Importance Weighting Correction of Regularized Least-Squares for Covariate and Target Shifts

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Abstract

In many real world problems, the training data and test data have different distributions. This situation is commonly referred as a dataset shift. The most common settings for dataset shift often considered in the literature are covariate shift and target shift. Importance weighting (IW) correction is a universal method for correcting the bias present in learning scenarios under dataset shift. The question one may ask is: does IW correction work equally well for different dataset shift scenarios? By investigating the generalization properties of the weighted kernel ridge regression (W-KRR) under covariate and target shifts we show that the answer is negative, except when IW is bounded and the model is well-specified. In the latter cases, a minimax optimal rates are achieved by importance weighted kernel ridge regression (IW-KRR) in both, covariate and target shift scenarios. Slightly relaxing the boundedness condition of the IW we show that the IW-KRR still achieves the optimal rates under target shift while leading to slower rates for covariate shift. In the case of the model misspecification we show that the performance of the W-KRR under covariate shift could be substantially increased by designing an alternative reweighting function. The distinction between misspecified and well-specified scenarios does not seem to be crucial in the learning problems under target shift.

1 Introduction

Perhaps the most common assumptions made in the statistical learning literature is that the (training and testing) data are drawn i.i.d. from a common probability distribution. However, this assumption needs not hold in a constantly changing world. Dataset shift naturally arises in many common learning scenarios. It is the case, for instance, in active learning problems, where the training data points are sampled by the learner at will, while the test input points are bounded to be sampled from the environment distribution [Pukelsheim, 2006, MacKay, 1992, Cortes et al., 2008]. Another example include domain adaptation, when training data is drawn from a source domain that differs from the target domain to which the learner is required to transfer its knowledge [Ben-David et al., 2007, Mansour et al., 2009b, Jiang and Zhai, 2007, Cortes and Mohri, 2014, Zhang et al., 2012].

The most common setting for dataset shift often considered in the literature are covariate shift and target shift. Covariate shift occurs when the conditional distribution of the label given the features are identical, allowing for different marginal distributions for training and testing instances. In target shift, training and testing conditional distributions of input given the output are the same, while the marginal output distributions could be different.

A common approach to address dataset shift is to consider the so-called importance weighted risk minimization for correcting the bias. The idea is to correct the notion of the risk in a way that matches the risk associated with the target (testing) distribution. While the risk correction seems natural, in some learning scenarios, it does not significantly improve over unweighted risk minimization, and sometimes leads to worse performance [Cortes et al., 2010].

Empirical and theoretical analyses of Importance Weighting correction under covariate shift was led by [Cortes et al., 2010]. The major issue of IW correction is the large values of the weighting function, which is unavoidable due to the fact that the regions of the input space with high testing probability are not properly covered by the training distribution. In order to measure the degree of singularity of the testing measure with respect to the training one, the notion of transfer-exponent was introduced in [Kpotufe and Martinet, 2021]. It was shown that the singularity, naturally presented in learning problems under covariate shift, imposes the limitation on the learning procedure which, in the minimax sense, is impossible to overcome. With this
result in mind, a natural question is whether IW adaptation (whenever IW is well defined) leads to slow learning rates or it maintains optimal learning rates and simply affects the constants in the generalization bounds. Recently [Ma et al., 2022] demonstrated the advantage of using truncated IW over uniform weights, by showing the optimality (up to the logarithmic factor) of the W-KRR with truncated weights under the weak assumption that the second moment of the IW is bounded. To the best of our knowledge the question of optimality of IW correction, when IW is not bounded, is still open.

Parametric models under covariate shift were studied by [Shimodaira, 2000], where it was shown that IW adaptation is the asymptotically optimal strategy (importance weighted MLE is consistent) when the target function is outside the hypothesis class, i.e., the model is misspecified. Although consistency becomes guaranteed by this modification, the weighted version of MLE is no longer asymptotically efficient. For well-specified models the situation is different. In this case, the asymptotically optimal strategy is uniform weighting \( w(x) = 1 \). The problem of IW under model misspecification was further investigated by [Wen et al., 2014]. Robustness to covariate shift for overparameterized models was studied in [Tripuraneni et al., 2021], where kernel methods with random feature approximation were considered.

