PAC-BAYESIAN BASED ADAPTATION FOR REGULARIZED LEARNING *

Prem Talwai
Operations Research Center
MIT

David Simchi-Levi
Institute for Data, Systems, and Society
MIT

ABSTRACT

In this paper, we propose a PAC-Bayesian a posteriori parameter selection scheme for adaptive regularized regression in Hilbert scales under general, unknown source conditions. We demonstrate that our approach is adaptive to misspecification, and achieves the optimal learning rate under sub-gaussian noise. Unlike existing parameter selection schemes, the computational complexity of our approach is independent of sample size. We derive minimax adaptive rates for a new, broad class of Tikhonov-regularized learning problems under general, misspecified source conditions, that notably do not require any conventional a priori assumptions on kernel eigendecay. Using the theory of interpolation, we demonstrate that the spectrum of the Mercer operator can be inferred in the presence of “tight” $L^\infty$ embeddings of suitable Hilbert scales. Finally, we prove, that under a $\Delta_2$ condition on the smoothness index functions, our PAC-Bayesian scheme can indeed achieve minimax rates. We discuss applications of our approach to statistical inverse problems and oracle-efficient contextual bandit algorithms.

Keywords Parameter selection, PAC-Bayesian, adaptive regularization

1 Introduction

Consider the classical learning problem:

$$Y = f^*(X) + \epsilon$$

(1)

where we wish to estimate the regression function $f^*$ in the presence of additive noise $\epsilon$ using a dataset $D = \{(X_1, Y_1), (X_2, Y_2), \ldots (X_n, Y_n)\}$ sampled i.i.d from a distribution $P$ over $\mathcal{X} \times \mathcal{Y}$. Typically this involves building a regularized estimate:

$$f_{D,\lambda} = q_\lambda(\{(X_i, Y_i)\}_{i=1}^n)$$

where $\{q_\lambda\}_{\lambda > 0}$ is some family of regularization functions that builds an estimate for $f^*$ using the data $D$. A popular scheme of regularization is Tikhonov (ridge) regression over a reproducing kernel Hilbert space (with kernel $K(x, y)$), where $f_{D,\lambda} = (C_D + \lambda)^{-1} \sum_{i=1}^n Y_i k(x_i, \cdot)$, with $C_D$ being the empirical kernel covariance matrix. This regularization scheme will be studied extensively in the second half of the paper.

The performance of a regularization scheme is typically quantified using the expected risk:

$$R(f_{D,\lambda}) = ||f_{D,\lambda} - f^*||^2_{L^2(P)}$$

It is well-known that achieving minimax convergence rates for $R(f_{D,\lambda, n})$ as $n \to \infty$, hinges on selecting an appropriate program for the regularizer $\lambda_n$. For example, when our hypothesis class is the Sobolev space $H^k(\mathbb{R}^d)$, then achieving...
the optimal convergence rate of $O\left(n^{-\frac{k}{d+k}}\right)$ relies on choosing the regularization program $\lambda_n \asymp n^{-\frac{k}{d+k}}$ in ridge-regression. Observe, here that this optimal choice requires a priori knowledge of the smoothness $k$. Typically, in practice, the true smoothness of the learning target $f^*$, may be unknown, hence we must make an a posteriori choice of $\lambda_n$ that adapts to unknown smoothness.

Several approaches have been proposed to tackle this issue of adaptivity in regularized learning. The most popular is Lepski’s balancing method [21, 25], which involves establishing upper bounds on the bias and variance of the $f_{D, \lambda_n}$ (as a function of $\lambda$), calculating candidate solutions $f_{D, \lambda_n}$, over a class of regularizers ($\lambda_{n,i} \in \Lambda_n$), and finally choosing the largest regularizer that satisfies a separation condition involving the variance upper bound (which intrinsically does not depend on the smoothness; see [25] for details). While this approach demonstrates strong theoretical guarantees, it involves the front-end calculation of $\log n$ candidate solutions, which may become prohibitively expensive as $n \to \infty$. While, Lepski’s original method was developed for full-information, Gaussian white noise settings, [10] extended these ideas to the learning setting, and developed a cross-validation based approach that splits the dataset into training and validation segments, and calculates regularized estimates using the training data, whose empirical risk is then evaluated on the test data. While their approach enjoys the similar theoretical guarantees in the statistical learning setting, it also requires the front-load calculation of a logarithmically growing set of candidate solutions. Recently, online stopping rules over Hilbert spaces have been proposed that seek to eliminate this frontload calculation [5, 31], but these typically require a priori information on the RKHS norm $\|f^*\|_K$ of the target function [31], which is typically unavailable, or are not adaptive to misspecification [5].

In this paper, we develop a PAC-Bayesian a posteriori parameter selection scheme that adapts to misspecification by randomizing the regularizer using a PAC-Bayesian posterior. Like, [10], our approach is based on cross-validation split in the dataset, however unlike their strategy, our parameter choice is simply the mean of a posterior distribution, and hence does not require the calculation of candidate set of solutions which grows with the sample size. Indeed, the only computational effort involved in implementing our approach stems from approximating the mean of continuous posterior distribution over the regularizer. This can be performed efficiently using a variety of methods such as Metropolis-Hastings [13], Langevin MCMC [23], and their variants [13], that do not require closed forms of the posterior density. In any implementation, the number of Monte Carlo samples needed to build an estimate on the posterior mean can be fixed, and is independent of the number of samples $n$. Moreover, unlike the stopping rules of [31] and [5], our method is adaptive to misspecification and does not require stringent assumptions on the function class.

We demonstrate that our approach achieves the minimax optimal rate in the presence of subgaussian noise and a doubling $(\Delta_2)$ condition on the bias and variance (as a function of the regularizer). In the second half of the paper, we present a general, concrete setting in which the latter condition is satisfied — Tikhonov regularization over variable Hilbert scales. We first derive novel optimal rates for the minimax expected risk in this setting, which allow for misspecification (i.e. the true function need not lie in an RKHS but simply a Hilbert scale with a possibly unknown index function), and are tractable to PAC-Bayesian adaptation in broad regimes. A notable feature in the latter analysis is that we do not impose the common assumption on kernel eigendecay [14, 22] typically required to establish minimax rates. Indeed, we demonstrate that if the embedding of an intermediate Hilbert scale is sufficiently “sharp” (characterized by the optimality of its index function in “covering” the decay of kernel spectral measure), then a Gagliardo-Nirenberg type inequality between the scales enables us to estimate kernel eigendecay via the Bernstein widths of the RKHS in $L^\infty$. To the best of our knowledge, this is the first work to establish minimax learning rates under general source conditions without appealing to any direct assumptions on the eigendecay or effective dimension of the Mercer operator. We close the paper with a brief discussion on the applicability of our work to problems in contextual bandits and statistical inverse problems.

## 2 PAC-Bayesian Based Adaptation

We present a PAC-Bayesian adaptation procedure for selecting an a posteriori choice of the regularization parameter $\lambda$. PAC-Bayesian approaches have found widespread use in the machine learning literature [18] since they were first formulated by McAllester [27], with applications ranging from sparse regression [2], matrix completion [1], sequential learning [16], and classification [17]. The widespread popularity of these approaches stems from their ability to elegantly adapt to uncertainty over wide parameter spaces via a simple posterior update as new data is processed. Their simple application is accompanied by strong theoretical guarantees, providing high-probability generalization bounds expressed solely in terms of the training data and other known/computable quantities, thus eliminating the need for the collection additional test-data; see [18] for a more detailed discussion.

Several PAC-Bayesian approaches have previously been proposed for model selection in learning settings [28, 41, 43]. These studies have traditionally considered either sparse regression [41], where the learning target lies in some un-
known low-dimensional subspace spanned by a sparse number of basis functions, or Gaussian process regression with unknown kernel hyperparameters [3]. In either case, a PAC-Bayesian posterior is applied to sample over admissible subspaces or kernel hyperparameters, and the contraction of this posterior towards the optimal parameter is demonstrated. Despite the proven success of these approaches in adapting to parameter uncertainty, the diversity of models sampled by the PAC-Bayesian posterior is still limited in these settings. For example, sampling over a family of squared-exponential Gaussian process priors with varying bandwidths still implicitly assumes that the target function is infinitely differentiable, and hence cannot adapt to the case of a regression target with finite smoothness.

In this paper, we develop a PAC-Bayesian approach that is based on sampling the regularization parameter \( \gamma \), rather than the underlying hypothesis class. As mentioned briefly in the introduction (and explored much deeper in section 3), the optimal choice of regularization parameter contains crucial information on the smoothness properties of the learning target. Our approach is based on accessing the “true” smoothness (model) class indirectly via sampling the choice of regularization parameter. Intuitively, the problem of converging to the true model is equivalent to approaching the optimal regularization program. However, unlike a posterior over function classes, a posterior over the space of regularizers (i.e. positive real numbers) avoids making even minimal parametric assumptions on the true model, and hence can effectively adapt to significant degrees of problem misspecification. The notion of stochastic SVMs was briefly discussed in [33, 36] for the classification setting, however their treatment only included estimates for the \( \xi \) parameter. Despite the proven success of these approaches in adapting to parameter uncertainty, the diversity of models sampled by the PAC-Bayesian posterior is still limited in these settings. For example, sampling over a family of squared-exponential Gaussian process priors with varying bandwidths still implicitly assumes that the target function is infinitely differentiable, and hence cannot adapt to the case of a regression target with finite smoothness.

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2.1 PAC-Bayesian Estimator

1. Split dataset \( D \) into train \( D_{\text{tr}} \) and test \( D_{\text{v}} \) sets, with \( |D_{\text{tr}}| = |D_{\text{v}}| = n \).
2. Choose an exponential prior \( \mu(\lambda) \sim \text{Exp}(\alpha) \) for some \( \alpha > 0 \),
3. Choose \( \gamma > 0 \). Using the validation set \( D_{\text{v}} \), build posterior distribution:
   \[
   \rho_{\gamma,n}(\lambda) \sim \frac{\exp\left(-\frac{\gamma}{n} \sum_{(X,Y)\in D_{\text{tr}}}(Y - f_{D_{\text{tr}},\lambda}(X))^2\right)\mu(\lambda)}{\int_0^\infty \exp\left(-\frac{\gamma}{n} \sum_{(X,Y)\in D_{\text{tr}}}(Y - f_{D_{\text{tr}},\lambda}(X))^2\right)\mu(\lambda)d\lambda}
   \]
   where \( f_{D_{\text{tr}},\lambda} = q_{\lambda}(D_{\text{tr}}) \) is the regularized estimate calculated using the training data.
4. Choose \( \hat{\lambda}_{2n} \) as:
   \[
   \hat{\lambda}_{2n} = \mathbb{E}_{\rho_{\gamma,n}}[\lambda]
   \]

2.2 Comparison to Existing Approaches

While our approach involves a cross-validation step inspired by [10], the most distinctive feature of our approach, relative to classical adaptation procedures like Lepski’s method or that of [10], is that the number of candidate regularizers to compute does not grow with the sample size \( n \). Indeed, the only computational bottleneck involved in the implementation of our approach stems from the need to estimate the mean of the continuous posterior distribution \( \rho_{\gamma,n} \). This can be done using a variety of popular sampling methods, such as Metropolis-Hastings ([18]), Langevin MCMC ([23]), and their variants ([13]). When using any of these methods, the number of Monte-Carlo samples used for estimating the average \( \hat{\lambda}_{2n} \) can be fixed independently of \( n \). Moreover, unlike online stopping rules, our method does not rely on stringent assumptions on the function class and is adaptive to misspecification. Finally, unlike randomized regularizers considered in [33, 36], our adaptation procedure provides an explicit parameter choice that demonstrates minimax optimal oracle bounds (see section 2.3).

