + \lambda \mathbf{M}^{-1})^{-1} \mathbf{M}^{-1} \theta^\star + (\hat{\Sigma}_P + \lambda \mathbf{M}^{-1})^{-1} \left(\frac{1}{n} \sum_{i=1}^n w_i \phi(x_i) \right).$$

By the triangle inequality, we have the upper bound $\|\hat{\theta} - \theta^\star\|_2^2 \leq 2(T_1 + T_2)$, where

$$T_1 := \|\lambda(\hat{\Sigma}_P + \lambda \mathbf{M}^{-1})^{-1} \mathbf{M}^{-1} \theta^\star\|_2^2, \quad \text{and} \quad T_2 := \|(\hat{\Sigma}_P + \lambda \mathbf{M}^{-1})^{-1} \left(\frac{1}{n} \sum_{i=1}^n w_i \phi(x_i) \right)\|_2^2.$$

In terms of this decomposition, it suffices to establish that the following bounds

$$T_1 \stackrel{(a)}{\leq} 2\lambda B \|f^\star\|_{\mathcal{H}}^2, \quad \text{and} \quad T_2 \stackrel{(b)}{\leq} \frac{40(\log n)\sigma^2}{n} \sum_{j=1}^\infty \frac{\mu_j}{\mu_j/B + \lambda}, \quad (29)$$

hold with probability at least $1 - 28 \frac{\kappa^2}{\lambda} e^{-\frac{n\lambda}{16\kappa^2}} - n^{-10}$.

5.1.1 Proof of the bound (29)(a)

We establish that this bound holds conditionally on the event $\mathcal{E}(\lambda)$. Following some algebraic manipulations, we have

$$\begin{aligned} T_1 &= \lambda^2 \|\mathbf{M}^{1/2}(\mathbf{M}^{1/2} \hat{\Sigma}_P \mathbf{M}^{1/2} + \lambda \mathbf{I})^{-1} \mathbf{M}^{-1/2} \theta^\star\|_2^2 \\ &\stackrel{(i)}{\leq} \lambda^2 \|f^\star\|_{\mathcal{H}}^2 \|\mathbf{M}^{1/2}(\mathbf{M}^{1/2} \hat{\Sigma}_P \mathbf{M}^{1/2} + \lambda \mathbf{I})^{-1}\|_2^2 \\ &\stackrel{(ii)}{\leq} \lambda \|f^\star\|_{\mathcal{H}}^2 \|\mathbf{M}^{1/2}(\mathbf{M}^{1/2} \hat{\Sigma}_P \mathbf{M}^{1/2} + \lambda \mathbf{I})^{-1/2}\|_2^2 \\ &\stackrel{(iii)}{\leq} 2\lambda \|f^\star\|_{\mathcal{H}}^2 \|\mathbf{M}^{1/2}(\mathbf{M}^{1/2} \Sigma_P \mathbf{M}^{1/2} + \lambda \mathbf{I})^{-1} \mathbf{M}^{1/2}\|_2 \end{aligned}$$

Here inequality (i) follows from the assumption that $\|f^\star\|_{\mathcal{H}} \leq \|f^\star\|_{\mathcal{H}}$ or equivalently $\|\mathbf{M}^{-1/2} \theta^\star\|_2 \leq \|f^\star\|_{\mathcal{H}}$; the second step (ii) uses the fact that $\mathbf{M}^{1/2} \hat{\Sigma}_P \mathbf{M}^{1/2} + \lambda \mathbf{I} \succeq \lambda \mathbf{I}$, and step (iii) follows from the fact that we are conditioning on the event $\mathcal{E}(\lambda)$.

Lemma 1 also guarantees that $\Sigma_P \succeq \frac{1}{B} \mathbf{I}$, whence

$$T_1 \leq 2\lambda \|f^\star\|_{\mathcal{H}}^2 \|\mathbf{M}^{1/2}(\frac{1}{B} \mathbf{M} + \lambda \mathbf{I})^{-1} \mathbf{M}^{1/2}\|_2 = 2\lambda \cdot \max_{j \geq 1} \left\{ \frac{\mu_j}{\frac{\mu_j}{B} + \lambda} \right\} \leq 2\lambda B \|f^\star\|_{\mathcal{H}}^2.$$

This establishes the claim (29)(a).

5.1.2 Proof of the bound (29)(b)

Define the random vector $W := (\hat{\Sigma}_P + \lambda \mathbf{M}^{-1})^{-1} \left(\frac{1}{n} \sum_{i=1}^n w_i \phi(x_i) \right)$. Conditioned on the covariates $\{x_i\}_{i=1}^n$, W is a zero-mean sub-Gaussian random variable with covariance operator

$$\mathbf{\Lambda} := \frac{\sigma^2}{n} (\hat{\Sigma}_P + \lambda \mathbf{M}^{-1})^{-1} \hat{\Sigma}_P (\hat{\Sigma}_P + \lambda \mathbf{M}^{-1})^{-1}.$$

Consequently, by the Hanson-Wright inequality in the RKHS (cf. Theorem 2.6 in the paper [2]), we have

$$\mathbb{P}[T_2 \geq 20(\log n) \text{trace}(\mathbf{\Lambda}) \mid \{x_i\}_{i=1}^n] \leq \frac{1}{n^{10}}, \quad (30)$$

where the probability is taken over the noise variables.

It remains to upper bound the trace. We have $\text{trace}(\mathbf{\Lambda}) = \text{trace}\left(\frac{\sigma^2}{n}(\widehat{\mathbf{\Sigma}}_P + \lambda \mathbf{M}^{-1})^{-1} \widehat{\mathbf{\Sigma}}_P (\widehat{\mathbf{\Sigma}}_P + \lambda \mathbf{M}^{-1})^{-1}\right)$, so that

$$\begin{aligned} \text{trace}(\mathbf{\Lambda}) &\leq \text{trace}\left(\frac{\sigma^2}{n}(\widehat{\mathbf{\Sigma}}_P + \lambda \mathbf{M}^{-1})^{-1}(\widehat{\mathbf{\Sigma}}_P + \lambda \mathbf{M}^{-1})(\widehat{\mathbf{\Sigma}}_P + \lambda \mathbf{M}^{-1})^{-1}\right) \\ &= \text{trace}\left(\frac{\sigma^2}{n}(\widehat{\mathbf{\Sigma}}_P + \lambda \mathbf{M}^{-1})^{-1}\right) = \text{trace}\left(\frac{\sigma^2}{n}(\mathbf{M}^{1/2}(\mathbf{M}^{1/2} \widehat{\mathbf{\Sigma}}_P \mathbf{M}^{1/2} + \lambda \mathbf{I})^{-1} \mathbf{M}^{1/2})\right). \end{aligned}$$

Under the event $\mathcal{E}(\lambda)$, we have $\mathbf{M}^{1/2} \widehat{\mathbf{\Sigma}}_P \mathbf{M}^{1/2} + \lambda \mathbf{I} \succeq \frac{1}{2}(\mathbf{M}^{1/2} \mathbf{\Sigma}_P \mathbf{M}^{1/2} + \lambda \mathbf{I})$, which implies

$$\begin{aligned} \text{trace}(\mathbf{\Lambda}) &\leq 2 \frac{\sigma^2}{n} \text{trace}\left(\mathbf{M}^{1/2}(\mathbf{M}^{1/2} \mathbf{\Sigma}_P \mathbf{M}^{1/2} + \lambda \mathbf{I})^{-1} \mathbf{M}^{1/2}\right) \\ &\stackrel{(i)}{\leq} 2 \frac{\sigma^2}{n} \text{trace}\left(\mathbf{M}^{1/2}\left(\frac{1}{B} \mathbf{M} + \lambda \mathbf{I}\right)^{-1} \mathbf{M}^{1/2}\right) \\ &\stackrel{(ii)}{=} 2 \frac{\sigma^2}{n} \sum_{j=1}^{\infty} \frac{\mu_j}{\frac{\mu_j}{B} + \lambda}. \end{aligned}$$

Here step (i) follows since $\mathbf{\Sigma}_P \succeq \frac{1}{B} \mathbf{I}$, and step (ii) follows from a direct calculation. Substituting this upper bound on the trace into the tail bound (30) yields the claimed bound (29)(b).

5.1.3 Proof of Lemma 1

We begin with the proof of the lower bound (28a). Since $\{\phi_j\}_{j \geq 1}$ is an orthonormal basis of $L^2(Q)$, we have

$$\mathbb{E}_{X \sim Q}[\phi(X)\phi(X)^\top] = \mathbb{E}_{X \sim P}[\rho(X)\phi(X)\phi(X)^\top] = \mathbf{I}.$$

Thus, the B -boundedness of the likelihood ratio (3) implies that

$$\mathbf{I} \preceq \mathbb{E}_{X \sim P}[B\phi(X)\phi(X)^\top] = B\mathbf{\Sigma}_P,$$

which is equivalent to the claim (28a).

Next we prove the lower bound (27). We introduce the shorthand notation

$$\widehat{\mathbf{\Sigma}}_\lambda := \mathbf{M}^{1/2} \widehat{\mathbf{\Sigma}}_P \mathbf{M}^{1/2} + \lambda \mathbf{I}, \quad \text{and} \quad \mathbf{\Sigma}_\lambda := \mathbf{M}^{1/2} \mathbf{\Sigma}_P \mathbf{M}^{1/2} + \lambda \mathbf{I}$$

along with the matrix $\mathbf{\Delta} := \mathbf{\Sigma}_\lambda^{-1/2}(\widehat{\mathbf{\Sigma}}_\lambda - \mathbf{\Sigma}_\lambda)\mathbf{\Sigma}_\lambda^{-1/2}$. Recalling that $\|\cdot\|_2$ denotes the ℓ_2 -operator norm of a matrix, we first observe that $\{\|\mathbf{\Delta}\|_2 \leq \frac{1}{2}\} \subseteq \mathcal{E}$. Consequently, it suffices to show that $\|\mathbf{\Delta}\|_2 \leq \frac{1}{2}$ with high probability.