Having in mind the difficulties associated with the IW correction for covariate shift, three relevant questions need to be addressed for the target shift: What is the effect of importance weighting correction applied to the target shift scenario, and how is it different from the IW correction applied under covariate shift? What are the effects of large values of the weighting function on the generalization properties of the IW correction? How important is it to distinguish the misspecified and well-specified scenarios under target shift to choose a more accurate weighting function? The paper aims to gain a better theoretical understanding of the nature of the bias associated with the different distributional shift scenarios and the role of the weights in the bias correction.

In the literature of target shift correction the main emphasis is in the estimation of the IW [Lipton et al., 2018; Azizzadenesheli et al., 2019; Garg et al., 2020], while the effectiveness of the importance-weighted risk minimizers remains under-explored. In the context of overparameterized deep neural networks optimized by stochastic gradient descent, it was empirically observed by [Byrd and Lipton, 2019] that importance weighting impacts only the early stage of training and the impact of importance weighting diminishes after the model separates (in classification settings) the training data. Theoretical insights into this phenomenon were given by [Xu et al., 2021]. Generalization bounds for the regularized algorithms under target shift was proposed by [Azizzadenesheli et al., 2019; Maity et al., 2020] provided the minimax analysis for the target shift problem for non-parametric binary classification.

In this paper, we study the theoretical properties of IW adaptation for kernel ridge regression (KRR) under both covariate and target shifts. Our technical tools are based on operator and spectral methods developed for kernel-based algorithms [Smale and Zhou, 2007; 2005; Caponnetto and De Vito, 2007; Zhang, 2002, 2005; Steinwart et al., 2009; Blanchard and Mücke, 2018].

The main contribution of the work is to derive the novel generalization bounds for the weighted kernel ridge regression when covariate and target shifts are presented. For the moderate covariate shift scenarios (when IW is bounded by \( W \)) we show that the kernel least squares corrected by the importance weights is optimal and matches the learning rates of KRR without covariate shift [Caponnetto and De Vito, 2007]. Relaxation of the boundedness condition (see the Assumption (5)) leads to the capacity independent rates of [Smale and Zhou, 2007; 2005], which is known to be sub-optimal for the smooth reproducing spaces (like Sobolev spaces). For the target shift the rates are still optimal. By analysing the general re-weighting procedure, we quantify the exact bias terms associated to different shifts. For the covariate shift the bias is the distance between the projections of the regression function w.r.t. the testing distribution and the distribution associated with the weighting function. When the regression function belongs to the hypothesis space, both of the projections are equal (thanks to the covariate shift assumption) and the bias term vanishes regardless of the weighting function used in risk minimization procedure. This partly explains the effectiveness of considering the large hypothesis spaces. Under the target shift the bias is related to the mismatch between the testing conditional output averages (regression function) and the conditional output averages induced by the weighting function. Unlike the covariate shift this bias can not be eliminated by considering the larger spaces.

The remainder of this paper is structured as follows. In Section 2 we briefly recall the learning problem under dataset shift, introduce some auxiliary notations and the importance weighted algorithms. Section 3 presents assumptions and the generalization bound of IW-KRR under covariate and target shifts. In Section 4 we study the generalization properties of alternative re-weighting algorithms.

### 2 The learning problem under distribution shift

Let \( X \) be a measurable space, which serves as an input space, \( Y \subset \mathbb{R} \) be an output space, and \( Z := X \times Y \) be the product space. We consider two probability distributions on \( Z \): one is the probability distribution \( \rho^t(x, y) \) of training data, and the other is the probability distribution \( \rho^v(x, y) \) of test data. Note that we use the notation \((x, y) \in X \times Y\) as variables and do not consider fixed quantities.
We consider the regression problem, where the task is to estimate the regression function \( f_{\rho^x} : X \to Y \) defined from the conditional distribution \( \rho^{x\mid y}(x|y) \) as

\[
f_{\rho^x}(x) := \int_Y y \, d\rho^{x\mid y}(y|x), \quad x \in X.
\] (1)

For this problem, we assume that we are given an i.i.d. sample of size \( n \in \mathbb{N} \) from the training distribution \( \rho^{tr} \) of \((x_1, y_1), \ldots, (x_n, y_n)\) as follows:

\[
(x_1, y_1), \ldots, (x_n, y_n) \overset{i.i.d.}{\sim} \rho^{tr} (x,y),
\]

and let \( z := \{ z_1, \ldots, z_n \} \in \mathbb{Z}^n \) with \( z_i := (x_i, y_i) \) denote the training dataset.