2.3 Oracle Bounds

We define the following growth condition:

**Definition 2.1.** A real-valued function \( \xi \) is said to satisfy the \( \Delta_2 \) condition if there exists constants \( D_1, D_2 > 0 \), such that:

\[
D_1 \xi(\lambda) \leq \xi(2\lambda) \leq D_2 \xi(\lambda) \quad \forall \lambda > 0
\]

(2)

Note, that if \( \xi \) is monotonic, one side of the \( \Delta_2 \) condition is trivial (this will typically be our setting). Moreover, suppose that we have the following high-probability bias-variance decomposition of \( R(f_{D,\lambda}) \), i.e:

\[
R(f_{D,\lambda}) \leq B(\lambda) + \Upsilon(\lambda)
\]

(3)
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with probability $1 - \delta$ on the draw of the training data. Here, $B(\lambda)$ is an upper bound on the bias (and hence nondecreasing in $\lambda$) and $\Upsilon(\lambda)$ is an upper bound on the variance (and hence is nonincreasing in $\lambda$), such that:

$$R(f_{D,\lambda_n^*}) \simeq B(\lambda_n^*) + \Upsilon(\lambda_n^*)$$

(4)

where $\lambda_n^*$ is the Tikhonov regularization program achieving the optimal rate. Our main result in this section states that when the additive noise $\epsilon$ in $P_\nu$ is subgaussian and the optimal expected risk satisfies the $\Delta_2$ condition, our PAC-Bayesian adaptation procedure recovers the optimal learning rate:

**Theorem 1.** Let $\{\lambda_n^*\}_{n=1}^\infty$ be a regularization program achieving the optimal $L^2(P_\nu)$ rate. Suppose $\epsilon \sim \text{SG}(\sigma^2)$, $B, \Upsilon$ in (3) satisfy the $\Delta_2$ condition for some constants $D_1^B, D_2^B, D_1^\Upsilon, D_2^\Upsilon$. Then, choosing $\gamma = \frac{\nu}{8\sigma^2}$, we have, with probability $1 - \delta$:

$$R(f_{D,\lambda_n}) \leq 3CR(f_{D,\lambda_n^*}) + \frac{32 \log \left( \frac{\nu}{\alpha^*} \right) + 40\alpha \lambda_n^* + 32 \log \frac{2}{\delta}}{\sigma^2_n}$$

where $C = \max \left\{ D_2^B, \frac{1}{D_1^B} \right\}$.

Hence, our oracle bound demonstrates that we can recover the optimal learning rate, as long as $R(f_{D,\lambda_n^*}) = \omega \left( n^{-1} \log \left( \frac{1}{\lambda_n^*} \right) \right)$, i.e. the optimal learning rate dominates $n^{-1} \log \left( \frac{1}{\lambda_n^*} \right)$ (the misspecification error). In section 3 we demonstrate that this optimality condition is readily satisfied for ridge regression over a broad class of smoothness priors.

3 Tikhonov Regularization over Hilbert Scales

We now present a concrete example of applicability of our adaptation procedure, by first deriving new minimax learning rates for a broad class of kernelized ridge regression problems, and then demonstrating that the developed PAC-Bayesian approach achieves these optimal rates under some weak growth assumptions. Throughout this section, we consider the following learning problem:

$$f_{\lambda,D} \in \arg \min_{f \in \mathcal{H}_K} \frac{1}{n} \sum_{(X,Y) \in D_n} (Y - f(X))^2 + \lambda ||f||_K^2$$

(5)

where $\mathcal{H}_K$ be a separable reproducing kernel Hilbert space (RKHS) on $\mathcal{X}$ (see e.g. [39] for a definition). A solution to this problem can be computed in closed form:

$$f_{\lambda,D} = (C_D + \lambda)^{-1} g_D$$

where $C_D = E_D[k(X,\cdot) \otimes k(Y,\cdot)]$ is the empirical covariance, and $g_D = \sum_{i=1}^n y_i k(x_i,\cdot)$. Before discussing our model framework and results, we begin with an overview of some mathematical preliminaries required for this section.

3.1 Hilbert Scales

Suppose the imbedding $I_\nu : \mathcal{H}_K \to L^2(\nu)$ of $\mathcal{H}_K$ into $L^2(\nu)$ is injective (here $\nu = P_\nu$ is the marginal on $\mathcal{X}$). Let $S_\nu = I_\nu^*$ be its adjoint. Then, it can be shown that $S_\nu$ is an integral operator given by:

$$S_\nu(f) = \int_{\mathcal{X}} k(x,\cdot)f(y) d\nu(y)$$

(6)

Using $S_\nu$ and $I_\nu$, we construct the following positive self-adjoint operators on $\mathcal{H}_K$ and $L^2(\nu)$, respectively:

$$C_\nu = S_\nu I_\nu = I_\nu^* I_\nu$$

$$T_\nu = I_\nu S_\nu = I_\nu I_\nu^*$$

We observe that $C_\nu$ and $T_\nu$ are nuclear (see Lemma 2.2/2.3 in [40]). Since, $T_\nu$ is nuclear and self-adjoint, it admits a spectral representation:

$$T_\nu = \sum_{j=1}^\infty \lambda_j e_j \langle e_j, \cdot \rangle_{L^2(\nu)}$$
where \( \{ \mu_j \}^\infty_{j=1} \subset (0, \infty) \) are nonzero eigenvalues of \( T_\nu \) (ordered nonincreasingly) and \( \{ e_j \}^\infty_{j=1} \subset L^2(\nu) \) form an orthonormal system of corresponding eigenfunctions. Note that formally, the elements \( e_j \) of \( L^2(\nu) \) are equivalence classes \( [e_j]_\nu \), whose members only differ on a set of \( \nu \)-measure zero—notationally, we consider this formalism to be understood here and simply write \( e_j \) to refer to elements in both \( H_K \), \( L^2(\nu) \), and their interpolation spaces (with the residence of \( e_j \) understood from context). Given a nonincreasing index function \( \phi : (0, |||T_\nu|||) \rightarrow \mathbb{R}_+ \), we define the Hilbert scales \( H_K^\phi \) as [20]:

**Definition 3.1.** Let \( \phi : (0, |||T_\nu|||) \rightarrow \mathbb{R}_+ \) be nondecreasing, continuous, with \( \psi(0) = 0 \). Then, the Hilbert scale \( H_K^\phi \) is the completion of the space:

\[
H_K^\phi = \left\{ f \in L^2(\nu) : \sum_{i=1}^\infty \frac{\langle f, e_i \rangle^2}{\phi(\mu_i)} < \infty \right\}
\]

with respect to the inner product \( \langle f, g \rangle = \sum_i \frac{\langle f, e_i \rangle \langle g, e_i \rangle}{\phi(\mu_i)} \).

It is easy to see that \( H_K^\phi \cong \text{ran}(\phi^{1\sharp}(T_\nu)) \). The subscript \( K \) in \( H_K^\phi \), reflects that \( \phi \) is acting on the spectrum of \( K \), when the kernel is fixed and understood from context, we will omit this subscript and simply denote the Hilbert scale \( H^\phi \).

We define:

\[
|||k_\phi|||_\infty = \sup_{x \in X} \sum_{i=1}^\infty \phi(\mu_i)x_i^2(x)
\]

where we allow \( |||k_\phi|||_\infty = \infty \). If \( |||k_\phi||| < \infty \), then it is easy to show that \( H_K^\phi \) is continuously embedded in \( L^\infty(X) \) with norm \( |||k_\phi|||_\infty \) (see e.g. Theorem 9 in [14] for the case of Holder source conditions).

The Hilbert scale \( H_K^\phi \) generalizes the notion of RKHS interpolation (power) spaces discussed in [40], which result from the specific choice of \( \phi(t) = t^\alpha \) for some \( \alpha \in (0, 1) \). Intuitively, the Hilbert scales can be viewed as a nonlinear transformation of the infinite-dimensional RKHS ellipsoid \( H_K \), realized by transforming the axes lengths with the index function \( \phi \). As we will see later, the growth properties of \( \phi \) play a fundamental role in specifying the smoothness of the elements of \( H_K \).

### 3.2 Rearrangement Invariant Spaces

Let \( (R, \mu) \) be a \( \sigma \)-finite measure space. For any measurable function \( f : (R, \mu) \rightarrow \mathbb{R} \), define \( \mu_f(\lambda) = \mu(\{ x \in R : |f(x)| > \lambda \}) \) to be the distribution function of \( f \) (in our context and most applications, \( \lambda \) is typically considered to be the Lebesgue measure). Two functions \( f \) and \( g \) are called *equimeasurable* (denoted by \( f \sim g \)) if \( \mu_f(\lambda) = \mu_g(\lambda) \) for all \( \lambda \).

**Definition 3.2.** A Banach function space \((B, || \cdot ||)\) over \((R, \mu)\) is rearrangement invariant if:

\[
||f||_X = ||g||_X \ \forall f, g \in X ; f \sim g
\]

Thus, norms in rearrangement invariant spaces are constant over equivalence classes of equimeasurable functions. We can associate each class with a function over \( \mathbb{R} \), called the decreasing rearrangement:

**Definition 3.3.** For any \( f \in X \), define \( f^* : \mathbb{R}^+ \rightarrow \mathbb{R}^+ \) as:

\[
f^*(\lambda) = \inf \{ x \in \mathbb{R}^+ : \mu_f(|f(x)|) < \lambda \}
\]

Clearly, if \( f \sim g \), then \( f^* = g^* \). We also define the maximal decreasing rearrangement \( f^{**} \) as \( f^{**}(t) = \frac{1}{t} \int_0^t f^*(s) \). A crucial component of our subsequent discussion relating Hilbert scales to rearrangement-invariant spaces relies on the fundamental function \( \phi : R(\mu) \rightarrow R^+ \) (where \( R(\mu) \) denotes the range of the measure \( \mu \) over \( R \)):

**Definition 3.4.**

\[
\phi(t) = |||\chi_E|||_X, \ \mu(E) = t
\]

Note, by rearrangement invariance, the choice of set \( E \) above is irrelevant. Intuitively, the fundamental function characterizes the relationship between the norm \( || \cdot ||_X \) and \( \mu \). We define two special spaces, the Lorentz space \( \Lambda_\phi \) and Marcinkiewicz space \( M_\phi \) with fundamental function \( \phi \):
We review some standard widths in approximation theory that describe the compactness of spaces in various norms.

Further if $\phi$ is concave, then we define the Lorentz space:

$$\Lambda_{\phi} = \{ g : \int_0^{\mu(R)} g^+(t) d\phi(t) < \infty \}$$

The Lorentz and Marcinkiewicz spaces are referred to as endpoint spaces, because they are respectively the largest and smallest spaces with fundamental function $\phi$. Formally, for any rearrangement invariant space $X$ with fundamental function $\phi$, we have:

$$\Lambda_{\phi} \subset X \subset M_{\phi}$$

$X$ is called ultrasymmetric if it can be obtained as an interpolation space between the Banach couple $(\Lambda_{\phi}, M_{\phi})$ (see e.g. [19] or more directly and recently [4] for a definition). Ultrasymmetric spaces are intermediate between the endpoint spaces $\Lambda_{\phi}$ and $M_{\phi}$, in the sense that bounded operators on these endpoint spaces are also bounded on $X$. Orlicz spaces $L^\Phi$, for example, are ultrasymmetric when $\phi = \frac{1}{\Phi(t)}$ has finite extension indices (Theorem 2/3 in [4]), which occurs for example when $\Phi$ satisfies the $\Delta_2$ condition in [2].