The matrix $\mathbf{\Delta}$ can be written as the normalized sum $\mathbf{\Delta} = \frac{1}{n} \sum_{i=1}^n \mathbf{Z}_i$, where the random operators

$$\mathbf{Z}_i := \mathbf{\Sigma}_\lambda^{-1/2} \mathbf{M}^{1/2} (\phi(x_i)\phi(x_i)^\top - \mathbf{\Sigma}_P) \mathbf{M}^{1/2} \mathbf{\Sigma}_\lambda^{-1/2}$$

are i.i.d. The operator norm of each term can be bounded as

$$\begin{aligned} \|\mathbf{Z}_i\|_2 &\leq 2 \sup_{x \in \mathcal{X}} \|\mathbf{\Sigma}_\lambda^{-1/2} \mathbf{M}^{1/2} \phi(x)\phi(x)^\top \mathbf{M}^{1/2} \mathbf{\Sigma}_\lambda^{-1/2}\|_2 = 2 \sup_{x \in \mathcal{X}} \|\mathbf{\Sigma}_\lambda^{-1/2} \mathbf{M}^{1/2} \phi(x)\|_2^2 \\ &\leq 2\kappa^2 \|\mathbf{\Sigma}_\lambda^{-1/2}\|_2^2 \leq \frac{2\kappa^2}{\lambda} =: L, \end{aligned} \tag{31}$$

where the final inequality follows from the assumption that $\sup_{x \in \mathcal{X}} \|\mathbf{M}^{1/2} \phi(x)\|_2^2 \leq \kappa^2$, and the fact that $\mathbf{\Sigma}_\lambda \succeq \lambda \mathbf{I}$.

On the other hand, the variance of \mathbf{Z}_i can be bounded as

$$\begin{aligned} \mathbb{E}[\mathbf{Z}_i^2] &\preceq \mathbb{E}[(\mathbf{\Sigma}_\lambda^{-1/2} \mathbf{M}^{1/2} \phi(X)\phi(X)^\top \mathbf{M}^{1/2} \mathbf{\Sigma}_\lambda^{-1/2})^2] \\ &= \mathbb{E}[\mathbf{\Sigma}_\lambda^{-1/2} \mathbf{M}^{1/2} \phi(X)\phi(X)^\top \mathbf{M}^{1/2} \mathbf{\Sigma}_\lambda^{-1} \mathbf{M}^{1/2} \phi(X)\phi(X)^\top \mathbf{M}^{1/2} \mathbf{\Sigma}_\lambda^{-1/2}] \end{aligned}$$

$$\begin{aligned}
&\preceq \mathbb{E} \left[\Sigma_\lambda^{-1/2} \mathbf{M}^{1/2} \phi(X) \phi(X)^\top \mathbf{M}^{1/2} \Sigma_\lambda^{-1/2} \right] \cdot \sup_{x \in \mathcal{X}} \left\{ \phi(x)^\top \mathbf{M}^{1/2} \Sigma_\lambda^{-1} \mathbf{M}^{1/2} \phi(x) \right\} \\
&\preceq \frac{\kappa^2}{\lambda} \Sigma_\lambda^{-1/2} \mathbf{M}^{1/2} \Sigma_P \mathbf{M}^{1/2} \Sigma_\lambda^{-1/2} =: \mathbf{V},
\end{aligned}$$

where the last inequality follows by applying the bound (31) on $\sup_{x \in \mathcal{X}} \|\Sigma_\lambda^{-1/2} \mathbf{M}^{1/2} \phi(x)\|_2^2$.

Suppose that we can show that

$$\text{trace}(\mathbf{V}) \leq \frac{\kappa^2}{\lambda} \cdot \frac{\kappa^2}{\lambda}; \quad (32a)$$

$$\|\mathbf{V}\|_2 \leq \frac{\kappa^2}{\lambda}. \quad (32b)$$

We can then apply a dimension-free matrix Bernstein inequality (see Lemma 8) with $t = 1/2$ to obtain the tail bound

$$\mathbb{P}[\|\Delta\|_2 \geq \frac{1}{2}] \leq 28 \frac{\kappa^2}{\lambda} \exp\left(-\frac{n\lambda}{16\kappa^2}\right),$$

as long as $n\lambda \geq 10\kappa^2$. Thus, the only remaining detail is to prove the bounds (32a) and (32b).

Proof of the bound (32a): Using the definition of \mathbf{V} , we have

$$\begin{aligned}
\text{trace}(\mathbf{V}) &= \frac{\kappa^2}{\lambda} \text{trace}\left(\Sigma_\lambda^{-1/2} \mathbf{M}^{1/2} \Sigma_P \mathbf{M}^{1/2} \Sigma_\lambda^{-1/2}\right) = \frac{\kappa^2}{\lambda} \mathbb{E}_P[\text{trace}(\Sigma_\lambda^{-1/2} \mathbf{M}^{1/2} \phi(x) \phi(x)^\top \mathbf{M}^{1/2} \Sigma_\lambda^{-1/2})] \\
&\leq \frac{\kappa^2}{\lambda} \cdot \frac{\kappa^2}{\lambda}.
\end{aligned}$$

Here we have again applied the bound $\sup_{x \in \mathcal{X}} \|\Sigma_\lambda^{-1/2} \mathbf{M}^{1/2} \phi(x)\|_2^2 \leq \kappa^2/\lambda$.

Proof of the bound (32b): Recalling the definition of Σ_λ , we see that $\|\Sigma_\lambda^{-1/2} \mathbf{M}^{1/2} \Sigma_P \mathbf{M}^{1/2} \Sigma_\lambda^{-1/2}\|_2 \leq 1$, and hence

$$\|\mathbf{V}\|_2 = \frac{\kappa^2}{\lambda} \|\Sigma_\lambda^{-1/2} \mathbf{M}^{1/2} \Sigma_P \mathbf{M}^{1/2} \Sigma_\lambda^{-1/2}\|_2 \leq \frac{\kappa^2}{\lambda},$$

which is the claimed upper bound on $\|\mathbf{V}\|_2$.

5.2 Proof of Theorem 4

We now turn to the proof of our guarantee on the truncated LR-reweighted estimator. At the core of the proof is a uniform concentration result, one that holds within a local ball

$$\mathcal{G}(r) := \{f \in \mathcal{H} \mid \|f - f^*\|_Q \leq r, \text{ and } \|f - f^*\|_{\mathcal{H}} \leq 3\|f^*\|_{\mathcal{H}}\}$$

around the true regression function f^* .

Lemma 2. *Fix any $r > 0$, we have*

$$\sup_{g \in \mathcal{G}(r)} \left\{ \|g - f^*\|_Q^2 + \frac{1}{n} \sum_{i=1}^n \rho_{\tau_n}(x_i) [(f^*(x_i) - y_i)^2 - (g(x_i) - y_i)^2] \right\} \leq \mathcal{M}(r) \quad (33)$$

with probability at least $1 - cn^{-10}$.

See Section 5.2.1 for the proof of this lemma.

Taking this lemma as given, we now complete the proof of the theorem. Define the regularized radius $\delta_\lambda := \sqrt{\delta_n^2 + 3\lambda\|f^*\|_{\mathcal{H}}^2}$, and denote by $\mathcal{E}(\delta_\lambda)$ the “good” event that the relation (33) holds at radius δ_λ . We

immediately point out an important property of the regularized radius δ_λ , namely $\mathcal{M}(\delta_\lambda) \leq (1/2) \cdot \delta_\lambda^2$. To see this, note that $r \mapsto \mathcal{M}(r)$ is non-increasing in r , and hence

$$\frac{\mathcal{M}(\delta_\lambda)}{\delta_\lambda} \leq \frac{\mathcal{M}(\delta_n)}{\delta_n} \leq \frac{1}{2}\delta_n \leq \frac{1}{2}\delta_\lambda.$$

Suppose that conditioned on $\mathcal{E}(\delta_\lambda)$, the following inequality holds

$$\inf_{f \in \mathcal{H}, f \notin \mathcal{G}(\delta_\lambda)} \frac{1}{n} \sum_{i=1}^n \rho_{\tau_n}(x_i) \left\{ (f(x_i) - y_i)^2 - (f^*(x_i) - y_i)^2 \right\} + \lambda \|f\|_{\mathcal{H}}^2 - \lambda \|f^*\|_{\mathcal{H}}^2 > 0. \quad (34)$$

It then follows that that $\|\hat{f} - f^*\|_Q \leq \delta_\lambda$, as desired. Consequently, the remainder of our proof is devoted to establishing that inequality (34) holds conditioned on $\mathcal{E}(\delta_\lambda)$.

Given any function $f \in \mathcal{H}$ and $f \notin \mathcal{G}(\delta_\lambda)$, there exists an $\alpha \geq 1$ such that $\tilde{f} := f^* + \frac{1}{\alpha}(f - f^*)$ lies in the set \mathcal{H} , and more importantly \tilde{f} lies on the boundary of $\mathcal{G}(\delta_\lambda)$. This follows from the convexity of the two sets \mathcal{H} and $\mathcal{G}(\delta_\lambda)$. Since \tilde{f} is a convex combination of f and f^* , Jensen's inequality implies that

$$\begin{aligned} & \rho_{\tau_n}(x_i) \left\{ (\tilde{f}(x_i) - y_i)^2 - (f^*(x_i) - y_i)^2 \right\} + \lambda \|\tilde{f}\|_{\mathcal{H}}^2 - \lambda \|f^*\|_{\mathcal{H}}^2 \\ & \leq \frac{1}{\alpha} \left\{ \rho_{\tau_n}(x_i) \left\{ (f(x_i) - y_i)^2 - (f^*(x_i) - y_i)^2 \right\} + \lambda \|f\|_{\mathcal{H}}^2 - \lambda \|f^*\|_{\mathcal{H}}^2 \right\}. \end{aligned}$$

Consequently, in order to establish the claim (34), it suffices to prove that the quantity

$$T := \frac{1}{n} \sum_{i=1}^n \rho_{\tau_n}(x_i) \left\{ (f^*(x_i) - y_i)^2 - (\tilde{f}(x_i) - y_i)^2 \right\} + \lambda \|f^*\|_{\mathcal{H}}^2 - \lambda \|\tilde{f}\|_{\mathcal{H}}^2$$

is negative. Since \tilde{f} lies on the boundary of $\mathcal{G}(\delta_\lambda)$, we can split the proof into two cases: (1) $\|\tilde{f} - f^*\|_Q = \delta_\lambda$, while $\|\tilde{f} - f^*\|_{\mathcal{H}} \leq 3\|f^*\|_{\mathcal{H}}$, and (2) $\|\tilde{f} - f^*\|_Q \leq \delta_\lambda$, while $\|\tilde{f} - f^*\|_{\mathcal{H}} = 3\|f^*\|_{\mathcal{H}}$.