We wish to construct an estimator \( f_z : X \to Y \) of the regression function \( f_{\rho^x} \) based on the training data \( z \). If the distributions are arbitrary, training data would be of no use to estimate the regression function (consider for instance distributions with disjoint support). Certain assumptions linking the training and testing distributions are required for the problem to be well defined. We consider the two following settings:

(i) **Covariate shift**, where \( \rho^{x\mid y}(x,y) \) and \( \rho^{x\mid y}(x,y) \) share the same conditional distribution of output \( y \) given input \( x \), but differ in their marginal distributions on the input space \( X \). More precisely, let \( \rho(y|x) \) and \( \rho(y|x) \) be the shared conditional distribution, and let \( \rho^{x\mid y}(x,y) \) and \( \rho^{x\mid y}(x,y) \) be the marginal distributions of \( \rho^{x\mid y}(x,y) \) and \( \rho^{x\mid y}(x,y) \) on \( X \), respectively:

\[
\rho^{x\mid y}(x,y) = \rho(y|x) \rho^{x\mid y}(x), \quad \rho^{x\mid y}(x,y) = \rho(x|y) \rho^{x\mid y}(x).
\]

(ii) **Target shift** where the conditional input distribution given output is invariant while the marginal output distribution changes from training to testing:

\[
\rho^{x\mid y}(x,y) = \rho(x|y) \rho^{x\mid y}(y), \quad \rho^{x\mid y}(x,y) = \rho(x|y) \rho^{x\mid y}(y).
\]

For any given function \( f : X \to Y \), consider the following risk functional

\[
\mathcal{E}_{\rho^x}(f) = \int_Z (f(x) - y)^2 \, d\rho^{x\mid y}(x,y).
\] (2)

It is well known that the minimizer of (2) over the space of square integrable functions is the regression function (1). The goal is to construct the function \( f_z \) from a finite size sample set \( z \) from \( \rho^{tr} \) such that \( \mathcal{E}_{\rho^x}(f_z) \) is close to \( \mathcal{E}_{\rho^x}(f_{\rho^x}) \) with high probability.

According to the empirical risk minimization principle [Vapnik, 1998], we replace the risk functional (2) with its finite sample approximation

\[
\mathcal{E}_{\rho^x}(f) = \frac{1}{n} \sum_{i=1}^n (f(x_i) - y_i)^2
\] (3)

based on the set \( z' = \{(x'_1, y'_1), \ldots, (x'_n, y'_n)\} \) sampled from \( \rho^{x\mid y} \). The empirical risk minimizer is then defined as the solution of (3) over some functional class \( \mathcal{H} \) called the **hypothesis space**. However, in the distribution shift scenarios samples from \( \rho^{x\mid y} \) are not available and the learning algorithm only receives the training set \( z \) drawn according to the measure \( \rho^{tr} \). To overcome this issue it is either possible to modify the training set \( z \) to make it resemble to samples coming from \( \rho^{x\mid y} \) or alternatively to change the notion of risk (2). The latter approach leads to the definition of importance weighted risk as follows. In particular, under the distribution shift and measure absolute continuity \( d\rho^{x\mid y} \ll d\rho^{tr} \) assumptions, defining \( w(x,y) = d\rho^{x\mid y}(x,y)/d\rho^{tr}(x,y) \) we build the following importance weighted risk

\[
\mathcal{E}_{\rho^x}(f) = \int_Z w(x,y)(f(x) - y)^2 \, d\rho^{tr}(x,y).
\]

and its empirical counterpart as

\[
\mathcal{E}_{\rho^x}(f) = \frac{1}{n} \sum_{i=1}^n w(x_i, y_i)(f(x_i) - y_i)^2.
\]