### 3.3 Approximation Widths

We review some standard widths in approximation theory that describe the compactness of spaces in various norms. The $n$th entropy number $e_n(\mathcal{X})$ of a compact set $\mathcal{X}$, is informally the smallest radius $\epsilon$ such that there exists an $\epsilon$-covering of $\mathcal{X}$ of at most $n$ balls. Precisely, we have:

$$e_n(\mathcal{X}) = \inf \{ \epsilon : \exists \{ x_i \}_{i=1}^n \subset \mathcal{X}; \ \text{s.t.} \ \mathcal{X} \subset \bigcup_{i=1}^n B(x_i, \epsilon) \}$$

We also define the $n$-Bernstein width of a Banach space $X$ compactly embedded in another space $Y$:

$$b_n(X, Y) = \sup_{\mathcal{X} \subset X, \dim(\mathcal{X}) \geq n+1} \inf_{\mathcal{Z} \subset Y} \frac{|| z ||_Y}{|| z ||_X}$$

Intuitively, the Bernstein width gives the radius of the largest $Y$-ball that may be inscribed in a unit $X$-ball in subspaces of dimension greater than $n$. When $X$ and $Y$ are both Hilbert spaces, then $b_n$ coincides with the $n+1$st singular number of the embedding $X \rightarrow Y$. For a detailed discussion of the relationships between various approximation widths and function space embeddings, we direct the reader to [11].

For a positive function $f : (0, \infty) \rightarrow (0, \infty)$, we define the dilation function $d_f : (0, \infty) \rightarrow (0, \infty)$ as:

$$d_f(t) = \sup_{s \in (0, \infty)} \frac{f(st)}{f(s)}$$

**Remark** (Notation). For any two Banach spaces $A$ and $B$, we write $A \hookrightarrow B$, if $A$ is continuously embedded in $B$, and $A \overset{\Delta}{\hookrightarrow} B$ if this embedding is further compact. We denote by $B(A)$ the unit ball in $A$. $\mathbb{E}_P[\cdot]$ denotes the sample expectation, and $C_D = \mathbb{E}_P[k(X, \cdot) \otimes k(X, \cdot)]$ denotes the sample covariance. We will denote by $f_{D, \lambda}$ the solution to [5] and $f_\lambda = (C_\nu + \lambda)^{-1} S_\nu f^*$, the regularized population solution. $F_d$ denotes the $d$-dimensional Fourier transform. $L^p(\mathcal{X}, \mu)$ denotes the $L^p$ space on the measure space $(\mathcal{X}, \mu)$ — the domain will be omitted in the notation if it is understood from context; likewise the measure will be omitted if it is equivalent to Lebesgue measure. $|| \cdot ||_2$ or $|| \cdot ||_{L^2(\nu)}$ are used to refer to norms in $L^2(\nu)$ (the latter if we want to make the space explicit); $|| \cdot ||_2$ or $|| \cdot ||_{L^2(\nu)}$ for the norm in Hilbert scale $\phi$, and $|| \cdot ||_{L^2(\nu)}$ for the RKHS $H_K$. Typically, we will take $\nu = P_X = P|_{\mathcal{X}}$ where $P$ is the data-generating measure, and denotes the “marginal on”. Finally, we will write $a(x) \preceq b(x)$ if $a(x) \leq b(x)$ almost surely. Finally, $\text{SG}(\sigma^2)$ is used to denote a subgaussian distribution with variance proxy $\sigma^2$.

### 3.4 Assumptions

Let $\phi$ and $\psi$ be two admissible index functions (i.e. $\phi$ and $\psi$ are nondecreasing, nonnegative, and continuous, with $\phi(0) = \psi(0) = 0$)
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Assumption 1. (1) $H_k \overset{c}{\hookrightarrow} H^\phi \overset{c}{\hookrightarrow} H^\psi \hookrightarrow L^\infty$; (2) $\frac{t}{\phi(t)}$ and $\frac{\phi(t)}{\psi(t)}$ are nondecreasing, and $\frac{1}{\psi(t)}$ is concave; (3) $\phi, \psi$ satisfy the $\Delta_2$ condition \([2]\) for some constants $D_1^\phi, D_2^\phi, D_1^\psi, D_2^\psi > 1$

Assumption 2. $f^* \in H^\phi$

Assumption 3*. $k$ is radial, i.e. $k(x, y) = \kappa(||x - y||)$ for some positive definite function $\kappa \in L^1(\mathbb{R})$, such that either $d_k(t) < \infty$ or $d_{F\kappa}(t) < \infty$ for all $t > 0$.

Assumption 4*. $X \subset \mathbb{R}^d$ is compact with $\epsilon_n(X) \asymp n^{-\frac{1}{d}}$ for $n \in \mathbb{N}$.

Assumption 5*. $\psi(t, F_{d\kappa}(t^{-\frac{1}{2}})) \asymp t$ as $t \to 0$

Assumption 1 dictates the relative growth rates of the index functions $\phi$ and $\psi$. Indeed, the compactness of the embedding $H^\phi \overset{c}{\hookrightarrow} H^\psi$ ensures that $\frac{\phi(t)}{\psi(t)} \to 0$ as $t \to 0$. Moreover, the first embedding $H_K \overset{c}{\hookrightarrow} H^\phi$ ensures that both $\frac{t}{\phi(t)} \to 0$ and $\frac{\phi(t)}{\psi(t)} \to 0$ as $t \to 0$. Intuitively, this condition implies that the norms are in $H_\psi$ and $H_\phi$ are weaker than those in our hypothesis class $H_K$, allowing us to study convergence in these larger spaces of sample estimators constructed in $H_K$. The second part of the assumption requiring $\frac{\phi(t)}{\psi(t)}$ to be nondecreasing extends this behavior as $t \to \infty$; collectively the two growth conditions characterize $\frac{1}{\phi}$ and $\frac{1}{\psi}$ as resembling a Young’s function; a requirement commonly imposed in the study of Orlicz spaces \([3]\). The requirement that $\frac{1}{\phi(t)}$ is additionally concave enables the application of a Gagliardo-Nirenberg type interpolation inequality \([24]\) that relates $\nu$ norms to those in $H_K$ and $L^2(\nu)$, which will be crucial in our analysis of uniform error rates. Finally, that index functions are $\Delta_2$ is found quite commonly in the literature on statistical inverse problems \([26, 37]\), where it has been used to demonstrate adaptivity of balancing strategies to unknown source conditions. It should be noted that all the growth conditions in Assumptions 1 are satisfied when $\phi = t^\alpha$ and $\psi = t^\beta$ are power functions with $0 < \alpha < \beta < 1$ (the so-called Holder source conditions).

Assumption 2 characterizes the smoothness of the learning target $f^*$. Note a distinctive feature of our analysis is that we allow $f^*$ to lie outside the hypothesis class $H_K$ (in light of Assumption 1). In practice, the smoothness index functions $\phi$ and $\psi$ are typically unknown, motivating the need for an adaptive learning procedure. Indeed, in Corollary 2\(a\) we demonstrate that as long as $\frac{1}{\psi(t)}$ is superlogarithmic as $t \to \infty$, our PAC-Bayesian adaptation algorithm achieves minimax optimal learning rates.

While Assumptions 3\(a\)\(c\)\(d\)\(e\) are not necessary for establishing the upper bound in Theorem 3\(a\) they are required to demonstrate its optimality. Namely, the radiality assumption on the kernel $k$ in Assumption 3\(e\) enables the tight estimation of the approximation widths of $H_K$ in $L^\infty$ via the compactness properties of the domain $X$, the latter of which are characterized by the asymptotic behavior of the entropy numbers specified in Assumption 3\(d\). The dilation condition can be satisfied either by the kernel or its $d$-dimensional Fourier transform; an example of the latter being the popular Matern kernel. This dilation condition is primarily for streamlining the analysis, it could be removed at the expense of requiring Assumption 3\(e\) to be satisfied instead by a dilation of the Fourier transform $F_{d\kappa}$ (this tradeoff is highlighted in Remark 3\(a\) in the Appendix). Similarly, the precise asymptotic behavior of the entropy numbers of $X$ is only included for simplicity; the general case would require replacing $F_{d\kappa(t^{-\frac{1}{2}})}$ with $F_{d\kappa(t^{-\frac{1}{2}})}(X)$ in Assumption 3\(e\).

Assumption 5\(a\) ensures that the index function $\psi$ is indeed the “optimal” choice for characterizing the embedding of our hypothesis class $H_K$ in $L^\infty$. It is important to note that while Assumptions 1 and 2\(b\) implicitly depend on the ambient measure $\nu$ (as the index functions act spectrally on the Mercer operator $T_\nu$), the optimality condition is independent of this measure, which is typically unknown in practice (and determined by the data-generating process). This contrasts with the conventional assumption on the exact decay rates of the eigenvalues $\mu_\nu(T_\nu)$ or the effective dimension \([7, 14]\) required to establish minimax optimal learning rates. Informally, the natural embedding of $H_K \overset{c}{\hookrightarrow} L^\infty$ in Assumption 1 combined with the condition in Assumption 5\(a\) on the decay of $\kappa$ (the “spectrum” of the kernel $K$ with respect to the Lebesgue measure) enables us to “infer” the decay of $\mu_\nu$ from that of $\kappa$ via the index function $\psi$. Moreover, in Lemma 2 we will demonstrate Assumption 5\(a\) is satisfied when the Marcinkiewicz space $M_\psi$ “tightly” contains the regularized transform $\frac{F_{d\kappa(t^{-\frac{1}{2}})}}{t}$, where $\Psi$ is the fundamental function of $L^\psi$, the Orlicz space with Young function $\psi$.

Lemma 2. Let $\Psi$ be the fundamental function of the Orlicz space $L^\psi$. Then, Assumption 5\(a\) implies that $\frac{F_{d\kappa(t^{-\frac{1}{2}})}}{t} \in M_\psi$, and $M_\psi$ is the smallest ultrasymmetric space containing $\frac{F_{d\kappa(t^{-\frac{1}{2}})}}{t}$ with fundamental function $\Psi$.

Intuitively, Lemma 2 ensures that the index function $\psi$ is optimal for characterizing the decay of $\kappa$ (and hence the smoothness of $k$). Indeed, recall from section 3\(a\)\(b\) that the Marcinkiewicz space $M_\psi$ is the largest rearrangement-invariant space with fundamental function $\Psi$ (which is closely related to the index function $\psi$ by definition, indeed
We first present our upper bound on the mean-square error in Theorem 3. The proof of Theorem 3 hinges on the following bias-variance decomposition, which illustrates that, up to a constant, 

\[ \Psi(t) = \frac{1}{\phi(t \nu)} \]. Hence, the assumption that \( M_\psi \) is the smallest such space containing \( \mathcal{F} \), implies that the fundamental function \( \Psi \) (and hence \( \psi \)) is “tight” in a sense for characterizing the smoothness of \( k \) (as \( \mathcal{F} \) lies at the “boundary” of the scale of spaces indexed by \( \Psi \)).

### 3.4.1 Related Work

Assumptions 1-5 can be viewed as a generalization of those in [14] to Hilbert scales. Namely, our source condition in Assumption 2 and embedding condition \( H^\psi \rightarrow L^\infty \) in Assumption 4 reduce to the corresponding source and embedding conditions in [14] with the choice of \( \phi(t) = t^\beta \) and \( \psi(t) = t^\alpha \) (using their notation). The additional embedding \( H^\psi \rightarrow H^\psi \) in Assumption 4 is not strictly necessary for the derivation of minimax rates, but helps simplify the analysis. Intuitively, this embedding ensures that \( f^* \) is bounded.