Case 1: $\|\tilde{f} - f^*\|_Q = \delta_\lambda$, while $\|\tilde{f} - f^*\|_{\mathcal{H}} \leq 3\|f^*\|_{\mathcal{H}}$. By adding and subtracting terms, we have

$$\begin{aligned} T &= \left[\frac{1}{n} \sum_{i=1}^n \rho_{\tau_n}(x_i) \left\{ (f^*(x_i) - y_i)^2 - (\tilde{f}(x_i) - y_i)^2 \right\} + \|\tilde{f} - f^*\|_Q^2 \right] - \|\tilde{f} - f^*\|_Q^2 + \lambda \|f^*\|_{\mathcal{H}}^2 - \lambda \|\tilde{f}\|_{\mathcal{H}}^2 \\ &\stackrel{(i)}{\leq} \mathcal{M}(\delta_\lambda) - \delta_\lambda^2 + \lambda \|f^*\|_{\mathcal{H}}^2 \stackrel{(ii)}{<} -\frac{1}{2}\delta_\lambda^2 + \lambda \|f^*\|_{\mathcal{H}}^2 \stackrel{(iii)}{<} 0, \end{aligned}$$

where step (i) follows from conditioning on the event $\mathcal{E}(\delta_\lambda)$, the equality $\|\tilde{f} - f^*\|_Q^2 = \delta_\lambda^2$, and non-positivity of $\lambda \|\tilde{f}\|_{\mathcal{H}}^2$; step (ii) follows from the property $\mathcal{M}(\delta_\lambda) \leq (1/2) \cdot \delta_\lambda^2$ and step (iii) uses the definitions of δ_λ and λ .

Case 2: $\|\tilde{f} - f^*\|_Q \leq \delta_\lambda$, while $\|\tilde{f} - f^*\|_{\mathcal{H}} = 3\|f^*\|_{\mathcal{H}}$. By the same addition and subtraction as above, we have

$$\begin{aligned} T &= \left[\frac{1}{n} \sum_{i=1}^n \rho_{\tau_n}(x_i) \left\{ (f^*(x_i) - y_i)^2 - (\tilde{f}(x_i) - y_i)^2 \right\} + \|\tilde{f} - f^*\|_Q^2 \right] - \|\tilde{f} - f^*\|_Q^2 + \lambda \|f^*\|_{\mathcal{H}}^2 - \lambda \|\tilde{f}\|_{\mathcal{H}}^2 \\ &\stackrel{(i)}{\leq} \mathcal{M}(\delta_\lambda) + \lambda \|f^*\|_{\mathcal{H}}^2 - \lambda \|\tilde{f}\|_{\mathcal{H}}^2 \\ &\stackrel{(ii)}{<} \frac{1}{2}\delta_\lambda^2 - 3\lambda \|f^*\|_{\mathcal{H}}^2, \end{aligned}$$

Here, step (i) again follows from the conditioning on the event $\mathcal{E}(\delta_\lambda)$ and the assumption that $\|\tilde{f} - f^*\|_Q \leq \delta_\lambda$. Step (ii) relies on the facts that property $\mathcal{M}(\delta_\lambda) \leq (1/2) \cdot \delta_\lambda^2$, $\|f^*\|_{\mathcal{H}} = \|f^*\|_{\mathcal{H}}$, and that $\|\tilde{f}\|_{\mathcal{H}} \geq 2\|f^*\|_{\mathcal{H}}$. The latter is a simple consequence of $\|\tilde{f} - f^*\|_{\mathcal{H}} = 3\|f^*\|_{\mathcal{H}}$ and the triangle inequality. Substitute in the definitions of δ_λ and λ to see the negativity of T .

Combine the two cases to finish the proof of the claim (34).

5.2.1 Proof of Lemma 2

Define the shifted function class $\mathcal{F}^\star := \mathcal{H} - f^\star$, along with its r -localized version

$$\mathcal{F}^\star(r) := \{h \in \mathcal{F}^\star \mid \|h\|_Q \leq r, \quad \text{and} \quad \|h\|_{\mathcal{H}} \leq 3\|f^\star\|_{\mathcal{H}}\}.$$

We begin by observing that

$$(f^\star(x_i) - y_i)^2 - (g(x_i) - y_i)^2 = 2w_i[g(x_i) - f^\star(x_i)] - (g(x_i) - f^\star(x_i))^2,$$

which yields the following equivalent formulation of our claim

$$\sup_{h \in \mathcal{F}^\star(r)} \left\{ \frac{1}{n} \sum_{i=1}^n \left[2w_i \rho_{\tau_n}(x_i) h(x_i) + \|h\|_Q^2 - \rho_{\tau_n}(x_i) h^2(x_i) \right] \right\} \leq \mathcal{M}(r). \quad (35)$$

By the triangle inequality, it suffices to show that $T_1 + T_2 \leq \mathcal{M}(r)$, where

$$T_1 := \sup_{h \in \mathcal{F}^\star(r)} \left| \frac{2}{n} \sum_{i=1}^n w_i \rho_{\tau_n}(x_i) h(x_i) \right|, \quad \text{and} \quad T_2 := \sup_{h \in \mathcal{F}^\star(r)} \left| \frac{1}{n} \sum_{i=1}^n \{ \|h\|_Q^2 - \rho_{\tau_n}(x_i) h^2(x_i) \} \right|.$$

More precisely, the core of our proof involves establishing the following two bounds:

$$T_1 \leq c\sigma \sqrt{\frac{V^2 \log^3(n)}{n}} \left\{ \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^\star\|_{\mathcal{H}}^2\} \right\}^{1/2} \quad \text{with probability at least } 1 - n^{-10}, \quad \text{and} \quad (36a)$$

$$T_2 \leq c\sqrt{\frac{V^2 \log^3(n)}{n}} \cdot \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^\star\|_{\mathcal{H}}^2\} \quad \text{with probability at least } 1 - n^{-10}. \quad (36b)$$

In conjunction, these two bounds ensure that

$$T_1 + T_2 \leq c\sqrt{\frac{V^2 \log^3(n)}{n}} \cdot \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^\star\|_{\mathcal{H}}^2\} + c\sqrt{\sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^\star\|_{\mathcal{H}}^2\} \frac{V^2 \log^3(n)}{n} \sigma^2}. \quad (37)$$

Since the kernel function is κ^2 -bounded, we have $\sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^\star\|_{\mathcal{H}}^2\} \leq \|f^\star\|_{\mathcal{H}}^2 \sum_{j=1}^{\infty} \mu_j \leq \kappa^2 \|f^\star\|_{\mathcal{H}}^2$, which together with the assumption $\sigma^2 \geq \kappa^2 \|f^\star\|_{\mathcal{H}}^2$ implies that $T_1 + T_2 \leq 2c\sqrt{\sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^\star\|_{\mathcal{H}}^2\} \frac{V^2 \log^3(n)}{n} \sigma^2}$. Therefore the bound (35) holds.

It remains to prove the bounds (36a) and (36b). The proofs make use of some elementary properties of the localized function class $\mathcal{F}^\star(r)$, which we collect here. For any $h \in \mathcal{F}^\star(r)$, we have

$$|h(x)| \leq \sqrt{10 \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^\star\|_{\mathcal{H}}^2\}}, \quad \text{and} \quad (38a)$$

$$\sum_{j=1}^{\infty} \frac{\theta_j^2}{\min\{r^2, \mu_j \|f^\star\|_{\mathcal{H}}^2\}} \leq 10, \quad \text{where } h = \sum_{j=1}^{\infty} \theta_j \phi_j. \quad (38b)$$

See Appendix C for the proof of these elementary claims.

5.2.2 Proof of inequality (36b)

We begin by analyzing the term T_2 . By the triangle inequality, we have the upper bound $T_2 \leq T_{2a} + T_{2b}$, where

$$T_{2a} := \sup_{h \in \mathcal{F}^\star(r)} \left| \|h\|_Q^2 - \mathbb{E}_P[\rho_{\tau_n}(X) h^2(X)] \right|, \quad \text{and}$$

$$T_{2b} := \sup_{h \in \mathcal{F}^*(r)} \left| \mathbb{E}_P[\rho_{\tau_n}(X)h^2(X)] - \frac{1}{n} \sum_{i=1}^n \rho_{\tau_n}(x_i)h^2(x_i) \right|.$$

Note that T_{2a} is a deterministic quantity, measuring the bias induced by truncation, whereas T_{2b} is the supremum of an empirical process. We split our proof into analysis of these two terms. In particular, we establish the following bounds:

$$T_{2a} \leq c \sqrt{\frac{V^2}{n}} \sum_{j=1}^{\infty} \min\{r^2, \mu_j\}, \quad \text{and} \quad (39a)$$

$$T_{2b} \leq c \sqrt{\frac{V^2 \log^2(n)}{n}} \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\} \quad \text{with probability at least } 1 - n^{-10}. \quad (39b)$$

Combining these two bounds yields the claim (36b).

Proof of inequality (39a): We begin by proving the claimed upper bound on T_{2a} . Note that

$$\begin{aligned} T_{2a} &\leq \sup_{h \in \mathcal{F}^*(r)} \left| \|h\|_Q^2 - \mathbb{E}_Q[\mathbb{1}\{\rho(X) \leq \tau_n\} h^2(X)] \right| = \sup_{h \in \mathcal{F}^*(r)} \mathbb{E}_Q \left[\mathbb{1}\{\rho(X) > \tau_n\} h^2(X) \right] \\ &\leq \mathbb{E}_Q \left[\mathbb{1}\{\rho(X) > \tau_n\} \right] \cdot \sup_{h \in \mathcal{F}^*(r)} \|h\|_{\infty}^2 \\ &\leq \frac{V^2}{\tau_n} \cdot 10 \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}, \end{aligned}$$

where the last step follows from a combination of Markov's inequality and the ℓ_{∞} -norm bound (38a). Recalling that $\tau_n = \sqrt{nV^2}$, the bound (39a) follows.

Proof of the bound (39b): We prove the claimed bound on T_{2b} by first bounding its mean $\mathbb{E}[T_{2b}]$, and then providing a high-probability bound on the deviation $T_{2b} - \mathbb{E}[T_{2b}]$.