In the following, we will study the properties of estimators belonging to the hypothesis space \( \mathcal{H} \) which is the so-called reproducing kernel Hilbert space defined as follows:

**Definition 1.** Let \( K : X \times X \to \mathbb{R} \) be continuous, symmetric, and positive semidefinite, i.e., for any finite set of distinct points \( \{ x_1, \ldots, x_n \} \subset X \), the matrix \( (K(x_i, x_j))_{i,j=1}^n \) is positive semidefinite. A Hilbert space \( \mathcal{H} \) of functions on \( X \) equipped with an inner-product \( \langle \cdot, \cdot \rangle_{\mathcal{H}} \) is called a reproducing kernel Hilbert space (RKHS) with reproducing kernel \( K \), if the following are satisfied:

1. For all \( x \in X \), we have \( K_x = K(\cdot, x) \in \mathcal{H} \);

2. For all \( x \in X \) and for all \( f \in \mathcal{H} \), \( f(x) = \langle f, K(\cdot, x) \rangle_{\mathcal{H}} \) (Reproducing property).

In what follows, we always assume that \( K \) is bounded, that is, \( \sup_{x \in X} K(x, x) \leq \kappa \). To avoid superfluous notations, we further assume \( \kappa \leq 1 \), noting that this can always be achieved by properly scaling the kernel function.

2.1 **Notations and Auxiliary Operators**

By \( L^2(X, \rho^x_X) \) and \( L^2(X, \rho^{tr}_X) \) we denote Lebesgue spaces of square-integrable functions with respect to \( \rho^x_X \) and \( \rho^{tr}_X \) with respective norms given by \( \| f \|_{\rho^x_X} = \left( \int_X f^2(x) \, d\rho^x_X(x) \right)^{\frac{1}{2}} \) and \( \| f \|_{\rho^{tr}_X} = \left( \int_X f^2(x) \, d\rho^{tr}_X(x) \right)^{\frac{1}{2}} \).

Let us recall introduce some operators related to the RKHS. Let \( T_v : \mathcal{H} \to \mathcal{H} \) and \( L_v : L^2(X, \nu) \to \mathcal{H} \) be the covari-
When IW is not known, it can be efficiently estimated from We now introduce the weighted kernel ridge regression algorithm. The W-KRR solution associated with the kernel $K$ is defined to be the minimizer of the following weighted regularization parameter known as a covariance operator $S_\mathcal{X}$. Following Smale and Zhou [2007] we define the sampling operator $S_\mathcal{X} : \mathcal{H} \rightarrow \mathbb{R}^n$ with a set $x = \{x_1, \ldots, x_n\} \subset \mathcal{X}$ as $(S_\mathcal{X} f)_i = f(x_i) = (f, K_{x_i})_{\mathcal{H}}$. Its adjoint operator $S_\mathcal{X}^* : \mathbb{R}^n \rightarrow \mathcal{H}$ is given by $S_\mathcal{X}^* (y) = \frac{1}{n} \sum_{i=1}^n y_i K_{x_i}$. 

### 2.2 Weighted risk minimization algorithm

We now introduce the weighted kernel ridge regression algorithm. The W-KRR solution associated with the kernel $K$ is defined to be the minimizer of the following weighted least-square optimization problem defined over a set of samples $z = \{(x_i, y_i)\}_{i=1}^n$ independently drawn according to $\rho^{x}$.

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

(4)

where $w(x, y) = \frac{\rho^{xy}(x,y)}{\rho^{x}}$ for some distribution $\rho^{x} \ll \rho^{x}$ and $\lambda = \lambda_n$ is any positive function of the number of samples $n$ known as a regularization parameter.

Thought the paper we assume that the importance weighting function is known and will be mainly concerned with the effects of weights on generalization properties of IW-KRR. When IW is not known, it can be efficiently estimated from the training data and unlabeled testing data.

The following lemma describes the solution of the minimization problem (4).