We emphasize that a distinctive feature of our analysis is that we do not make any assumption on the eigendecay of \( T_\nu \), or its effective dimension. Indeed, while [7, 8] established learning rates in the stronger \( \| \cdot \|_K \) norm for more general regularization schemes, their analysis only considered Holder-type source conditions and hinged on a particular asymptotic eigendecay of \( T_\nu \) (which depends on the unknown measure \( \nu = P|_X \)). [32, 33] consider general source conditions similar to this paper (and for more general regularization schemes), although they too place conditions on the decay of the effective dimension of \( T_\nu \) (which is strongly related to its eigendecay). Recently, [22] considered Lepski-based parameter selection strategy for general regularization schemes, and demonstrated that known estimates on the effective dimension of \( T_\nu \) can be effectively leveraged for adapting to misspecification.

To the best of our knowledge, this is the first work to establish minimax learning rates under general source conditions without appealing to any direct assumptions on the eigendecay or effective dimension of the Mercer operator \( T_\nu \). Instead, our approach leverages the \( L^\infty \) embedding of the Hilbert scale \( H^\psi \) and a compatibility condition between \( \psi \) and the Fourier transform of the kernel (Assumption 5) to infer spectral information on \( T_\nu \). In a sense, our analysis demonstrates that, via an interpolation inequality, evaluating the tightness of the embedding \( H^\psi \rightarrow L^\infty \) is in a sense equivalent to evaluating the optimality of \( \psi \) in characterizing the decay of the Fourier transform \( \mathcal{F} \) (via the Marcinkiewicz space \( M_\phi \psi \); see Lemma 2). When \( \psi \) is indeed optimal, the interpolation inequality (Lemma D.1) provides the correct “change of measure”. However, this delicate relationship hinges on the radiality of the kernel, and does not obviously extend to more general kernel families.

### 3.5 Results

We first present our upper bound on the mean-square error in Theorem 3.

**Theorem 3.** Suppose Assumptions 1-5 hold and \( \epsilon \sim \text{SG}(\sigma^2) \) in (1). Choosing \( \lambda_n \sim (\phi(\psi^{-1}) (n-1) \), we obtain, with probability \( 1 - 2 \delta \),

\[ \| f_D, \lambda_n - f^* \|_{L^2(\nu)} \leq \log(\delta^{-1}) \sqrt{\phi((\psi^{-1}) (n-1))} \]  

This can be extended to the case of subexponential noise (satisfying the common Bernstein condition) in light of the proof of Lemma B.3 (see Remark following Lemma B.3). However, in order to match the subgaussian framework under which the PAC-Bayesian adaptation scheme was developed, we simply suppose the noise is subgaussian here.

Intuitively, this function \( \phi \circ (\psi^{-1}) \) appearing in (9) can be viewed as capturing the “ratio” between the capacities of the Hilbert scales \( H^\psi \) and \( H^\psi \). For example, when \( \phi(t) = t^\beta \) and \( \psi(t) = t^\alpha \) are power functions (with \( \alpha, \beta \in (0, 1) \)), \( \phi \circ (\psi^{-1}) = t^{\alpha - \beta} \), and we see that the exponent captures precisely the contribution of \( \beta \) to the sum \( \alpha + \beta \), which geometrically reflects the relative distances of \( H^\beta \) to \( H^\alpha \) and \( H^\psi \), respectively (recall that \( H^\psi \subset H^\beta \subset H^\alpha \) by Assumption 1). When this ratio is high (i.e. \( H^\beta \) is much closer to \( H^\alpha \) than \( H^\psi \)), the hypothesis class approximates the true \( f^* \in H^\beta \) relatively well and hence we achieve a fast learning rate. When, this ratio is near its maximal value of \( 1 \), i.e. \( H^\beta \) and \( H^\alpha \) are very close, we essentially can only surmise that \( f^* \) is bounded (as \( H^\alpha \rightarrow L^\infty \), and therefore the hypothesis class may only provide a very coarse approximation to \( H^\beta \), causing the sample estimator \( f_{D, \lambda} \in H^\beta \) to converge very slowly to the limit point \( f^* \).

The proof of Theorem 3 hinges on the following bias-variance decomposition, which illustrates that, up to a constant, both components of the error can be controlled purely in terms of the index functions \( \phi \) and \( \psi \):

**Lemma 4.** Suppose Assumptions 1-5 hold and \( \epsilon \sim \text{SG}(\sigma^2) \) in (1). Then:

\[ \| f^* - f_{D, \lambda} \|_{L^2(\nu)} \leq \| f^* \|_{\phi} \sqrt{\phi(\lambda)} + \sqrt{\frac{1152 \log(2\delta^{-1}) \sigma^2 \| k_\nu \|_{L^2(\nu)}^2 \| f^* \|_{\phi}^2}{n\psi(\lambda)}} \]
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with probability $1 - 3\delta$.

As noted above, we observe here that the kernel only appears in \[10\] via the constant term $\|k\|_\infty$, and hence $k$ does not influence the asymptotic behavior of the upper bound as $\lambda \to 0$. This surprising absence of the kernel (beyond a constant), can be attributed to the embedding conditions in Assumption \[1\] which ensure that (via a Gagliardo-Nirenberg type inequality) uniform bounds on the bias depend only on the ratios between norms in $\mathcal{H}^\psi$, and $\mathcal{H}^\phi$ and $\mathcal{H}_K$, respectively. Moreover, due to relative growth rates of the index functions implied by compactness, these capacity ratios depend solely on $\phi$ and $\psi$.

We now discuss the optimality of the upper bound in Theorem 3. The derivation of a minimax lower bound matching widths of \[9\] is significantly more involved and hinges crucially on the sharpness of the embedding $U \hookrightarrow L^\infty$, which in turn depends on the compactness properties of the domain $X \subseteq \mathbb{R}^d$ (captured by the entropy condition in Assumption \[4\]) and the smoothness of the kernel $k$. Unlike the derivation of the upper bound, we cannot reduce this analysis simply to a comparison of the index functions, as we must demonstrate the maximality of the spectral function $\psi$ in “stretching” the functions in $\mathcal{H}_K$. Informally, we need to ensure that the enlarged (infinite-dimensional) ellipsoid $\psi(\mathcal{H}_K)$ is “maximal” in $L^\infty$, otherwise our use of $\mathcal{H}^\psi$ as a proxy for $L^\infty$ in the derivation of \[9\] is suboptimal (i.e. $\|\cdot\|_{\mathcal{H}^\psi}$ may provide a very coarse approximation of $\|\cdot\|_\infty$). We quantify this maximality via estimating the Bernstein widths of $\mathcal{H}_K$ in $L^\infty$, which can then be compared to the eigenvalues $\mu_i$ (the Bernstein widths of $\mathcal{H}_K$ in $L^2(\nu)$; see e.g. Prop. 5 in \[24\]) via the Gagliardo interpolation inequality. The latter widths are independent of the measure $\nu$ and therefore depend only on the smoothness of $k$ (captured by its Fourier decay) and the compactness of $X$. Intuitively, the embedding $\mathcal{H}^\psi \hookrightarrow L^\infty$ is sharp (and our learning rate in \[9\] is optimal) if the index function $\psi$ provides the correct “change-of-measure” from $\nu$ to the $d$-dimensional Lebesgue measure.

**Theorem 5.** There exists a distribution $P$ on $X \times \mathbb{R}$ with $P|X = \nu$, $\|f_p\|_\phi \leq B_\phi$, $\|f_p\|_\infty \leq B_\infty$, and $\epsilon \sim \mathbb{S}\mathbb{G}(\sigma^2)$ such that, for any learning algorithm $D \mapsto f_D$, we have with $P$-probability not less than $1 - \frac{432e(D)^2}{U_{d,\infty,\phi}\sigma^2\log 2}$,

$$\|f_D - f_p\|_{L^2(\nu)} \geq \sqrt{\delta \phi((\phi\psi)^{-1}(n^{-1}))},$$

where $U_{d,\infty,\phi}$ does not depend on $n$ or $T$ and $u = \log_{D_\phi} T$.

Moreover, equipped with Lemma \[4\] it is easy to see that when the index functions $\phi$ and $\psi$ satisfy the $\Delta_2$ condition as in Assumption \[1\] then the hypotheses of Theorem \[3\] are satisfied, and hence we achieve the optimal learning rate as long as $\psi(t) \log(t^{-1}) \to 0$ as $t \to 0$, i.e. $\psi$ decays to 0 faster than $-\frac{\log t}{\log \tau}$. This is the case for example, when $\psi = t^\beta$ is a power function for $\beta \in (0, 1)$ (as in \[12\]).

**Corollary 5.1.** Suppose Assumptions \[1\][3\] are satisfied and $\psi(t) \log(t^{-1}) \to 0$ as $t \to 0$. Then, the PAC-Bayesian adaptation algorithm achieves the optimal learning rate, i.e.

$$R(f_{\lambda_2n,D}) \asymp R(f_{\lambda_2n,D}),$$

where $\lambda_{2n} \asymp (\phi\psi)^{-1}\left(\frac{1}{2n}\right)$.

### 4 Conclusion

In this paper, we develop a PAC-Bayesian adaptation scheme for regularized regression. Our approach proposes a a posteriori choice for the regularization parameter, based on calculating the expectation of a PAC-Bayesian posterior distribution with exponentially weighted risks. Unlike existing adaptation procedures, the computational effort of our approach does not grow with the sample size $n$. We derive oracle bounds for our adaptation strategy that recover the optimal learning rate over a large class of regularization instances.

In the second part of the paper, we derive novel minimax learning rates for ridge regression over Hilbert scales with general source conditions. A notable feature of our analysis is that we do not impose the conventional conditions on eigendecay rates, and instead present a new approach based on estimating the Bernstein widths of the kernel class in $L^\infty$ to demonstrate minimax optimality.