Bound on the mean: By a standard symmetrization argument (see e.g., Chapter 4 in the book [21]), we have the upper bound

$$\mathbb{E}[T_{2b}] \leq \frac{2}{n} \mathbb{E} \left[\sup_{h \in \mathcal{F}^*(r)} \left| \sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) h^2(x_i) \right| \right],$$

where $\{\varepsilon_i\}_{i=1}^n$ is an i.i.d. sequence of Rademacher variables. Now observe that

$$\sup_{h \in \mathcal{F}^*(r)} \left| \sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) h^2(x_i) \right| \leq \sup_{\tilde{h}, h \in \mathcal{F}^*(r)} Z(h, \tilde{h}), \quad \text{where } Z(h, \tilde{h}) := \left| \sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) \tilde{h}(x_i) h(x_i) \right|.$$

Writing $\tilde{h} = \sum_{j=1}^{\infty} \tilde{\theta}_j \phi_j$, we have

$$\begin{aligned} Z(h, \tilde{h}) &= \left| \sum_{j=1}^{\infty} \tilde{\theta}_j \left\{ \sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) \phi_j(x_i) h(x_i) \right\} \right| \\ &\leq \left| \sum_{j=1}^{\infty} \frac{\tilde{\theta}_j}{\sqrt{\min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}}} \cdot \sqrt{\min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}} \left\{ \sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) \phi_j(x_i) h(x_i) \right\} \right| \\ &\leq \sqrt{10} \left\{ \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\} \cdot \left\{ \sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) \phi_j(x_i) h(x_i) \right\}^2 \right\}^{1/2}, \end{aligned}$$

where the final step follows by combining the Cauchy–Schwarz inequality with the bound (38b). We now repeat the same argument to upper bound the inner term involving h ; in particular, we have

$$\begin{aligned} \left\{ \sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) \phi_j(x_i) h(x_i) \right\}^2 &= \left\{ \sum_{k=1}^{\infty} \theta_k \left(\sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) \phi_j(x_i) \phi_k(x_i) \right) \right\}^2 \\ &\leq 10 \cdot \sum_{k=1}^{\infty} \min\{r^2, \mu_k \|f^*\|_{\mathcal{H}}^2\} \left(\sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) \phi_j(x_i) \phi_k(x_i) \right)^2. \end{aligned}$$

Putting together the pieces now leads to the upper bound

$$\begin{aligned} \frac{2}{n} \sup_{h \in \mathcal{F}^*(r)} \left| \sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) h^2(x_i) \right| &\leq \frac{2}{n} \sup_{h, \tilde{h} \in \mathcal{F}^*(r)} Z(h, \tilde{h}) \\ &\leq \frac{20}{n} \left\{ \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\} \cdot \sum_{k=1}^{\infty} \min\{r^2, \mu_k \|f^*\|_{\mathcal{H}}^2\} \left(\sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) \phi_j(x_i) \phi_k(x_i) \right)^2 \right\}^{1/2}. \end{aligned}$$

By taking expectations of both sides and applying Jensen’s inequality, we find that

$$\mathbb{E}[T_{2b}] \leq \frac{20}{n} \left\{ \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\} \cdot \sum_{k=1}^{\infty} \min\{r^2, \mu_k \|f^*\|_{\mathcal{H}}^2\} \mathbb{E}_{X, \varepsilon} \left(\sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) \phi_j(x_i) \phi_k(x_i) \right)^2 \right\}^{1/2}. \quad (40)$$

We now observe that

$$\begin{aligned} \mathbb{E}_{X, \varepsilon} \left[\left(\sum_{i=1}^n \varepsilon_i \rho_{\tau_n}(x_i) \phi_j(x_i) \phi_k(x_i) \right)^2 \right] &= \sum_{i=1}^n \mathbb{E}_{X, \varepsilon} \left[\varepsilon_i^2 \rho^2(x_i) \mathbb{1}\{\rho(x_i) \leq \tau_n\} \phi_j^2(x_i) \phi_k^2(x_i) \right] \\ &\leq \sum_{i=1}^n \mathbb{E}_{X, \varepsilon} [\rho^2(x_i)] \leq nV^2, \end{aligned}$$

where we have used the fact that $\|\phi_j\|_{\infty} \leq 1$ for all $j \geq 1$. Substituting this upper bound into our earlier inequality (40) yields

$$\mathbb{E}[T_{2b}] \leq 20 \sqrt{\frac{V^2}{n}} \cdot \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}. \quad (41)$$

Bounding the deviation term: Recall that for any $h \in \mathcal{F}^*$, we have $\|h\|_{\infty} \leq \sqrt{10 \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}}$. Consequently, we have

$$\begin{aligned} \sup_{h \in \mathcal{F}^*(r)} \left| \mathbb{E}_Q[\mathbb{1}\{\rho(X) \leq \tau_n\} h^2(X)] - \rho_{\tau_n}(x_i) h^2(x_i) \right| &\leq 10 \tau_n \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\} \\ &= 10 \sqrt{nV^2} \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}. \end{aligned}$$

In addition, we have

$$\begin{aligned} \sup_{h \in \mathcal{F}^*(r)} \sum_{i=1}^n \mathbb{E} \left[\left\{ \mathbb{E}_Q[\mathbb{1}\{\rho(X) \leq \tau_n\} h^2(X)] - \rho_{\tau_n}(x_i) h^2(x_i) \right\}^2 \right] &\leq \sup_{h \in \mathcal{F}^*(r)} \sum_{i=1}^n \mathbb{E} [\rho^2(x_i) \mathbb{1}\{\rho(x_i) \leq \tau_n\} h^4(x_i)] \\ &\leq 100nV^2 \left(\sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\} \right)^2, \end{aligned}$$

where we have applied the ℓ_∞ -norm bound (38a) as well as the V^2 -condition on the likelihood ratio. These two facts together allow us to apply Talagrand's concentration results (cf. Lemma 9) and obtain

$$\mathbb{P}\left[T_{2b} \geq \mathbb{E}[T_{2b}] + \frac{t}{n}\right] \leq \exp\left(-\frac{t^2}{3000nV^2\left(\sum_{j=1}^{\infty} \min\{r^2, \mu_j\|f^\star\|_{\mathcal{H}}^2\}\right)^2 + 900\sqrt{nV^2}\sum_{j=1}^{\infty} \min\{r^2, \mu_j\|f^\star\|_{\mathcal{H}}^2\}t}\right). \quad (42)$$

Completing the proof of the bound (39b): We now have the ingredients to complete the proof of the claim (39b). In particular, by combining the upper bound (41) on the mean with the deviation bound (42), we find that

$$T_{2b} \leq c\sqrt{\frac{V^2 \log^2(n)}{n}} \sum_{j=1}^{\infty} \min\{r^2, \mu_j\|f^\star\|_{\mathcal{H}}^2\} \quad \text{with probability at least } 1 - n^{-10},$$

as claimed in equation (39b).

5.2.3 Proof of inequality (36a)

Now we focus on the first term $T_1 = \sup_{h \in \mathcal{F}^\star(r)} \left| \frac{1}{n} \sum_{i=1}^n w_i \rho_{\tau_n}(x_i) h(x_i) \right|$. Define the truncated noise variables $\tilde{w}_i := w_i \mathbb{1}\{|w_i| \leq 5\sigma\sqrt{\log n}\}$. By sub-Gaussian concentration, we have $w_i = \tilde{w}_i$ for all $i = 1, 2, \dots, n$ with probability at least $1 - n^{-12}$. Hence, we have

$$\sup_{h \in \mathcal{F}^\star(r)} \left| \frac{1}{n} \sum_{i=1}^n w_i \rho_{\tau_n}(x_i) h(x_i) \right| = Z := \sup_{h \in \mathcal{F}^\star(r)} \left| \frac{1}{n} \sum_{i=1}^n \tilde{w}_i \rho_{\tau_n}(x_i) h(x_i) \right|$$

with the same probability. Thus, it suffices to control the random variable Z . As before, we first control the mean $\mathbb{E}[Z]$ and then the deviation $Z - \mathbb{E}[Z]$.

Bounding the mean: In terms of the basis expansion $h = \sum_{j=1}^{\infty} \theta_j \phi_j$, we have

$$Z = \sup_{h \in \mathcal{F}^\star(r)} \left| \sum_{j=1}^{\infty} \theta_j \left\{ \sum_{i=1}^n \tilde{w}_i \rho_{\tau_n}(x_i) \phi_j(x_i) \right\} \right| \leq \left\{ 10 \sum_{j=1}^{\infty} \min\{r^2, \mu_j\|f^\star\|_{\mathcal{H}}^2\} \cdot \left[\sum_{i=1}^n \tilde{w}_i \rho_{\tau_n}(x_i) \phi_j(x_i) \right]^2 \right\}^{1/2},$$

where we have followed the same argument used in the proof of the bound (39b). Taking expectations on both sides and applying Jensen's inequality yields

$$\begin{aligned} \mathbb{E}[Z] &\leq \frac{1}{n} \left\{ 10 \sum_{j=1}^{\infty} \min\{r^2, \mu_j\|f^\star\|_{\mathcal{H}}^2\} \cdot \mathbb{E} \left[\sum_{i=1}^n \tilde{w}_i \rho_{\tau_n}(x_i) \phi_j(x_i) \right]^2 \right\}^{1/2} \\ &\leq \left\{ 10 \sum_{j=1}^{\infty} \min\{r^2, \mu_j\|f^\star\|_{\mathcal{H}}^2\} \cdot \sum_{i=1}^n \mathbb{E} \left[\tilde{w}_i^2 \rho^2(x_i) \mathbb{1}\{\rho(x_i) \leq \tau_n\} \phi_j^2(x_i) \right] \right\}^{1/2} \\ &\leq \sqrt{10 \sum_{j=1}^{\infty} \min\{r^2, \mu_j\|f^\star\|_{\mathcal{H}}^2\} n V^2 \sigma^2}. \end{aligned} \quad (43)$$

Bound on the deviation $Z - \mathbb{E}[Z]$: Recalling the definition of the truncated noise variables $\tilde{w}_i = w_i \mathbb{1}\{|w_i| \leq 5\sigma\sqrt{\log n}\}$, we begin with the sup-norm bound

$$\sup_{h \in \mathcal{F}^\star(r)} \left| \tilde{w}_i \rho_{\tau_n}(x_i) h(x_i) \right| \leq 5\sigma\sqrt{\log n} \cdot \tau_n \sqrt{10 \sum_{j=1}^{\infty} \min\{r^2, \mu_j\|f^\star\|_{\mathcal{H}}^2\}}$$

$$= 5\sigma\sqrt{\log n} \cdot \sqrt{nV^2} \sqrt{10 \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}}.$$

We have the variance bound

$$\begin{aligned} \frac{1}{n} \sup_{h \in \mathcal{F}^*(r)} \sum_{i=1}^n \mathbb{E} \left[\left(\tilde{w}_i \rho_{\tau_n}(x_i) h(x_i) \right)^2 \right] &\leq \sup_{h \in \mathcal{F}^*(r)} \mathbb{E} \left[\tilde{w}_i^2 \rho^2(x_i) \mathbb{1}_{\{\rho(x_i) \leq \tau_n\}} h^2(x_i) \right] \\ &\leq 10V^2\sigma^2 \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}, \end{aligned}$$

where we again used the ℓ_∞ -norm bound (38a). Applying Talagrand's inequality (cf. Lemma 9) guarantees that

$$Z \leq \mathbb{E}[Z] + c \sqrt{\frac{\log^3(n)}{n}} \sqrt{V^2\sigma^2 \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}}. \quad (44)$$

for a universal constant c .

Completing the proof: We now substitute the upper bound on the mean (43) into the tail bound (44) to conclude that

$$Z \leq c \left\{ \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\} \frac{V^2 \log^3(n)}{n} \sigma^2 \right\}^{1/2}$$

with probability exceeding $1 - n^{-11}$. From our earlier analysis, the random variable Z is equal to T_1 with probability at least $1 - n^{-12}$, so that we conclude that the same bound applies to T_1 with probability at least $1 - n^{-10}$. This completes the proof of the claimed bound (36a).