**Lemma 2.** For any $\lambda > 0$, the solution $f_{z,\lambda}^{W}$ exist and unique. Moreover.

$$f_{z,\lambda}^{W} = \left( S_\mathcal{X}^T M_w S_\mathcal{X} + \lambda \right)^{-1} S_\mathcal{X}^T M_w y$$

(5)

where $y = (y_1, \ldots, y_n)$, $w = (w(x_1, y_1), \ldots, w(x_n, y_n))$ with $w(x, y) = d\rho^x(x,y)/d\rho^x(x,y)$ and $M_w$ is the diagonal matrix with main diagonal entries $w(x_i, y_i), i = 1, \ldots, n$.

**Proof.** The proof can be found in [Smale and Zhou 2004, Theorem 2].

Assuming that the matrix $M_w$ have full rank the solution (5) can be equivalently written in a more traditional form as

$$f_{z,\lambda}^{W} = \sum_{i=1}^{n} \alpha_i K(\cdot, x_i), \quad \alpha = (K_{xx} + n\lambda M_1/w)^{-1} y,$$

where $K_{xx}$ is the covariance matrix whose entries are given by $K_{ij} = K(x_i, x_j)$. Depending on the observation weight we rescale the regularizer accordingly: the higher the weight of observation, the less we regularize.

### 3 Learning Guarantees for IW-KRR

Let $f_\mathcal{H}$ and $f_{\mathcal{H}}'$ be the projections of the regression function $f_{\rho^X}$ onto the closure of $\mathcal{H}$ in $L^2(X, \rho^X)$ and $L^2(X, \rho^X')$ respectively.

We first introduce some basic assumptions common for both covariate and target shift scenarios.

**Assumption 1.** There exist $r > 0$ and $R > 0$ such that $\|L^{-r}f_\mathcal{H}\|_{\rho^X} \leq R$.

Finiteness of $\|L^{-r}f_\mathcal{H}\|_{\rho^X}$ is a common source condition in the inverse problem literature [Smale and Zhou 2004, 2007, De Vito et al. 2005, Caponnetto 2006] and characterizes the regularity of the target function $f_\mathcal{H}$. A bigger $r$ corresponds to higher regularity and can lead to faster convergence rates. In particular, for $r = 0$, we are making no assumption, while for $r = 1/2$, we are requiring $f_\mathcal{H} \in \mathcal{H}$, since $\|L^{1/2}f\|_\mathcal{H} = \|f\|_{\rho^X}$. For $r \geq 1/2$ the image of the integral operator $L^{r} \left(L^2(X, \rho^X)\right)$ becomes a subset of $\mathcal{H}$, which implies that the minimization of risk functional (2) over $\mathcal{H}$ has at least one solution in $\mathcal{H}$. This is referred to as the attainable case.

**Assumption 2.** For some $s \in (0, 1]$ we assume that

$$E_s := 1 \vee \sup_{\lambda \in [0,1]} \sqrt{N(\lambda)} \lambda^s < \infty,$$

where $N(\lambda) := \text{Tr} \left[ T(T + \lambda)^{-1} \right]$.

The constant $E_s$ characterizes the marginal distribution $\rho^X$ through $N(\lambda)$ also termed as degrees of freedom [Zhang 2005], or effective dimension [Caponnetto and De Vito 2007]. It satisfied, for instance, when eigenvalues of $T$, $\mu_i(T)$, have asymptotic order $O(i^{-1/s})$. In general, the eigenvalue assumption is a tighter measure for the complexity of the RKHS than more classical covering, or entropy.
number assumptions [Steinwart et al., 2009]. For \( s = 1 \), \( E_s \) is always bounded as \( \mathbb{N}(\lambda) \lambda \leq \kappa = 1 \). This is referred to as the capacity independent setting.

### 3.1 Importance Weighting Correction under Covariate Shift

**Assumption 3.** Let \( w_X = d\rho^W_X / d\rho^Y_X \). For some \( q \in [0, 1] \) there exist positive constants \( W \) and \( \sigma \) depending on \( q \) such that for all integer \( m \geq 2 \)

\[
\left( \int_X w_X(x) \frac{m-1}{m} d\rho^W_X(x) \right)^q \leq \frac{1}{2} m! W_X^{m-2} \sigma^2_X. \tag{6}
\]

**Remark 3.** When \( q = 0 \) it corresponds to the case when \( w_X(x) \) is uniformly bounded over \( X \). In this case \( W = \sup_{x \in X} w_X(x) \) and \( \sigma^2 = \int w_X(x) d\rho^W_X = \int w_X^2(x) d\rho^W_X \).