The need for smoothness-adaptive learning approaches extends beyond the framework of offline regression or statistical estimation. In recent years, several studies have demonstrated that online decision-making problems can be successfully reduced to offline (i.i.d) regression problems via a suitable schedule of oracle calls \[15, 20, 38\]. Potential misspecification in the target function class is quite prevalent in these settings, as the ambient measure governing the data-generating process is non-stationary and influenced by the history of the learner’s actions. Thus, we hope that the adaptive regression approaches proposed in this paper find broader use in improving model selection and combating misspecification in the face of real-time decisions.
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A Proof of Theorem 1 and Lemma 2

Proof of Theorem 1 Our proof is heavily motivated by that of Theorem 3.1 in [2], and hence we highlight the components that depart from the latter. We consider the empirical risk over the test data: \( \{X_i\}_{i=1}^n \). Since this dataset is fixed here, we omit specifying it in the estimator and simply write \( f_\lambda \). For \( i \in [n] \) and \( \lambda > 0 \), define:

\[
T_i = (Y_i - f^*(X_i))^2 - (Y_i - f_\lambda(X_i))^2
\]

Observe that:

\[
E[T_i | X_i] = E[(2\epsilon_i + f^*(X_i) - f_\lambda(X_i))(f_\lambda(X_i) - f^*(X_i))|X_i] = -(f_\lambda(X_i) - f^*(X_i))^2
\]

Hence, by the subgaussianity of \( \epsilon_i \equiv Y_i - f^*(X_i) \), we have that for \( \nu > 0 \):

\[
E[\exp(\nu(T_i - E[T_i | X_i]))|X_i] \leq \exp(4\nu^2\sigma^2(f^*(X_i) - f_\lambda(X_i))^2)
\]

Hence, we have that \( T_i + (f_\lambda(X_i) - f^*(X_i))^2 \) is conditionally SG\((4\sigma^2(f^*(X_i) - f_\lambda(X_i))^2)\). Hence, choosing \( \nu = \frac{2}{n} \) for \( \gamma > 0 \), we have that:

\[
E\left[\exp\left(\frac{2}{n} \sum_{i=1}^n T_i - E[T_i | X_i]\right) | X_i\right] \leq \exp\left(\frac{4\gamma^2\sigma^2}{n^2} \sum_{i=1}^n (f^*(X_i) - f_\lambda(X_i))^2\right)
\]
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Now, define:
\[
\begin{align*}
    r_D(f) &= \frac{1}{n} \sum_{i=1}^{n} (Y_i - f(X_i))^2 \\
    R_D(f) &= \frac{1}{n} \sum_{i=1}^{n} (f^*(X_i) - f(X_i))^2
\end{align*}
\]

Then, we obtain:
\[
\int_{0}^{\infty} \mathbb{E} \left[ \exp \left( \gamma (r_D(f^*) - r_D(f_\lambda)) + \beta_1 R_D(f_\lambda) + \log \frac{\delta}{2} \right) \right] d\mu(\lambda) \leq \frac{\delta}{2}
\]
where \( \beta_1 = \gamma - \frac{4\nu^2 \alpha^2}{n} \). Similarly, we have that:
\[
\int_{0}^{\infty} \mathbb{E} \left[ \exp \left( \gamma (r_D(f_\lambda)) - r_D(f^*) - \beta_2 R_D(f_\lambda) + \log \frac{\delta}{2} \right) \right] d\mu(\lambda) \leq \frac{\delta}{2}
\]
where \( \beta_2 = \gamma + \frac{4\nu^2 \alpha^2}{n} \). (by considering \(-T_i\)). Then, following identical steps as in the proof of Theorem 3.1 in [2] (see p.141; equations (4.5)-(4.6) therein), we can obtain, via a change of measure and application of Jensen’s inequality that, with probability \(1 - \delta\) (with respect to the draw of the data):
\[
R_D(f_{\lambda_{2n}}) \leq \inf_{\rho \leq \mu} \frac{\beta_2 \int R_D(f_\lambda) d\rho(\lambda) + 2(KL(\rho||\mu) + \log \frac{2}{\delta})}{\beta_1}
\]
We note that choosing \( \gamma = \frac{2}{\alpha^2 n} \), this becomes:
\[
R_D(f_{\lambda_{2n}}) \leq \inf_{\rho \leq \mu} 3 \int R_D(f_\lambda) d\rho(\lambda) + \frac{32}{\sigma^2 n} (KL(\rho||\mu) + \log \frac{2}{\delta}) \tag{11}
\]
Take expectations of both sides with respect to \( D \sim P^n \). Then, we obtain:
\[
R(f_{\lambda_{2n}}) \leq \inf_{\rho \leq \mu} 3 \int R(f_\lambda) d\rho(\lambda) + \frac{32}{\sigma^2 n} (KL(\rho||\mu) + \log \frac{2}{\delta}) \tag{12}
\]
Now, we consider the uniform measure \( \rho \) on \([\lambda_{2n}^2, 2\lambda_{2n}^2]\). Noting that on the support of \( \rho \), we have:
\[
R(f_\lambda) \leq B(\lambda) + \Upsilon(\lambda) \tag{13}
\]
\[
\leq B\left(2\lambda_{2n}^2\right) + \Upsilon\left(\frac{\lambda_{2n}^2}{2}\right) \tag{14}
\]
\[
\leq B^B\left(\lambda_{2n}^2\right) + \Upsilon\left(\frac{\lambda_{2n}^2}{D_1^B}\right) \tag{15}
\]
where \(13\) and \(15\) follow from the definition of \( B, \Upsilon \) in [3], \(14\) follow from the fact that \( B \) is nondecreasing and \( \Upsilon \) nonincreasing in \( \lambda \), and \(13\). Hence, substituting \( \rho \) into \(12\), and observing that \( KL(\rho||\mu) = \log \left(\frac{\sqrt{2}}{\sigma \lambda_{2n}}\right) + \frac{5\lambda_{2n}^2}{4} \), we obtain our result.

**Proof of Lemma 2** We recall that the fundamental function of the Orlicz space \( L^{\Psi} \) is \( \Psi = \frac{1}{\psi^{-1}(t^{-1})} \). Hence, by Assumption 5 we have that:
\[
1 \geq \frac{\mathcal{F}_{d;\eta}(t^{\frac{1}{\psi}})}{t^{1/\psi - 1}} = \frac{1}{\psi^{-1}(t^{-1})} \cdot \left( \frac{\mathcal{F}_{d;\eta}(t^{\frac{1}{\psi}})}{t} \right)^{\ast} \tag{16}
\]
where the last inequality follows from the fact that \( \mathcal{F}_{d;\eta}(\cdot) \) is nonincreasing. Therefore, since \( \psi \) satisfies the \( \Delta_2 \) condition \(2\), and \( \Psi \) has finite nonzero extension indices (see p.274 of [3] for a definition), we have by Lemma 2.16 in [12] that \( \mathcal{F}_{d;\eta}(t^{\frac{1}{\psi}}) \in M_{\Psi} \). To see that \( M_{\Psi} \) is the largest ultrasmooth space with fundamental function \( \Psi \) containing \( \mathcal{F}_{d;\eta}(t^{\frac{1}{\psi}}) \), we proceed by contradiction and suppose this is not the case. Then, we apply Theorem 2.1 in [50], to deduce
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that for any such space $G$, there is an interpolation space $E$ between $L^1(\mathbb{R})$ and $L^\infty(\mathbb{R})$ (with respect to the measure $\frac{dt}{t}$) that is rearrangement invariant, such that:

$$\| \frac{\mathcal{F}_E(t^\frac{1}{2})}{t} \|_G = \| \frac{\mathcal{F}_E(t^\frac{1}{2})}{\Gamma_\psi^{-1}(t^{-1})} \|_E$$

Now, since $E$ is rearrangement invariant, it follows by (16) that there exists a $c > 0$, such that, for any $s > 0$ and set $F$ of measure $s$, $c\phi_E(s) = \|c\chi_F\|_E \leq \| \frac{\mathcal{F}_E(t^\frac{1}{2})}{\Gamma_\psi^{-1}(t^{-1})} \|_E$, where $\phi_E$ is the fundamental function of $E$. Since $\phi_E$ is nondecreasing, it follows that $\phi_E$ must therefore be eventually constant, which implies that $E \cong L^\infty$, which is a contradiction. \hfill \Box

B Proof of Theorem 3

The main effort in the proof of Theorem 3 involves proving Lemma 4, from which the Theorem 3 easily follows; hence we will begin with the proof of Lemma 4. We start with the following bound on the bias:

Lemma B.1.

$$\|f^* - f_\lambda\|^2_{L^2(\nu)} \leq \phi(\lambda)\|f^*\|^2_\phi$$

Proof. Since $f \in H^\phi$, we have that there exists a $\{a_i\}_{i=1}^\infty \in \ell^2$ such that:

$$f^* = \sum_i a_i \phi^\frac{1}{2}(\mu_i) e_i$$

Hence,

$$f^* - f_\lambda = \sum_{i=1}^\infty \frac{a_i \lambda \phi^\frac{1}{2}(\mu_i)}{\mu_i + \lambda} e_i$$

Therefore, by the Cauchy-Schwartz inequality:

$$\|f^* - f_\lambda\|^2_{L^2(\nu)} \leq \sum_{i=1}^\infty \left( \frac{a_i \lambda \phi^\frac{1}{2}(\mu_i)}{\mu_i + \lambda} \right)^2 \leq \left( \sup_{i} \frac{\lambda^2 \phi(\mu_i)}{(\mu_i + \lambda)^2} \right) \sum_{i=1}^\infty a_i^2 \leq \left( \sup_{i} \frac{\lambda^2 \phi(\mu_i)}{(\mu_i + \lambda)^2} \right) \|f^*\|^2_\phi$$

Now, observe that for $\mu_i < \lambda$:

$$\sup_{i: \mu_i < \lambda} \frac{\lambda^2 \phi(\mu_i)}{(\mu_i + \lambda)^2} \leq \phi(\lambda)$$

as $\phi$ is nondecreasing. For $\mu_i \geq \lambda$, we have that:

$$\sup_{i: \mu_i \geq \lambda} \frac{\lambda^2 \phi(\mu_i)}{(\mu_i + \lambda)^2} = \sup_{i: \mu_i \geq \lambda} \frac{\lambda^2 \mu_i^2 \phi(\mu_i)}{\mu_i^2 (\mu_i + \lambda)^2} \leq \sup_{i: \mu_i \geq \lambda} \frac{\lambda^2 \mu_i^2 \phi(\lambda)}{\mu_i^2 (\mu_i + \lambda)^2} \leq \phi(\lambda)$$

where the second inequality follows from the fact that $\frac{\phi(t)}{t^2}$ is nonincreasing (from Assumption 1). Putting this together, we obtain our result. \hfill \Box

Lemma B.2.

$$\|f^* - f_\lambda\|^2_{L^\infty} \leq \frac{\phi(\lambda)\|k_\psi\|^2_{L^\infty} \|f^*\|^2_\phi}{\psi(\lambda)}$$
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Proof. We have from (17):

$$\|f^* - f_\lambda\|_\infty^2 \leq \sum_{i=1}^\infty \frac{a_i \phi(\mu_i)^2 e_i(\cdot)}{\mu_i + \lambda}$$

where (19) follows from the fact that for any $h$ that $\phi(t)$ is decreasing for $t \geq \lambda$ and $\frac{\phi(t)}{\psi(t)}$ is increasing for $t < \lambda$ by Assumption [1]

Proof. We begin with a standard decomposition applied in the proof of Theorem 16 in [14] and Theorem 7 in [42]. We first observe that:

$$\|f - f_{D,\lambda}\|_{L^2(\nu)} = \|f - f_{D,\lambda}\|_K$$

with probability $1 - 3\delta$

Proof. We begin with a standard decomposition applied in the proof of Theorem 16 in [14] and Theorem 7 in [42]. We first observe that:

$$f_\lambda - f_{D,\lambda} = f_\lambda - (C_D + \lambda)^{-1} g_D = (C_D + \lambda)^{-1} ((C_D + \lambda) f_\lambda - g_D)$$

where $g_D = \sum_{i=1}^n y_i k(x_i, \cdot) \in H_K$. Hence, we have that:

$$\|f_\lambda - f_{D,\lambda}\|_{L^2(\nu)} = \|f_{\lambda} - (C_D + \lambda)^{-1} g_D\|_K$$

where (19) follows from the fact that for any $f \in H_K$, $(I_\nu f, I_\nu f)_K = \langle f, C_\nu f \rangle_K$ and (6), and (20) follows from (18) and algebraic manipulation. It is easy to see that:

$$\|C_\nu f\|_K^2 \leq 1$$

We now analyze second factor in (20). Indeed, we have that:

$$(C_\nu + \lambda)^{-\frac{1}{2}} (C_D + \lambda)^{-1} (C_\nu + \lambda)^{-\frac{1}{2}} = \left(I - (C_\nu + \lambda)^{-\frac{1}{2}} (C_D + \lambda)^{-\frac{1}{2}} (C_\nu + \lambda)^{-\frac{1}{2}}\right)^{-1}$$