6 Discussion

In this paper, we study RKHS-based non-parametric regression under covariate shift. In particular, we focus on two broad families of covariate shift problems: (1) the uniformly B -bounded family, and (2) the χ^2 -bounded family. For the uniformly B -bounded family, we prove that the unweighted KRR estimate—with properly chosen regularization parameter—achieves optimal rate convergence for a large family of RKHSs with regular eigenvalues. In contrast, the naïve constrained kernel regression estimator is provably suboptimal under covariate shift. In addition, for the χ^2 -bounded family, we demonstrate via careful simulations that unweighted KRR is suboptimal, and to remedy this, we propose a likelihood-ratio-reweighted KRR with proper truncation that attains the minimax lower bound over this larger family of covariate shift problems.

Our study is an initial step towards understanding the statistical nature of covariate shift. Below we single out several interesting directions to pursue in the future. First, it is of great importance to extend the study to other classes of regression functions, e.g., high dimensional linear regression, decision trees, etc. Second, while it is natural to measure discrepancy between source-target pairs using likelihood ratio, this is certainly not the only possibility. Various measures of discrepancy have been proposed in the literature, and it is interesting to see what the corresponding optimal procedures are. Lastly, on a technical end, it is also interesting to see whether one can remove the uniform boundedness of the eigenfunctions in the unbounded likelihood ratio case, and retain the optimal rate of convergence.

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A Proof of Theorem 2

Let δ_n be the smallest positive solution to the inequality $c'\sigma^2 B \frac{d(\delta)}{n} \leq \delta^2$, where $c' > 0$ is some large constant. We decompose the proof into two steps. First, we construct the lower bound instance, namely the source, target distributions, and the corresponding orthonormal basis. Second, we apply the Fano method to prove the lower bound.

Step 1: Constructing the lower bound instance. Let Q be a uniform distribution on $\{\pm 1\}^{+\infty}$. For the source distribution P , we set it as follows: with probability $1/B$, we sample x uniformly on $\{\pm 1\}^{+\infty}$, and with probability $1 - 1/B$, we set $x = 0$. It can be verified that the pair (P, Q) has B -bounded likelihood ratio. Corresponding to the target distribution Q , we take $\phi_j(x) = x_j$ for every $j \geq 1$. In other words, we consider a linear kernel.

Step 2: Establishing the lower bound. In order to apply Fano’s method, we first need to construct a packing set of the function class $\mathcal{B}_{\mathcal{H}}(1)$. For a given radius $r > 0$, consider the r -localized ellipse

$$\mathcal{E}(r) := \left\{ \theta \mid \sum_{j=1}^{\infty} \frac{\theta_j^2}{\min\{r^2, \mu_j\}} \leq 1 \right\}.$$

It is straightforward to check that for any $\theta \in \mathcal{E}(r)$, the function $f = \sum_{j=1}^{\infty} \theta_j \phi_j$ lies in $\mathcal{B}_{\mathcal{H}}(1)$. This set $\mathcal{E}(r)$ admits a large packing set in the ℓ_2 -norm, as claimed in the following lemma.

Lemma 3. *For any $r \in (0, \delta_n]$, there exists a set $\{\theta^1, \theta^2, \dots, \theta^M\} \subseteq \mathcal{E}(r)$ with $\log M = d_n/64$ such that*

$$\|\theta^j - \theta^k\|_2^2 \geq \frac{r^2}{4} \quad \text{for any distinct pair of indices } j \neq k.$$

See Lemma 4 in the paper [22].

Having constructed the packing, we then need to control the pairwise KL divergence. Fix an index $j \in [M]$. Let $P \times \mathcal{L}_j$ denote the joint distribution over the observed data $\{(x_i, y_i)\}_{1 \leq i \leq n}$ when the true function arises from θ^j . Then for any pair of distinct indices $j \neq k$, we have the upper bound

$$\begin{aligned} \text{KL}(P \times \mathcal{L}_j \| P \times \mathcal{L}_k) &= \frac{n}{2\sigma^2} \cdot \mathbb{E}_{X \sim P} \left[((\theta^j - \theta^k)^\top \phi(X))^2 \right] \stackrel{(i)}{=} \frac{n}{2\sigma^2 B} \|\theta^j - \theta^k\|_2^2 \\ &\stackrel{(ii)}{\leq} \frac{2nr^2}{\sigma^2 B}, \end{aligned}$$

where step (i) follows from the definition of P ; and step (ii) follows from applying the triangle inequality, and the fact that $\|\theta\|_2 \leq r$ for all $\theta \in \mathcal{E}(r)$.

Consequently, we arrive at the lower bound $\inf_{\hat{f}} \sup_{f^* \in \mathcal{F}} \mathbb{E}[\|\hat{f} - f^*\|_Q^2] \geq \frac{r^2}{8}$, valid for any sample size satisfying the condition

$$\frac{2nr^2}{\sigma^2 B} + \log 2 \leq \frac{1}{2} \log M = \frac{d_n}{128}. \quad (45)$$

By the definition of a regular kernel, we have $d_n \geq c \frac{n\delta_n^2}{B\sigma^2}$ for a universal constant c . Furthermore, since δ_n satisfies the lower bound $\delta_n^2 \geq c' \frac{\sigma^2 B}{n}$, the condition (45) is met by setting $r^2 = c_1 \delta_n^2$ for some sufficiently small constant $c_1 > 0$.

B Proof of Theorem 3

Let the sample size $n \geq 1$ and likelihood ratio bound $B \geq 1$ be given. Our failure instance relies on a function class \mathcal{F}_n , together with a pair of distributions (P, Q) . The function class \mathcal{F}_n is the unit ball of a RKHS with finite-rank kernel, over the hypercube $\{-1, +1\}^n$. The kernel is given by $\mathcal{K}(x, z) := \sum_{j=1}^n \mu_j \phi_j(x) \phi_j(z)$. The eigenfunctions and eigenvalues are

$$\phi_j(x) = x_j, \quad \text{and} \quad \mu_j = \frac{1}{j^2}, \quad \text{for } j = 1, \dots, n.$$

To be clear, the function class is given by

$$\mathcal{F}_n := \left\{ f := \sum_{j=1}^n \theta_j \phi_j \mid \sum_{j=1}^n \frac{\theta_j^2}{\mu_j} \leq 1 \right\}.$$

The target distribution, Q , is the uniform distribution on $\{-1, +1\}^n$. The source distribution is a product distribution, $P = \otimes_{j=1}^n P_j$. We take P_j to be uniform on $\{+1, -1\}$, when $j > 1$. On the other hand, the first coordinate follows the distribution

$$P_1 := \left(1 - \frac{1}{B}\right) \delta_0 + \frac{1}{B} \text{Unif}(\{-1, +1\}).$$

It is immediate that (P, Q) have B -bounded likelihood ratio.

Given this set-up, our first step is to reduce the lower bound to the separation of a single coordinate of the parameter associated with the empirical risk minimizer and a single coordinate of the parameter associated with a hard instance in the function class of interest \mathcal{F}_n . We introduce a one-dimensional minimization problem that governs this separation problem and allows us to establish our result.

B.1 Reduction to a one dimensional separation problem

To establish our lower bound it suffices to consider the following “hard” function

$$f_{\text{hard}}^*(x) = x_1 = \sum_{j=1}^n (\theta_{\text{hard}}^*)_j \phi_j(x), \quad \text{where } \theta_{\text{hard}}^* = (1, 0, \dots, 0) \in \mathbb{R}^n.$$

Since $\phi_j(x) = x_j$ and $\mu_j = j^{-2}$, it follows that $f_{\text{hard}}^* \in \mathcal{F}_n$. We can write $\hat{f}_{\text{erm}}(x) = \sum_{j=1}^n (\hat{\theta}_{\text{erm}})_j x_j$, where we defined

$$\hat{\theta}_{\text{erm}} := \arg \min \left\{ \sum_{i=1}^n \left(\sum_{j=1}^n \theta_j x_{ij} - y_i \right)^2 \mid \sum_{j=1}^n \frac{\theta_j^2}{\mu_j} \leq 1 \right\}. \quad (46)$$

Putting these pieces together, we see that

$$\sup_{f^* \in \mathcal{F}_n} \mathbb{E} \left[\|\hat{f}_{\text{erm}} - f^*\|_Q^2 \right] \geq \mathbb{E} \left[\|\hat{f}_{\text{erm}} - f_{\text{hard}}^*\|_Q^2 \right] \stackrel{(i)}{=} \mathbb{E} \left[\|\hat{\theta}_{\text{erm}} - \theta_{\text{hard}}^*\|_2^2 \right] \stackrel{(ii)}{\geq} \mathbb{E} \left[((\hat{\theta}_{\text{erm}})_1 - \theta_1^*)^2 \right]. \quad (47)$$

Above, the relation (i) is a consequence of Parseval’s theorem, along with the orthonormality of $\{\phi_j\}_{j=1}^n$ in $L^2(Q)$. Inequality (ii) follows by dropping terms corresponding to indices $j > 1$. Therefore, in view of display (47), it suffices to show that:

$$\mathbb{P} \left\{ ((\hat{\theta}_{\text{erm}})_1 - 1)^2 \geq c_3 \frac{B^3}{n^2} \right\} \geq \frac{1}{2}. \quad (48)$$

B.2 Proof of one-dimensional separation bound (48)

We begin with a proof outline.

Proof outline To establish (48), we can assume $(\hat{\theta}_{\text{erm}})_1 \in [0, 1]$; otherwise, the lower bound follows trivially, provided c_2 is sufficiently small, in particular, $c_2 \leq \sqrt[3]{1/c_3}$. We introduce a bit of notation:

$$\hat{\Sigma}_P := \frac{1}{n} \sum_{i=1}^n x_i x_i^\top \quad \text{and} \quad v := \frac{1}{n} \sum_{i=1}^n w_i x_i.$$

Thus, we can further restrict the empirical risk minimization problem (46) to

$$\begin{aligned} \tilde{\theta} &:= \arg \min \left\{ \sum_{i=1}^n \left(\sum_{j=1}^n \theta_j x_{ij} - y_i \right)^2 \mid \sum_{j=1}^n \frac{\theta_j^2}{\mu_j} \leq 1, \quad \theta_1 \in [0, 1] \right\} \\ &= \arg \min \left\{ (\theta - \theta^*)^T \hat{\Sigma}_P (\theta - \theta^*) - 2v^T (\theta - \theta^*) \mid \sum_{j=1}^n \frac{\theta_j^2}{\mu_j} \leq 1, \quad \theta_1 \in [0, 1] \right\}. \end{aligned} \quad (49)$$

Indeed, in order to prove inequality (48), it suffices to show that

$$\mathbb{P} \left\{ (\tilde{\theta}_1 - 1)^2 \geq c_3 \frac{B^3}{n^2} \right\} \geq \frac{1}{2}. \quad (50)$$

Let us define an auxiliary function $g: [0, 1] \rightarrow \mathbb{R}$, given by

$$g(t) := \inf \left\{ (\theta - \theta^*)^T \hat{\Sigma}_P (\theta - \theta^*) - 2v^T (\theta - \theta^*) \mid \sum_{j=1}^n \frac{\theta_j^2}{\mu_j} \leq 1, \quad \theta_1 = t \right\}. \quad (51)$$

By definition (49), the choice $\tilde{\theta}$ minimizes this objective, and therefore $\inf_{t \in [0, 1]} g(t) = g(\tilde{\theta}_1)$. The next two lemmas concern the minimum value and minimizer of g . Lemma 4, which we prove in section B.4.1, bounds the minimal value from above. Lemma 5, demonstrates that there is an interval of length order $\sqrt{B^3/n^2}$ on which the function g is bounded away from the minimal value. We prove this result in Section B.4.2.

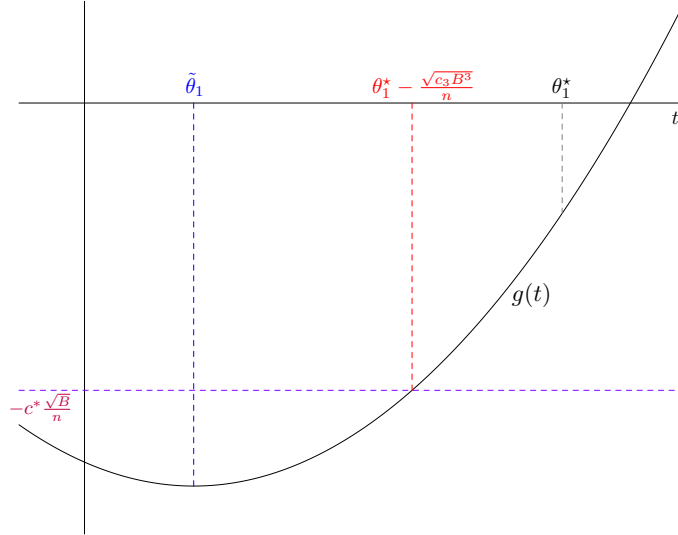


Figure 4. Pictorial representation of lower bound argument, separating the first coordinate of empirical risk minimizer, $\tilde{\theta}_1$, from the true population minimizer θ_1^* . Lemma 4 establishes the upper bound, depicted in purple above, on the minimal value of g . Lemma 5 establishes an interval, shown between the red dashed line and θ_1^* above, which excludes $\tilde{\theta}_1$. This allows us to ensure that θ_1^* and $\tilde{\theta}_1$ are sufficiently separated.

Lemma 4 (Minimal value of empirical objective). *There is a constant $c^* > 0$ such that*

$$g(\tilde{\theta}_1) \leq -c^* \frac{\sqrt{B}}{n}$$

holds with probability at least 3/4.

Lemma 5 (Separation from θ_1^*). *There exists a constant $c_3 > 0$ such that*

$$\inf_{\substack{t \in [0,1] \\ (1-t)^2 \leq c_3 B^3/n^2}} g(t) > -c^* \frac{\sqrt{B}}{n}. \quad (52)$$

where probability at least $3/4$.

Note that the constant c^* used in Lemmas 4 and 5 is the same. Thus—after union bounding over the two error events—with probability at least $1/2$,

$$g(\tilde{\theta}_1) < \inf_{\substack{t \in [0,1] \\ (1-t)^2 \leq c_3 B^3/n^2}} g(t).$$

Recalling that $\tilde{\theta}_1 \in [0, 1]$, we conclude on this event that $(1 - \tilde{\theta}_1)^2 \geq c_3 \frac{B^3}{n^2}$, which furnishes (50), and thereby establishes the required result. To complete the proof, it then remains to establish the auxiliary lemmas stated above. Before doing so, we record a useful lemma, which will be used multiple times later.

B.3 A useful lemma

Lemma 6. *For any quantity $\alpha \in (\frac{B}{4n^2}, \frac{B}{4})$, with probability at least $1 - c_1 \exp(-c_2 \frac{B^{1/2}}{\alpha^{1/2}})$, one has*

$$c \frac{B^{1/2}}{\alpha^{1/2}} \frac{1}{n} \leq \sum_{j=2}^n \frac{(v_j)^2}{1 + \frac{\alpha}{B\mu_j}} \leq C \frac{B^{1/2}}{\alpha^{1/2}} \frac{1}{n}.$$

Here $c_1, c_2, C, c > 0$ are absolute constants.

Proof. For each $j \geq 1$, define $\eta_j := (1 + \frac{\alpha}{B\mu_j})^{-1}$. We focus on controlling the term

$$\sum_{j=2}^n \eta_j [(\sqrt{n}v_j)^2 - 1].$$

Recall from the definition of v that $v_j = \frac{1}{n} \sum_{i=1}^n w_i x_{ij}$. Under the construction of the lower bound instance, we have $\sqrt{n}v_j \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1)$. Therefore $(\sqrt{n}v_j)^2 - 1$ is a mean-zero sub-exponential random variable. This allows us to invoke Bernstein's inequality to obtain

$$\mathbb{P} \left(\left| \sum_{j=2}^n \eta_j [(\sqrt{n}v_j)^2 - 1] \right| \geq t \right) \leq 2 \exp \left\{ -c \min \left(\frac{t^2}{\sum_{j \geq 2} \eta_j^2}, \frac{t}{\max_j \eta_j} \right) \right\},$$

where $c > 0$ is some universal constant.

We claim that there exist three constants $C_1, C_2, C_3 > 0$ such that

$$\max_{j=2, \dots, n} \eta_j \leq 1; \quad (53a)$$

$$\sum_{j=2}^n \eta_j^2 \leq C_1 \frac{B^{1/2}}{\alpha^{1/2}}; \quad (53b)$$

$$C_2 \frac{B^{1/2}}{\alpha^{1/2}} \leq \sum_{j=2}^n \eta_j \leq C_3 \frac{B^{1/2}}{\alpha^{1/2}}. \quad (53c)$$

As a result, we can $t = c_0 \frac{B^{1/2}}{\alpha^{1/2}}$ with c_0 sufficiently small to arrive at the desired conclusion.

We are left with proving the claimed relations (53). The first relation (53a) is trivial. We provide the proof of the third inequalities (53c); the proof of the middle one (cf. relation (53b)) follows by a similar argument. Since $\alpha \in (\frac{B}{4n^2}, \frac{B}{4})$, we can decompose the sum into

$$\sum_{j=2}^n \eta_j = \sum_{j=2}^{\lfloor \sqrt{B/\alpha} \rfloor} \frac{1}{1 + \frac{\alpha}{B\mu_j}} + \sum_{j=\lfloor \sqrt{B/\alpha} \rfloor + 1}^n \frac{1}{1 + \frac{\alpha}{B\mu_j}}.$$

Recall that $\mu_j = j^{-2}$. We thus have $1 \geq \frac{\alpha}{B\mu_j}$ for $j \leq \lfloor \sqrt{B/\alpha} \rfloor$ and $1 \leq \frac{\alpha}{B\mu_j}$ for $j \geq \lfloor \sqrt{B/\alpha} \rfloor$. These allow us to upper bound $\sum_{j=2}^n \eta_j$ as

$$\sum_{j=2}^n \eta_j \leq \lfloor \sqrt{B/\alpha} \rfloor + \frac{B}{\alpha} \sum_{j=\lfloor \sqrt{B/\alpha} \rfloor + 1}^n \frac{1}{j^2} \leq C_3 \frac{B^{1/2}}{\alpha^{1/2}}.$$

Similarly, we have the lower bound

$$\sum_{j=2}^n \eta_j \geq \sum_{j=2}^{\lfloor \sqrt{B/\alpha} \rfloor} \frac{1}{1 + \frac{\alpha}{B\mu_j}} \geq \frac{1}{2} \lfloor \sqrt{B/\alpha} \rfloor \geq C_2 \frac{B^{1/2}}{\alpha^{1/2}}.$$

This finishes the proof. \square

B.4 Proof of auxiliary lemmas

In order to facilitate the proofs of these lemmas, it is useful to decompose $\theta = (\theta_1, \theta_R) \in \mathbb{R} \times \mathbb{R}^{n-1}$. Additionally, we consider the constraint set

$$\mathcal{C}(t) := \left\{ \theta_R \in \mathbb{R}^{n-1} \mid \sum_{j=2}^n \frac{\theta_j^2}{\mu_j} \leq 1 - t^2 \right\}, \quad \text{where } t \in [0, 1].$$

This set plays a key role. In view of definition (51), we can write

$$g(t) = \inf_{\theta_R \in \mathcal{C}(t)} \left\{ \begin{bmatrix} t-1 \\ \theta_R \end{bmatrix}^\top \widehat{\Sigma}_P \begin{bmatrix} t-1 \\ \theta_R \end{bmatrix} - 2 \begin{bmatrix} t-1 \\ \theta_R \end{bmatrix}^\top v \right\}, \quad (54)$$

where above we have used $\theta^* = (1, 0, \dots, 0)$. Finally, we will use the diagonal matrix of kernel eigenvalues $\mathbf{M} := \text{diag}(\mu_1, \mu_2, \dots, \mu_n)$, repeatedly.

B.4.1 Proof of Lemma 4

We show that with probability at least $3/4$,

$$g(\omega) \leq -c^* \frac{\sqrt{B}}{n}, \quad \text{where } \omega := \sqrt{1 - \frac{B^{3/2}}{n}}. \quad (55)$$

When $n^2 \geq B^3$, we have $\omega \in [0, 1]$. Since $\inf_{t \in [0, 1]} g(t) \leq g(\omega)$, the display (55) implies the result.