by the same algebraic manipulation as in the proof of Theorem 16 in [14] (for the sake of space, we avoid repeating the argument verbatim here). Hence, estimating the middle factor in (20) boils down to estimating the concentration of $(C_\nu + \lambda)^{-\frac{1}{2}} (C_D + \lambda)^{-\frac{1}{2}} (C_\nu + \lambda)^{-\frac{1}{2}}$. We first note that:

$$(C_\nu + \lambda)^{-\frac{1}{2}} (C_D - C_\nu) (C_\nu + \lambda)^{-\frac{1}{2}} = E_X[h(X, \cdot) \otimes h(X, \cdot)] - E_D[h(X, \cdot) \otimes h(X, \cdot)]$$

where $h(x, \cdot) = (C_\nu + \lambda)^{-\frac{1}{2}} k(x, \cdot)$. Note, by Lemma [12] we have that $\|h(x, \cdot)\|_K \leq \sqrt{\sum_{k}^\nu ||k||^2 \psi(\lambda)}$. Then, analogously to Lemma 17 in [14], we may demonstrate that:

$$(C_\nu + \lambda)^{-\frac{1}{2}} (C_D - C_\nu) (C_\nu + \lambda)^{-\frac{1}{2}} \leq \frac{2}{3}$$

with probability $1 - 2\delta$, when $n \geq 8 \log(\delta^{-1}) ||k^\nu||_\infty^2 g_X \psi(\lambda)^{-1}$, where $g_\lambda = \log(2eN(\lambda)\left(1 + \frac{\lambda}{1 + n}\right))$, where $N(\lambda) = \text{tr}(C_\nu (C_\nu + \lambda)^{-1})$ Applying a Neumann series expansion, we obtain (like in [14]):

$$\|(C_\nu + \lambda)^{\frac{1}{2}} (C_D + \lambda)^{-1} (C_\nu + \lambda)^{\frac{1}{2}} = \|(I - (C_\nu + \lambda)^{-\frac{1}{2}} (C_D + \lambda)^{-\frac{1}{2}} (C_\nu + \lambda)^{-\frac{1}{2}}\) \leq 3$$

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for \( n \geq 8 \log(\delta^{-1}) ||\psi||_\infty^2 g_\lambda \psi(\lambda)^{-1} \). Now, it remains to bound the third factor in (20). We observe that we may write:

\[
(C_\nu + \lambda)^{-\frac{1}{2}} ((C_\nu + \lambda) f_\lambda - g_D) = (C_\nu + \lambda)^{-\frac{1}{2}} ((C_\nu + \lambda) f_\lambda + S_\nu f^* - g_D) = E_D[h(x, \cdot) (f_\lambda(X) - Y)] - E_Y[h(x, \cdot) (f_\lambda(X) - Y)]
\]

which follow by the definition of \( f_\lambda \) and \( h(x, \cdot) \). In order to estimate this concentration, we compute absolute moments:

\[
E_X E_Y[||(h(X, \cdot) (f_\lambda(X) - Y))||^p_K] \leq E_X E_Y[||(h(X, \cdot) (f_\lambda(X) - f^*(X) + f^*(X) - Y))||^p_K] \\
\leq 2p^{-1} E_X E_Y[||(h(X, \cdot)||^p_K ||(f_\lambda(X) - f^*(X))||^p + ||f^*(X) - Y||^p)] \\
\leq 2p^{-1} E_X E_Y[||(h(X, \cdot)||^p_K ||(f_\lambda(X) - f^*(X))||^p + \frac{1}{2} ||f^*(X) - 1||^p] 
\]

where in the last line we have used the fact \( Y|X \) is \( \sigma^2 \) – subgaussian and Proposition 3.2 in \[34\]. Applying Lemmas D.2 and B.2 it follows that:

\[
E_X E_Y[||(h(X, \cdot) (f_\lambda(X) - Y))||^p_K] \leq 2p^{-1} \left( \frac{1}{\psi(\lambda)} \left( \frac{||k||_2^2 ||f^*||_\phi}{2} \right)^p + p \Gamma \left( \frac{p}{2} \right) \left( \frac{2||k||_2^2 \sigma^2}{\psi(\lambda)} \right)^{\frac{p}{2}} \right) \\
\leq 2p^{-1} \left( \frac{1}{\psi(\lambda)} \left( \frac{||k||_2^2 ||f^*||_\phi}{2} \right)^p + p \Gamma \left( \frac{p}{2} \right) \left( \frac{2||k||_2^2 \sigma^2}{\psi(\lambda)} \right)^{\frac{p}{2}} \right) \\
\leq \frac{p ||k||_2^2 R^2}{\lambda} 
\]

with \( L = \frac{2||f^*||_\phi ||k||_\phi}{\psi(\lambda)} \) and \( R^2 = \frac{2||f^*||_\phi ||k||_\phi}{\psi(\lambda)} \). (21) follows from the fact that \( \frac{\phi(\lambda)}{\psi(\lambda)} \rightarrow 0 \) as \( \lambda \rightarrow 0 \). Hence, applying Theorem 26 in \[14\], we have that:

\[
||((C_\nu + \lambda)^{-\frac{1}{2}} ((C_\nu + \lambda) f_\lambda - g_D))||_K^2 \leq \frac{32 \log(2\delta^{-1})}{n} \left( \frac{2||k||_2^2 ||f^*||_\phi^2}{\psi(\lambda)} + \frac{4||k||_2^2 ||f^*||_\phi^2}{n \psi(\lambda)} \right) \leq \frac{128 \log(2\delta^{-1}) \sigma^2 ||k||_2^2 ||f^*||_\phi^2}{n \psi(\lambda)} 
\]

with probability \( 1 - \delta \). Putting this all together, we have that:

\[
||f_\lambda - f_D, \lambda||_{L^2(\nu)} \leq \sqrt{\frac{1152 \log(2\delta^{-1}) \sigma^2 ||k||_2^2 ||f^*||_\phi^2}{n \psi(\lambda)}} 
\]

with probability \( 1 - 3\delta \), when \( n \geq 8 \log(\delta^{-1}) ||\psi||_\infty^2 g_\lambda \psi(\lambda)^{-1} \). We demonstrate that this latter condition is eventually met, when the regularization program is \( \lambda_n \approx (\psi(\lambda))^{-1}(n^{-1}) \). Indeed, we have that:

\[
\frac{8 \log(\delta^{-1}) ||\psi||_\infty^2 g_\lambda}{n \psi(\lambda)} = \frac{8 \log(\delta^{-1}) ||\psi||_\infty^2}{n \psi(\lambda)} \log \left( 2eN(\lambda_n) \left( 1 + \frac{\lambda_n}{||f^*||_\phi} \right) \right) \leq \frac{16 \log(\delta^{-1}) ||\psi||_\infty^2}{n \psi(\lambda)} \log \left( 2eN(\lambda_n) \right) \leq \frac{16 \log(\delta^{-1}) ||\psi||_\infty^2}{n \psi(\lambda)} \log \left( \psi(\lambda)^{-1} \right) 
\]

where the last line follows by Lemma D.3. Hence, it is sufficient to demonstrate that \( \log \left( \frac{\psi(\lambda_n)^{-1}}{n \psi(\lambda)} \right) \) for the regularization program. Indeed, since \( \lambda_n \approx (\psi(\lambda))^{-1}(n^{-1}) \), we have that:

\[
\frac{\log \left( \frac{\psi(\lambda_n)^{-1}}{n \psi(\lambda)} \right)}{\psi(\lambda)} \approx \phi(\lambda_n) \cdot \log \left( \psi(\lambda_n)^{-1} \right) \leq \frac{\phi(\lambda_n)}{\psi(\lambda)} \rightarrow 0
\]

by Assumption I.

**Remark.** Note that in light of the proof of Lemma B.3 and the application of the Theorem 26 in \[14\] (which was designed for subexponential noise), an almost identical proof can be applied when the noise satisfies a Bernstein-type subexponential condition (in a sense, applying Theorem 26 from \[14\] here required us to frame the subgaussian noise as subexponential).
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Proof of Lemma 4: This follows immediately by combining Lemma B.3 with Lemma B.1.

Proof of Theorem 3: Follows immediately from the Lemma 4 after substituting the choice of regularizer (which was proposed via balancing).

C Proof of Theorem 5

Lemma C.1.

\[ b_{n-1}(\mathcal{H}_K, L^\infty) \leq \|k^\psi\|_\infty^2 \left( \frac{t}{\psi} \right) (\mu_n) \]

Proof. We first note that since \( t(\psi) \) is concave by Assumption 1, we have by the Gagliardo-Nirenberg interpolation inequality (Lemma B.1), that for all \( f \in \mathcal{H}_K \):

\[ \frac{\|f\|^2_\nu}{\|f\|^2_\nu} \leq \left( \frac{t}{\psi} \right) \left( \frac{\|f\|^2_\psi}{\|f\|^2_{\mathcal{H}_K}} \right) \]

By the embedding condition \( \mathcal{H}_\psi \hookrightarrow L^\infty \), we have hence have that:

\[ \frac{\|f\|^2_\nu}{\|f\|^2_\nu} \leq \|k^\psi\|_\infty^2 \left( \frac{t}{\psi} \right) \left( \frac{\|f\|^2_\psi}{\|f\|^2_{\mathcal{H}_K}} \right) \]

Hence, we have that:

\[ \sup_{\text{dim}(Z) \geq n} \inf_{f \in Z \cap \mathcal{H}_K} \frac{\|f\|^2_\nu}{\|f\|^2_\nu} \leq \sup_{\text{dim}(Z) \geq n} \inf_{f \in Z \cap \mathcal{H}_K} \|k^\psi\|_\infty^2 \left( \frac{t}{\psi} \right) \left( \frac{\|f\|^2_\psi}{\|f\|^2_{\mathcal{H}_K}} \right) \]

\[ = \|k^\psi\|_\infty^2 \left( \frac{t}{\psi} \right) \left( \sup_{\text{dim}(Z) \geq n} \inf_{f \in Z \cap \mathcal{H}_K} \frac{\|f\|^2_\psi}{\|f\|^2_{\mathcal{H}_K}} \right) \]

where the last step follows from the fact that \( t(\psi) \) is nondecreasing and continuous. Hence, by the definition of the Bernstein width (3.3), and Proposition 5 in [24], we obtain our result.

Lemma C.2.

\[ b_{n-1}(\mathcal{H}_K, L^\infty) \geq \sqrt{C_d F_d K(n^{\frac{d}{2}})} \]

where \( C_d > 0 \) is constant depending on the dimension \( d \) and independent of \( n \).