Proof of bound (55): From the proof of Lemma 1, if we set $\lambda := C \frac{\log n}{n}$ for some constant $C > 0$, then we have

$$\frac{1}{2}(\Sigma_P + \lambda \mathbf{M}^{-1}) \preceq \widehat{\Sigma}_P + \lambda \mathbf{M}^{-1} \preceq \frac{3}{2}(\Sigma_P + \lambda \mathbf{M}^{-1}), \quad (56)$$

with probability at least $1 - \frac{1}{n}$. Consequently, for any vector θ obeying $\theta^\top \mathbf{M}^{-1} \theta \leq 1$, we have the upper bound

$$(\theta - \theta^*)^\top \widehat{\Sigma}_P (\theta - \theta^*) = (\theta - \theta^*)^\top \left(\widehat{\Sigma}_P + \lambda \mathbf{M}^{-1} \right) (\theta - \theta^*) - \lambda (\theta - \theta^*)^\top \mathbf{M}^{-1} (\theta - \theta^*)$$

$$\begin{aligned}
&\leq \frac{3}{2} (\theta - \theta^\star)^\top (\Sigma_P + \lambda \mathbf{M}^{-1}) (\theta - \theta^\star) - \lambda (\theta - \theta^\star)^\top \mathbf{M}^{-1} (\theta - \theta^\star) \\
&= \frac{3}{2} (\theta - \theta^\star)^\top \Sigma_P (\theta - \theta^\star) + \frac{\lambda}{2} (\theta - \theta^\star)^\top \mathbf{M}^{-1} (\theta - \theta^\star) \\
&\leq \frac{3}{2} (\theta - \theta^\star)^\top \Sigma_P (\theta - \theta^\star) + 2\lambda,
\end{aligned}$$

where the final inequality holds since $(\theta - \theta^\star)^\top \mathbf{M}^{-1} (\theta - \theta^\star) \leq 4$. Applying this result with the vector $\theta = (\omega, \theta_R)^\top$ yields

$$\begin{aligned}
g(\omega) &\leq \min_{\theta_R \in \mathcal{C}} \left\{ \frac{3}{2} \begin{bmatrix} \omega - 1 \\ \theta_R \end{bmatrix}^\top \Sigma_P \begin{bmatrix} \omega - 1 \\ \theta_R \end{bmatrix} - 2 \begin{bmatrix} \omega - 1 \\ \theta_R \end{bmatrix}^\top v + 2\lambda \right\} \\
&= T_1(\omega) + T_2(\omega) + 2\lambda + \min_{\theta_R \in \mathcal{C}} T_3(\theta_R).
\end{aligned} \tag{57}$$

Above, we have defined

$$T_1(\omega) := \frac{3}{2} \frac{(\omega - 1)^2}{B}, \quad T_2(\omega) := -2v_1(\omega - 1), \quad \text{and} \quad T_3(\theta_R) := \frac{3}{2} \|\theta_R\|_2^2 - 2v_R^\top \theta_R, \tag{58}$$

and we have used the decomposition $v = (v_1, v_R)^\top$. We now bound each of these three terms in turn.

Controlling the term $T_1(\omega)$: Recall $\omega \in [0, 1]$ satisfies the equality $1 - \omega^2 = \frac{B^{3/2}}{n}$. Consequently, we have

$$T_1(\omega) = \frac{3}{2} \frac{(1 - \omega)^2}{B} \leq \frac{3}{2} \frac{(1 - \omega^2)^2}{B} = \frac{3}{2} \frac{B^2}{n^2}. \tag{59}$$

Controlling the term $T_2(\omega)$: For the second term, by definition of ω , we have

$$T_2(\omega) = 2v_1(1 - \omega) \leq 2|v_1|(1 - \omega) \leq 2|v_1|(1 - \omega^2) = 2|v_1| \cdot \frac{B^{3/2}}{n}. \tag{60}$$

We have the following lemma to control the size of $|v_1|$.

Lemma 7. *The following holds true with probability at least 0.99*

$$\left| \frac{1}{n} \sum_{i=1}^n w_i x_{i1} \right| \leq \frac{10}{\sqrt{nB}}.$$

Proof. In view of the construction of the lower bound instance, we can calculate

$$\mathbb{E} \left[\left(\frac{1}{n} \sum_{i=1}^n w_i x_{i1} \right)^2 \right] = \frac{1}{n^2} \sum_{i=1}^n \mathbb{E} [w_i^2 x_{i1}^2] = \frac{1}{nB}.$$

The claim then follows from Chebyshev's inequality. \square

Lemma 7 demonstrates that $|v_1| \leq \frac{10}{\sqrt{nB}}$, with probability at least 99/100. Therefore, on this event, the bound (60) guarantees

$$T_2(\omega) \leq 20 \frac{B}{n^{3/2}}. \tag{61}$$

Controlling the term $T_3(\theta_r)$: Our final step is to upper bound the constrained minimum $\min_{\theta_R \in \mathcal{C}} T_3(\theta_R)$. Since this minimization problem is strictly feasible, Lagrange duality guarantees that

$$\begin{aligned} \min_{\theta_R \in \mathcal{C}} T_3(\theta_R) &= \min_{\theta_R} \max_{\xi \geq 0} \left\{ \frac{3}{2} \|\theta_R\|_2^2 - 2v_R^\top \theta_R + \xi(\theta_R^\top M_R^{-1} \theta_R - \frac{B^{3/2}}{n}) \right\} \\ &= \max_{\xi \geq 0} \min_{\theta_R} \left\{ \frac{3}{2} \|\theta_R\|_2^2 - 2v_R^\top \theta_R + \xi(\theta_R^\top M_R^{-1} \theta_R - \frac{B^{3/2}}{n}) \right\}. \end{aligned}$$

The inner minimum is achieved at $\theta_R = [\frac{3}{2} \mathbf{I} + \xi M_R^{-1}]^{-1} v_R$, so that we have established the equality

$$\min_{\theta_R \in \mathcal{C}} T_3(\theta_R) = \max_{\xi \geq 0} \left\{ -\xi \frac{B^{3/2}}{n} - v_R^\top [\frac{3}{2} \mathbf{I} + \xi M_R^{-1}]^{-1} v_R \right\} = \max_{\xi \geq 0} \left\{ -\xi \frac{B^{3/2}}{n} - \sum_{j=2}^n \frac{(v_j)^2}{\frac{3}{2} + \frac{\xi}{\mu_j}} \right\}.$$

It remains to analyze the maximum over the dual variable ξ , and we split the analysis into two cases.

- Case 1: First, suppose that the maximum is achieved at some $\xi^* \geq \frac{1}{B}$. In this case, we have

$$\max_{\xi \geq 0} \left\{ -\xi \frac{B^{3/2}}{n} - \sum_{j=2}^n \frac{(v_j)^2}{\frac{3}{2} + \frac{\xi}{\mu_j}} \right\} \leq -\xi^* \frac{B^{3/2}}{n} \leq -\frac{B^{1/2}}{n}.$$

- Case 2: Otherwise, we may assume that the maximum achieved at some $\xi^* \in [0, \frac{1}{B}]$, in which case we have

$$\max_{\xi \geq 0} \left\{ -\xi \frac{B^{3/2}}{n} - \sum_{j=2}^n \frac{(v_j)^2}{\frac{3}{2} + \frac{\xi}{\mu_j}} \right\} \leq -\sum_{j=2}^n \frac{(v_j)^2}{\frac{3}{2} + \frac{\xi^*}{\mu_j}} \leq -\sum_{j=2}^n \frac{(v_j)^2}{\frac{3}{2} + \frac{1}{B\mu_j}} \leq -c \frac{B^{1/2}}{n},$$

where $c > 0$ is a constant. Here in view of Lemma 6, the last inequality holds with probability at least 0.9 as long as B is sufficiently large.

Combining the two cases, we arrive at the conclusion that as long as B is sufficiently large, with probability at least 0.9,

$$\min_{\theta_R \in \mathcal{C}} T_3(\theta_R) \leq -c_1 \frac{B^{1/2}}{n} \quad (62)$$

for some constant $c_1 > 0$.

Completing the proof: We can now combine bounds (59), (61), and (62) on the terms T_1, T_2, T_3 , respectively. Note that when $n \geq 7B^{3/2} \geq 7$, all three events and the upper bound (57) hold simultaneously, with probability $1 - (\frac{1}{n} + \frac{1}{100} + \frac{1}{10}) \geq 3/4$. Therefore, we obtain

$$\begin{aligned} g(\omega) &\leq \frac{3}{2} \frac{B^2}{n^2} + 20 \frac{B}{n^{3/2}} - c_1 \frac{B^{1/2}}{n} + C \frac{\log n}{n} \\ &\leq -\frac{c_1}{2} \frac{B^{1/2}}{n}. \end{aligned}$$

The final inequality above holds, since $B \geq c_1(\log n)^2$ and $n \geq 7B^{3/2}$, for sufficiently large $c_1 > 0$.

B.4.2 Proof of Lemma 5

We will prove the slightly stronger claim that with probability at least 3/4, we have

$$\inf_{\substack{t \in [0,1] \\ 1-t^2 \leq \beta B^{3/2}/n}} g(t) > -c^* \frac{\sqrt{B}}{n} \quad (63)$$

To see that this proves the claim, note that $\sup_{t \in [0,1]} \frac{(1-t^2)^2}{(1-t)^2} = 4$. Therefore, if $(1-t)^2 \leq \frac{\beta^2}{4} \frac{B^3}{n^2}$, then $(1-t^2)^2 \leq \beta^2 \frac{B^3}{n^2}$. Hence, (63) proves the claim as soon as $c_3 = \beta^2/4$.

Proof of bound (63): On the event (56), if $\theta = (\theta_1, \theta_R)^\top$ obeys $\theta^\top \mathbf{M}^{-1} \theta \leq 1$, then we have the lower bound

$$\begin{aligned}
(\theta - \theta^*)^\top \widehat{\Sigma}_P (\theta - \theta^*) &= (\theta - \theta^*)^\top \left(\widehat{\Sigma}_P + \lambda \mathbf{M}^{-1} \right) (\theta - \theta^*) - \lambda (\theta - \theta^*)^\top \mathbf{M}^{-1} (\theta - \theta^*) \\
&\geq \frac{1}{2} (\theta - \theta^*)^\top (\Sigma_P + \lambda \mathbf{M}^{-1}) (\theta - \theta^*) - \lambda (\theta - \theta^*)^\top \mathbf{M}^{-1} (\theta - \theta^*) \\
&= \frac{1}{2} (\theta - \theta^*)^\top \Sigma_P (\theta - \theta^*) - \frac{\lambda}{2} (\theta - \theta^*)^\top \mathbf{M}^{-1} (\theta - \theta^*) \\
&\geq \frac{1}{2} (\theta - \theta^*)^\top \Sigma_P (\theta - \theta^*) - 2\lambda,
\end{aligned}$$

valid when $\lambda = C \frac{\log n}{n}$ for some constant $C > 0$. Consequently, we have

$$\begin{aligned}
g(\theta_1) &\geq \min_{\theta_R \in \mathcal{C}(\theta_1)} \left\{ \frac{1}{2} (\theta - \theta^*)^\top \Sigma_P (\theta - \theta^*) - 2 (\theta - \theta^*)^\top v - 2\lambda \right\} \\
&= \min_{\theta_R \in \mathcal{C}(\theta_1)} \left\{ \frac{1}{2} \frac{(\theta_1 - 1)^2}{B} - 2v_1(\theta_1 - 1) + \frac{1}{2} \|\theta_R\|_2^2 - 2v_R^\top \theta_R - 2\lambda \right\} \\
&\geq -T_2(\theta_1) - 2\lambda + \min_{\theta_R \in \mathcal{C}(\theta_1)} \left\{ \frac{1}{2} \|\theta_R\|_2^2 - 2v_R^\top \theta_R \right\}.
\end{aligned} \tag{64}$$

where the last line identifies $-2v_1(\theta_1 - 1)$ with $T_2(\theta_1)$ (cf. definition (58)).

We separate the proof into two cases—mainly to get around the duality issue.

Case 1: $\theta_1 = 1$. In this case, we have

$$g(\theta_1) \geq -2\lambda = -\frac{2C \log n}{n}. \tag{65}$$

Case 2: $\theta_1 \in [0, 1)$. We lower bound the terms in equation (64) in turn.

- **Lower bounding $T_2(\theta_1)$.** For any $0 < 1 - \theta_1^2 \leq \beta \frac{B^{3/2}}{n}$, the following relation

$$T_2(\theta_1) \geq -2|v_1| \cdot |\theta_1 - 1| \stackrel{(i)}{\geq} -2|v_1| \cdot (1 - \theta_1^2) \stackrel{(ii)}{\geq} -20\beta \frac{B}{n^{3/2}}$$

holds with probability at least 0.99. Here step (i) uses the fact that

$$|\theta_1 - 1| = |1 - \sqrt{1 - (1 - \theta_1^2)}| \leq 1 - \theta_1^2 \quad \text{for all } \theta_1 \in [0, 1],$$

and step (ii) relies on Lemma 7 and the constraint $1 - \theta_1^2 \leq \beta \frac{B^{3/2}}{n}$.

- **Lower bounding $\min_{\theta_R \in \mathcal{C}'(\theta_1)} \{\frac{1}{2} \|\theta_R\|_2^2 - 2v_R^\top \theta_R\}$.** When $\theta_1 \in [0, 1)$, the constraint set $\mathcal{C}'(\theta_1)$ has non-empty interior, and the minimization over θ_R is strictly feasible. In this case, strict duality holds so that

$$\begin{aligned}
\min_{\theta_R \in \mathcal{C}'(\theta_1)} \left\{ \frac{1}{2} \|\theta_R\|_2^2 - 2v_R^\top \theta_R \right\} &= \max_{\xi \geq 0} \left\{ -\xi(1 - \theta_1^2) - \sum_{j=2}^n \frac{(v_j)^2}{\frac{1}{2} + \frac{\xi}{\mu_j}} \right\} \\
&\geq -[n(1 - \theta_1^2)]^{-2/3} (1 - \theta_1^2) - \sum_{j=2}^n \frac{(v_j)^2}{\frac{1}{2} + \frac{(n(1 - \theta_1^2))^{-2/3}}{\mu_j}} \\
&= -\frac{(1 - \theta_1^2)^{1/3}}{n^{2/3}} - \sum_{j=2}^n \frac{(v_j)^2}{\frac{1}{2} + \frac{(n(1 - \theta_1^2))^{-2/3}}{\mu_j}}.
\end{aligned}$$

Here the second line arises from a particular choice of ξ , namely $\xi = (n(1 - \theta_1^2))^{-2/3}$. Since $1 - \theta_1^2 \leq \beta \frac{B^{3/2}}{n}$, we further have

$$\begin{aligned} -\frac{(1 - \theta_1^2)^{1/3}}{n^{2/3}} - \sum_{j=2}^n \frac{(v_j)^2}{\frac{1}{2} + \frac{(n(1 - \theta_1^2))^{-2/3}}{\mu_j}} &\geq -\frac{\beta^{1/3} B^{1/2}}{n} - \sum_{j=2}^n \frac{(v_j)^2}{\frac{1}{2} + \frac{(\beta B^{3/2})^{-2/3}}{\mu_j}} \\ &= -\frac{\beta^{1/3} B^{1/2}}{n} - \sum_{j=2}^n \frac{(v_j)^2}{\frac{1}{2} + \frac{1}{\beta^{2/3} B \mu_j}} \\ &\geq -\tilde{C} \frac{\beta^{1/3} B^{1/2}}{n}, \end{aligned}$$

where $\tilde{C} > 0$ is a constant. Here, since B is sufficiently large, Lemma 6 guarantees that the last inequality holds with probability at least 0.9.

Combining the two cases above, we arrive at the conclusion that for any $1 - \theta_1^2 \leq \beta \frac{B^{3/2}}{n}$,

$$g(\theta_1) \geq -20\beta \frac{B}{n^{3/2}} - 2C \frac{\log n}{n} - \tilde{C} \frac{\beta^{1/3} B^{1/2}}{n}.$$

Under the assumptions that $B \geq C_1(\log n)^2$ and $n \geq C_2 B^{3/2}$ for some sufficiently large constants $C_1, C_2 > 0$, we can choose β sufficiently small so as to make sure that

$$g(\theta_1) \geq -c^* \frac{B^{1/2}}{n} \quad \text{for all} \quad 1 - \theta_1^2 \leq \beta \frac{B^{3/2}}{n}.$$

C Proofs of the bounds (38)

By definition, $h \in \mathcal{F}^*$ has the upper bound $\|h\|_{\mathcal{H}} \leq 3\|f^*\|_{\mathcal{H}}$. In terms of the expansion $h = \sum_{j=1}^{\infty} \theta_j \phi_j$, this constraint is equivalent to the bound $\sum_{j=1}^{\infty} \theta_j^2 / \mu_j \leq 9\|f^*\|_{\mathcal{H}}^2$. In addition, the constraint $\|h\|_Q \leq r$ implies that $\sum_{j=1}^{\infty} \theta_j^2 \leq r^2$. In conjunction, these two inequalities imply that

$$\sum_{j=1}^{\infty} \frac{\theta_j^2}{\min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}} \leq 10,$$

as claimed in inequality (38b).

We now use this inequality to establish the bound (38a). For any $x \in \mathcal{X}$, we have

$$\begin{aligned} |h(x)| &= \left| \sum_{j=1}^{\infty} \theta_j \phi_j(x) \right| = \left| \sum_{j=1}^{\infty} \frac{\theta_j}{\sqrt{\min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}}} \cdot \sqrt{\min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}} \phi_j(x) \right| \\ &\stackrel{(i)}{\leq} \sqrt{\sum_{j=1}^{\infty} \frac{\theta_j^2}{\min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}}} \sqrt{\sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\} \phi_j^2(x)} \\ &\stackrel{(ii)}{\leq} \sqrt{10 \sum_{j=1}^{\infty} \min\{r^2, \mu_j \|f^*\|_{\mathcal{H}}^2\}}. \end{aligned}$$

Here step (i) uses the Cauchy–Schwarz inequality, whereas step (ii) follows from the previous claim (38b) and the assumption that $|\phi_j(x)| \leq 1$.

D Performance guarantees for LR-reweighted KRR

In this section, we present the performance guarantee for the LR-reweighted KRR estimate with truncation for all ranges of σ^2 .

Similar to the large noise regime, we define

$$\mathcal{M}^{\text{new}}(\delta) := c_0 \sqrt{\frac{\sigma^2 V^2 \log^3(n)}{n} \Psi(\delta, \mu)} \left(\sqrt{\frac{\Psi(\delta, \mu)}{\sigma^2}} + 1 \right). \quad (66)$$

Our theorem applies to any solution $\delta_n^{\text{new}} > 0$ to the inequality $\mathcal{M}^{\text{new}}(\delta) \leq \delta^2/2$.

Theorem 5. *Consider a kernel with sup-norm bounded eigenfunctions (19), and a source-target pair with $\mathbb{E}_P[\rho^2(X)] \leq V^2$. Then the estimate $\hat{f}_\lambda^{\text{rw}}$ with truncation $\tau_n = \sqrt{nV^2}$ and regularization $\lambda \|f^*\|_{\mathcal{H}}^2 = \delta_n^2/3$ satisfies the bound*

$$\|\hat{f}_\lambda^{\text{rw}} - f^*\|_Q^2 \leq \delta_n^2 \quad (67)$$

with probability at least $1 - c n^{-10}$.

Proof. Inspecting the proof of Theorem 4 (in particular, equation (37)), one has with high probability that

$$\sup_{g \in \mathcal{G}(\delta_n)} \left\{ \|g - f^*\|_Q^2 + \frac{1}{n} \sum_{i=1}^n \rho_{\tau_n}(x_i) [(f^*(x_i) - y_i)^2 - (g(x_i) - y_i)^2] \right\} \leq \mathcal{M}^{\text{new}}(\delta_n).$$

Repeating the analysis in Section 5.2 with $\delta_\lambda = \delta_n$ yields the desired claim. \square

E Auxiliary lemmas

The following lemma provides concentration inequalities for the sum of independent self-adjoint operators, which appeared in the work [11].

Lemma 8. *Let $\mathbf{Z}_1, \mathbf{Z}_2, \dots, \mathbf{Z}_n$ be i.i.d. self-adjoint operators on a separable Hilbert space. Assume that $\mathbb{E}[\mathbf{Z}_1] = \mathbf{0}$, and $\|\mathbf{Z}_1\|_2 \leq L$ for some $L > 0$. Let \mathbf{V} be a positive trace-class operator such that $\mathbb{E}[\mathbf{Z}_1^2] \preceq \mathbf{V}$, and $\|\mathbb{E}[\mathbf{Z}_1^2]\|_2 \leq R$. Then one has*

$$\mathbb{P}\left(\left\|\frac{1}{n} \sum_{i=1}^n \mathbf{Z}_i\right\|_2 \geq t\right) \leq \frac{28 \text{trace}(\mathbf{V})}{R} \cdot \exp\left(-\frac{nt^2/2}{R + Lt/3}\right), \quad \text{for all } t \geq \sqrt{R/n} + L/(3n).$$

Next, we turn attention to bounding the maxima of empirical processes. Let X_1, X_2, \dots, X_n be independent random variables. Let \mathcal{F} be a countable class of functions uniformly bounded by b . Assume that for all i and all $f \in \mathcal{F}$, $\mathbb{E}[f(X_i)] = 0$. We are interested in controlling the random variable $Z := \sup_{f \in \mathcal{F}} \sum_{i=1}^n f(X_i)$, for which the variance statistics $v^2 := \sup_{f \in \mathcal{F}} \mathbb{E}[(f(X_i))^2]$ is crucial. Now we are in position to state the classical Talagrand's concentration inequalities; see the paper [7].

Lemma 9. *For all $t > 0$, we have*

$$\mathbb{P}(Z \geq \mathbb{E}[Z] + t) \leq \exp\left(-\frac{t^2}{2(v^2 + 2v\mathbb{E}[Z]) + 3vt}\right). \quad (68)$$