Proof. Let \( \{z_i\}_{i=1}^{2n} \subset \mathcal{X} \) be a set of \( 2n \) distinct points in \( \mathcal{X} \). Consider the subspace \( Z = \text{span}\{k(z_i, \cdot)\}_{i=1}^{2n} \subset \mathcal{H}_K \). Since, \( k \) is positive definite by assumption, we have that \( \text{dim}(Z) = 2n \). Since \( \mathcal{H}_K \) is a Hilbert space, \( Z \) is isomorphic to \( L^2(\mathbb{R}^{2n}, \mu_2) \) (with the Euclidean norm). By Theorem 3.1 in [43] (see also Theorem 1 in [29]), there exists a subspace \( \tilde{Z} \subset Z \) of dimension \( n \) and constant \( C > 0 \), such that:

\[ \|z\|_{\mathcal{H}_K} \leq \sqrt{\frac{C}{2}} M^*(B(L^\infty) \cap Z) \]

for all \( z \in \tilde{Z} \cap B(L^n) \) (we will absorb additional constants into \( C \) throughout this proof). Here, \( M^*(B(L^\infty) \cap Z) \) denotes the mean width of \( B(L^\infty) \cap Z \) given by:

\[ M^*(B(L^\infty) \cap Z) = \int_{\partial B(Z)} \sup_{x \in B(L^\infty) \cap Z} (x, y)_{K} dS_{2n}(y) \]

where \( S_{2n}(\cdot) \) is the canonical uniform measure over the unit sphere in \( Z \). Let \( \gamma_{2n} \) denote the standard Gaussian measure on \( \mathbb{R}^{2n} \), and \( \mu_{2n} \) its pushforward onto \( Z \) via the canonical isomorphism. We write \( g = \sum_{i=1}^{2n} a_i(g) k(z_i, \cdot) \)
We now wish to upper bound $|q|$ where

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where again we recall that the overhead constant $C_1 > 0$:

$$M^*(B_\infty \cap Z) = \int_{\partial B(Z)} \sup_{f \in B(L^\infty) \cap Z} \langle f, g \rangle dS_{2n}(g)$$

$$= \frac{C_1}{\sqrt{2n}} \int_Z \sup_{f \in B(L^\infty) \cap Z} \langle f, g \rangle d\mu_{2n}(g)$$

$$= \frac{C_1}{\sqrt{2n}} \int_Z \sup_{f \in B(L^\infty) \cap Z} \left( \sum_{i=1}^{2n} a_i(g)k(z_i, \cdot) \right) d\mu_{2n}(g)$$

$$= \frac{C_1}{\sqrt{2n}} \int_Z \left( \sum_{i=1}^{2n} a_i(g)f(z_i) \right) d\mu_{2n}(g)$$

$$\leq \frac{C_1}{\sqrt{2n}} \int_Z \left( \sum_{i=1}^{2n} a_i(g) \right) d\mu_{2n}(g)$$

since $|f(z_i)| \leq 1$ as $f \in B(L^\infty)$. Now, observe that $g \in \partial B(Z)$ iff $a(g) \cdot (K_{2n}a(g)) = 1$, where $a(g) = [a_1(g), \ldots, a_{2n}(g)]^T$ and $(K_{2n})_{ij} = k(z_i, z_j)$ is the kernel Gram matrix on $\{z_i\}_{i=1}^{2n}$. Hence, performing a change of variables (and renaming), we obtain, for a constant $C_1 > 0$:

$$M^*(B(L^\infty) \cap Z) \leq \frac{C_1}{\sqrt{2n}} \int_{R^{2n}} |K_{2n}^{-1/2}a_1| d\gamma_{2n}(a)$$

$$\leq C_1 \int_{R^{2n}} \sqrt{||K_{2n}^{-1/2}||_2} |a_1| d\gamma_{2n}(a)$$

$$\leq C_1 \sqrt{2n ||K_{2n}^{-1}||_2}$$

since $\int_{R^{2n}} |a|^2 d\gamma_{2n}(a) = 2n$ as $\gamma_{2n}$ is standard normal. Hence, putting this all together, we have:

$$\|z\|_K \leq \sqrt{C_3n ||K_{2n}^{-1}||_2}$$

for all $z \in \tilde{Z} \cap B(L^\infty)$. Hence, for all $z \in \tilde{Z}$, we have that:

$$\|z\|_K \leq \sqrt{C_3n ||K_{2n}^{-1}||_2 \|z\|_\infty}$$

where $C_3 = CC_1$. By the definition of the Bernstein width, we therefore have:

$$b_{n-1}(H_K, L^\infty) \geq \sqrt{\frac{C}{n ||K_{2n}^{-1}||_2}}$$

(23)

We now wish to upper bound $||K_{2n}^{-1}||_2$—we do this by using the following lower bound on the minimum eigenvalue of $K_{2n}$, given in Theorem 12.3 of [44]:

$$\lambda_{\min}(K_{2n}) \geq C_d \left( \frac{12.76d}{q_z} \right)^d \mathcal{F}_d(\frac{12.76d}{q_z})$$

where $q_z = \min_{i \neq j} \|z_i - z_j\|$ and $C_d > 0$ is an absolute constant depending only on the dimension $d$. We choose a maximal $2n$-set $\{z_i\}_{i=1}^{2n}$, so that $q_z$ is the packing number $p_n(\mathcal{X})$ of the domain $\mathcal{X}$. From the standard equivalence $p_n(\mathcal{X}) \approx \epsilon_n(\mathcal{X})$ and Assumption 4, we have that:

$$\lambda_{\min}(K_{2n}) \geq C_{dn} \mathcal{F}_d(\frac{12.76d(2n)^{1/2}}{q_z})$$

From the integral expression for the $d$-dimensional Fourier transform (see e.g. Theorem 5.26 in [44]), and the dilation condition in Assumption 5, we therefore have that:

$$\lambda_{\min}(K_{2n}) \geq C_{dn} \mathcal{F}_d(\frac{12.76d(n^{1/2})}{q_z})$$

where again we recall that the overhead constant $C_d > 0$ depends only on the ambient dimension in Assumption 4. Noting that $||K_{2n}^{-1}||_2 \leq \lambda_{\min}^{-1}(K_{2n})$ and plugging back into (23), we have that:

$$b_{n-1}(H_K, L^\infty) \geq \sqrt{C_{dn} \mathcal{F}_d(n^{1/2})}$$
Corollary C.2.1.

\[ \mu_n \geq \psi^{-1}(n^{-1}) \]

**Proof.** From Lemma C.1 and Lemma C.2, we have that:

\[ \frac{t}{\psi} \left( \mu_n \right) \geq b_{n-1}^2 (\mathcal{H}_K; L^\infty) \geq \mathcal{F}_d k(n^{\frac{1}{d}}) \]  

(24)

Now, from Assumption 5**, we have that:

\[ \psi^{-1}(t^{-1}) = \psi^{-1} \left( \left( \frac{t}{\psi} \right)^{-1} \left( \psi^{-1}(t^{-1}) \right) \right) \]

\[ = \left( \frac{t}{\psi} \right)^{-1} \left( \mathcal{F}_d k(t^{\frac{1}{d}}) \right) \]

Hence, combining this with (24), we have that:

\[ \mu_n \geq \psi^{-1}(n^{-1}) \]

\[ \square \]

**Remark.** Observe, that in light of the proof of Lemma C.2, Corollary C.2.1 would still hold if in Assumption 5**, \( \mathcal{F}_d k(t^{-\frac{1}{d}}) \) was replaced by \( \mathcal{F}_d k \left( 12.76d \left( \frac{2}{t} \right)^{\frac{1}{d}} \right) \). However, in order to streamline the analysis, we have chosen the simpler assumption, as also discussed in section 5.4.

**Proof of Theorem 5** We follow the general outline of the proof of Theorem 2 in [14] that was earlier utilized in [9] and [7]. Our goal is to construct a sequence of probability measures \( \{P_j\}_{j=1}^M \) on \( X \times \mathbb{R} \) with \( P_j|X = \nu \) (i.e. the measures share the same marginal on \( X \)) that are hard to learn, i.e. their regression functions \( f_j \) satisfy the source conditions but are sufficiently “well spread out” in \( L^2(\nu) \) so that it is sufficiently hard to distinguish between these functions given only the sample data. We make these ideas more precise in the subsequent analysis. Our candidate regression functions take the following form — for some fixed \( \epsilon \in (0, 1) \) and \( m \in \mathbb{N} \), we consider the element:

\[ f_\omega = 2 \sqrt{8\epsilon} \frac{1}{m} \sum_{i=1}^m \omega_i e_{i+m} \]

where \( \omega \in \{0, 1\}^m \) is some binary string. Since the sum is finite, we have that \( f \in \mathcal{H}_K \subset L^\infty \cap \mathcal{H}^\phi \). We will demonstrate that \( ||f||_\phi \leq B_\phi \) and \( ||f||_\infty \leq B_\infty \) for sufficiently large choices of \( m \). Indeed, we have that:

\[ ||f_\omega||^2_\phi = \frac{32\epsilon}{m} \sum_{i=1}^m \phi^2(\mu_{i+m}) \leq \frac{32\epsilon}{\phi(\mu_{2m})} \]

\[ ||f_\omega||^2_\infty \leq ||k^\phi||^2_\infty ||f_\omega||^2_\psi \leq \frac{32||k^\phi||^2_\infty \epsilon}{\psi(\mu_{2m})} \]

Now, by Corollary C.2.1, we have that:

\[ ||f_\omega||^2_\psi \leq \frac{32\epsilon}{\phi^{-1} \left( \frac{C_\psi m^{-1}}{2} \right)} \]

\[ ||f_\omega||^2_\infty \leq \frac{64||k^\phi||^2_\infty \epsilon}{C_\phi^d m^{-1}} \]

where \( C_d > 0 \) depends only \( d \). Hence, by the \( \Delta_2 \) condition on \( \phi \) and \( \psi \), we have that \( ||f||^2_\phi \leq B_\phi^2 \) and \( ||f||^2_\infty \leq B_\infty^2 \), when:

\[ m \leq \min \left\{ \frac{C_d B_\phi^2}{64||k^\phi||^2_\infty \epsilon}, \left( \psi \left( \phi^{-1} \left( \frac{32\epsilon}{C_d B_\phi^2} \right) \right) \right)^{-1} \right\} \]

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(where we have renamed the constant $C_d$, as we will throughout this proof). By Assumption [1] we have that $\frac{\phi(t)}{\psi(t)} \to 0$ as $t \to 0$. Hence, for sufficiently small $t > 0$, we have that $\frac{\phi^{-1}(t)}{t} = \frac{\phi^{-1}(t)}{\psi(\phi^{-1}(t))} \geq 1$. Hence, we may choose $\epsilon_1 \in (0, 1)$, such that for $\epsilon \in (0, \epsilon_1)$, we have $\|f\|_\infty^2 \leq B_\infty^2$ and $\|f\|_2^2 \leq B_\infty^2$, when:

$$m \leq \frac{U_{d, \infty, \phi}}{\psi(\phi^{-1}(\epsilon))}$$

where $U_{d, \infty, \phi} > 0$ is a constant depending only on $d, B_\infty, B_d$ that we have again extracted via the $\Delta_2$ condition on $\psi$ and $\phi$. We can ensure that there is an $\epsilon_2 > 0$ satisfying this bound by choosing $\epsilon \leq \epsilon_2 = \min\{1, \phi(\psi^{-1}(U_{d, \infty, \phi}))\}$.

Moreover, we have for any two binary strings $\omega^{(1)}, \omega^{(2)} \in \{0, 1\}^m$:

$$\|f_{\omega^{(1)}} - f_{\omega^{(2)}}\|_{2, \psi(\nu)}^2 = \frac{32\epsilon}{m} \sum_{i=1}^m (\omega_i^{(1)} - \omega_i^{(2)})^2 \leq 32\epsilon$$

Now, observe that if we choose $\epsilon \leq \epsilon_3 = \min\{\epsilon_2, \phi^{-1}(\psi(\frac{U_{d, \infty, \phi}}{9}))\}$, and choose $m_\epsilon = \lfloor \frac{U_{d, \infty, \phi}}{\psi(\phi^{-1}(\epsilon))} \rfloor$ like before, we have $m_\epsilon \geq 9$. Then, by the Gilbert-Varshamov bound (see e.g. Lemma 24 in [14]), there exists a $M_\epsilon \geq 2 \frac{m_\epsilon}{\epsilon}$, and some binary strings $\omega^{(1)}, \omega^{(2)}, \ldots, \omega^{(M_\epsilon)}$, such that:

$$\sum_{i=1}^{m_\epsilon} (\omega_i^{(k)} - \omega_i^{(l)})^2 \geq \frac{m_\epsilon}{8}$$

for all $k, l \in [M_\epsilon]$. Therefore, we have:

$$\|f_{\omega^{(k)}} - f_{\omega^{(l)}}\|_{2, \psi(\nu)}^2 \geq 4\epsilon$$

(25)

for $k, l \in [M_\epsilon]$. We now construct measures $\{P_j\}_{j=1}^{M_\epsilon}$ on $\mathcal{X} \times \mathcal{Y}$ such that $P_j|_{\mathcal{X}} = \nu = P_X$, with $\mathbb{E}[Y|X] = f_{\omega^{(j)}}(X)$ and $Y \sim P_{\mathcal{Y}|\mathcal{X}} = \mathcal{N}(0, \sigma^2)$ for $(X, Y) \sim P_{\mathcal{X}}$ and all $j \in [M_\epsilon]$. The measures $P_j$ are clearly conditionally $\sigma^2$-subgaussian. Letting $P_0$ be such that $f_{\omega^{(0)}} = 0$. Then, we have that:

$$\frac{1}{M_\epsilon} \sum_{i=1}^{M_\epsilon} \text{KL}(P_i^n || P_0^n) = \frac{n}{2\sigma^2 M_\epsilon} \sum_{i=1}^{M_\epsilon} \|f_i - f_0\|_{2, \psi(\nu)}^2 \leq \frac{16n\epsilon}{\sigma^2} \equiv \alpha^*$$

Thus, for any measurable function $\Theta : (\mathcal{X} \times \mathbb{R})^n \to \{0, 1, \ldots, M_\epsilon\}$, we have by Theorem 20 in [14] that:

$$\max_{j \in [M_\epsilon]} P_j(\Theta(D) \neq j) \geq \frac{\sqrt{M_\epsilon}}{1 + \sqrt{M_\epsilon}} \left(1 - \frac{48n\epsilon}{\sigma^2 \log M_\epsilon} - \frac{1}{2 \log M_\epsilon}\right)$$

(26)

Note that $M_\epsilon \geq 2 \frac{m_\epsilon}{\epsilon} \geq \frac{U_{d, \infty, \phi}}{9\psi(\phi^{-1}(\epsilon))}$ using the definition of $m_\epsilon$ and the fact that $m_\epsilon \geq 9$. Substituting this into (26) we obtain:

$$\max_{j \in [M_\epsilon]} P_j(\Theta(D) \neq j) \geq \frac{\sqrt{M_\epsilon}}{1 + \sqrt{M_\epsilon}} \left(1 - \frac{432n\epsilon_\tau}{U_{d, \infty, \phi}\sigma^2 \log 2} - \frac{1}{2 \log M_\epsilon}\right)$$

Now, we choose $\epsilon_\tau = \tau \phi((\phi \psi)^{-1}(n^{-1}))$ where $\tau < 1$ has been chosen so that $\epsilon_\tau \leq \epsilon_3$. Define:

$$\Theta(D) \equiv \arg \min_{j \in [M_\epsilon]} \|f_D - f_j\|_{2, \psi(\nu)}$$

Then for any $j \neq \Theta(D)$, we have by (25):

$$2\sqrt{\epsilon_\tau} \leq \|f_{\Theta(D)} - f_j\|_{2, \psi(\nu)} \leq \|f_D - f_{\Theta(D)}\|_{2, \psi(\nu)} + \|f_D - f_j\|_{2, \psi(\nu)} \leq 2\|f_D - f_j\|_{2, \psi(\nu)}$$

Thus, we have:

$$\max_{j \in [M_\epsilon]} P_j(\|f_D - f_j\|_{2, \psi(\nu)} \geq \sqrt{\epsilon_\tau}) \geq \max_{j \in [M_\epsilon]} P_j(\Theta(D) \neq j) \geq \frac{\sqrt{M_\epsilon}}{1 + \sqrt{M_\epsilon}} \left(1 - \frac{432n\epsilon_\tau}{U_{d, \infty, \phi}\sigma^2 \log 2} - \frac{1}{2 \log M_\epsilon}\right) \geq \frac{\sqrt{M_\epsilon}}{1 + \sqrt{M_\epsilon}} \left(1 - \frac{1}{2 \log M_\epsilon}\right)$$

after substituting the choice of $\epsilon_\tau$ and letting $C_\tau = \frac{432\tau D_\epsilon^n}{U_{d, \infty, \phi}\sigma^2 \log 2}$ (where $u = \log_{D_\psi} \tau$). Observing that $M_\epsilon \to \infty$ as $\epsilon_\tau \to 0$ (as $n \to \infty$), we obtain our result.\)
D Auxiliary Results

Lemma D.1. Suppose $\frac{t}{\psi(t)}$ is concave. Then, if Assumption $[\text{(1)}]$ holds, we have for all $f \in \mathcal{H}_K$:

$$\frac{\|f\|_2^2}{\|f\|_K^2} \leq \frac{t}{\psi\left(\frac{\|f\|_{L^2(\nu)}}{\|f\|_K}\right)}$$

Proof. Follows immediately from Proposition 7 in [24] with $\kappa = \sqrt{t}$ and $\phi = \sqrt{\psi(t)}$ (here are $\kappa$ and $\phi$ are the notation used in their paper and do not coincide with the objects $\kappa$ and $\phi$ in this paper).

Lemma D.2.

$$\sup_{x \in X} \|\left((C_\nu + \lambda)^{-\frac{1}{2}} k(x, \cdot)\right)\|_K \leq \sqrt{\frac{\|k\psi\|_2^2}{\psi(\lambda)}}$$

Proof. We first note that, for any linear operator $T$ on $\mathcal{H}_K$, we have:

$$\sup_{x \in X} \|Tk(x, \cdot)\|_K = \sup_{\|f\|_K = 1, x \in X} \langle Tk(x, \cdot), f \rangle_K$$

$$= \sup_{\|f\|_K = 1, x \in X} \langle k(x, \cdot), T^* f \rangle_K$$

$$= \sup_{\|f\|_K = 1, x \in X} \langle T^* f(x), \rangle_K$$

$$= \sup_{\|f\|_K = 1} \|T^* f\|_K$$

Hence, since $(C_\nu + \lambda)^{-\frac{1}{2}}$ is self-adjoint, we have by the interpolation inequality (Lemma D.1), that:

$$\left\|\left((C_\nu + \lambda)^{-\frac{1}{2}} f\right)\right\|_\infty^2 \leq \frac{\|k\psi\|_2^2 \|\left((C_\nu + \lambda)^{-\frac{1}{2}} f\right)\|_K^2}{\psi\left(\|\left((C_\nu + \lambda)^{-\frac{1}{2}} f\right)\|_K\right)}$$

(27)

Taking the supremum over $f \in \mathcal{H}_K$, and noting that (27) is jointly increasing in $\|\left((C_\nu + \lambda)^{-\frac{1}{2}} f\right)\|_2$ and $\|\left((C_\nu + \lambda)^{-\frac{1}{2}} f\right)\|_K$ by the fact that $\frac{t}{\psi(t)}$ is concave and nondecreasing in Assumption $[\text{(1)}]$ we obtain:

$$\|\left((C_\nu + \lambda)^{-\frac{1}{2}} f\right)\|_\infty^2 \leq \frac{\|k\psi\|_2^2}{\psi(\lambda)}$$

where we have used the fact that $\sup_{f \in \mathcal{H}_K} \|\left((C_\nu + \lambda)^{-\frac{1}{2}} f\right)\|_2 = \sup_{f \in \mathcal{H}_K} \|k\psi\|_2^2 (C_\nu + \lambda)^{-\frac{1}{2}} f\|_K^2$.

Lemma D.3.

$$N(\lambda) \equiv \text{tr}(C_\nu (C_\nu + \lambda)^{-1}) \leq \frac{1}{\psi(\lambda)}$$

Proof. First, we note that, since $\mathcal{H}_\psi \hookrightarrow L^\infty$, we have that:

$$\|k\psi\|_\infty = \left\|\sum_{i=1}^\infty \psi(\mu_i) e_i^2(\cdot)\right\|_\infty < \infty$$

Hence, integrating both sides against $\nu$, we obtain:

$$\sum_{i=1}^\infty \psi(\mu_i) < \infty$$
Adaptive PAC-Bayesian Regularization

from which we may deduce that $\psi(\mu_i) \leq i^{-1}$, or $\mu_i \leq \psi^{-1}(i^{-1})$. Combined with Corollary C.2.1 we obtain

$$
\mu_i \asymp \psi^{-1}(i^{-1}).
$$

Therefore, there exist $C_1, C_2 > 0$, such that:

$$
\mathcal{N}(\lambda) \equiv \text{tr}(C_\nu(C_\nu + \lambda)^{-1})
$$

$$
\leq \sum_{i=1}^{\infty} \frac{\mu_i}{\mu_i + \lambda}
$$

$$
\leq \sum_{i=1}^{\infty} \frac{C_1 \psi^{-1}(i^{-1})}{C_2 \psi^{-1}(i^{-1}) + \lambda}
$$

$$
\leq \int_0^{\infty} \frac{C_1 \psi^{-1}(t^{-1})}{C_2 \psi^{-1}(t^{-1}) + \lambda} dt
$$

$$
= \int_0^{\infty} \frac{C_1}{C_2 + \frac{\lambda}{\psi^{-1}(t^{-1})}} dt
$$

$$
= \int_0^{\psi(\lambda)^{-1}} \frac{C_1}{C_2 + \frac{\psi^{-1}(\psi(\lambda))}{\psi^{-1}(t^{-1})}} dt + \int_{\psi(\lambda)^{-1}}^{\infty} \frac{C_1}{C_2 + \frac{\psi^{-1}(\psi(\lambda))}{\psi^{-1}(t^{-1})}} dt
$$

We observe that, by Assumption 1 we have that:

$$
2\psi^{-1}\left(\frac{x}{D_1}\right) \leq \psi^{-1}(x) \leq 2\psi^{-1}\left(\frac{x}{D_2}\right)
$$

Hence, for $t > \psi(\lambda)^{-1}$, we have:

$$
\frac{\psi^{-1}(\psi(\lambda))}{\psi^{-1}(t^{-1})} = \frac{\psi^{-1}(t\psi(\lambda)t^{-1})}{\psi^{-1}(t^{-1})} \geq 2^{\log_{D_1}(t\psi(\lambda))}
$$

Observing that $2^{\log_{D_1}(t\psi(\lambda))} = (t\psi(\lambda))^r$, where $r \equiv \log_{D_1}(2)$ Hence, we have:

$$
\mathcal{N}(\lambda) \leq \int_0^{\psi(\lambda)^{-1}} \frac{C_1}{C_2 + \frac{\psi^{-1}(\psi(\lambda))}{\psi^{-1}(t^{-1})}} dt + \int_{\psi(\lambda)^{-1}}^{\infty} \frac{C_1}{C_2 + \frac{\psi^{-1}(\psi(\lambda))}{\psi^{-1}(t^{-1})}} dt
$$

$$
\leq \frac{C_1 \psi(\lambda)^{-1}}{C_2} + \int_{\psi(\lambda)^{-1}}^{\infty} \frac{C_1}{C_2 + (\psi(\lambda))^r} dt
$$

$$
\leq \frac{C_1 \psi(\lambda)^{-1}}{C_2} + \psi(\lambda)^{-1} \int_1^{\infty} \frac{C_1}{C_2 + s^r} ds
$$

$$
\leq \frac{C_3}{\psi(\lambda)}
$$

after noting that the second integral converges since $r = \log_{D_1}(2) > 1$ (as $\frac{t}{\psi(t)}$ is nondecreasing by Assumption 1).