The condition above is weaker than more traditional boundedness condition usually considered in the literature. It is not hard to check that the Assumption 3 is satisfied when \( 2\rho^W_X \{ x : w_X(x) \geq t \} \leq W_X \sigma^2_X \exp(-\rho^W_X t \) \), restricting the behavior of large values of the Radon–Nikodym derivative.

The condition 3 can be written equivalently as a condition on the Rényi Divergence [Mansour et al. 2009a, Cortes et al., 2010] as follows

\[
H_{(m-1)/q}(\rho^W_X \| \rho^Y_X) \leq \frac{1}{m-1} \left( \log m! + \log \left( \frac{W_X^{m-2} \sigma^2_X}{2} \right) \right)
\]

where

\[
H_a(\rho^W_X \| \rho^Y_X) = \frac{1}{a} \log \int_X w(x)^a d\rho^W_X(x)
\]

is the Rényi Divergence with parameter \( a \). Notice that for each fixed \( q > 0 \), we are imposing the growth condition on the Rényi Divergence w.r.t. the parameter \( m \).

Now we are ready to state our main results for the weighted kernel ridge regression under covariate shift.

**Theorem 4** (IW-KRR under Covariate Shift). For \( M > 0 \), let \( \rho^W \) and \( \rho^Y \) be the distributions on \( X \times [-M, M] \), satisfying the covariate shift assumption and Assumptions 1-3. Furthermore, let \( n \) and \( \lambda \) satisfy the constraints \( \lambda \leq \| T \| \) and

\[
\lambda = \left( \frac{8E_s(\sqrt{W_X + \sigma_X}) \log (\frac{2}{\delta})}{\sqrt{n}} \right)^{\frac{2}{\lambda+\frac{2}{\lambda}}} \tag{7}
\]

for \( \delta \in (0, 1) \), \( q \in [0, 1] \) and \( s \in (0, 1] \). Then, for \( r \geq 0.5 \), with probability greater than \( 1 - \delta \), it holds

\[
\| f^W_{r, \lambda} - f_H \|_{\rho^W_X} \leq C \left( \frac{8E_s(\sqrt{W_X + \sigma_X}) \log (\frac{2}{\delta})}{\sqrt{n}} \right)^{\frac{2}{\lambda+\frac{2}{\lambda}}} \tag{8}
\]

where \( C = 3 (M + R) \).

Some comments are in order.

First, the optimal choice of the regularization parameter depends on the characteristics of the weighting function. Compared to the standard learning scenario [Caponnetto and De Vito, 2007] [Caponnetto, 2006], under covariate shift, when importance weighting correction is applied, the optimal regularizer is usually bigger depending on the \( V_X \) and \( \sigma_X \).

Second, equation (7) together with the condition \( \lambda \leq \| T \| \) can be equivalently given as a condition on the number of observations as follows

\[
\sqrt{n} \geq 8E_s(\sqrt{W_X + \sigma_X})\| T \|^{-\frac{2}{\lambda+\frac{2}{\lambda}}} \log \left( \frac{6}{\delta} \right).
\]

Third, slow tail decay of importance weighting function does not go in favor of importance weighting adaptation. To see this lets consider two extreme cases when \( q = 0 \) and \( q = 1 \). When \( q = 0 \), \( w \) is bounded and \( \| f^W_{r, \lambda} - f_H \|_{\rho^W_X} \) has asymptotic rate of convergence \( O(n^{-\frac{2}{\lambda+\frac{2}{\lambda}}}) \) for \( s \in (0, 1] \), which is optimal in the minimax sense of Caponnetto and De Vito (2007). The rate of convergence of importance weighted empirical risk minimizer achieves the same order as those attained by empirical risk minimizer in absence of covariate shift. For \( q = 1 \), the probability of large values of \( w \) decays exponentially and the best learning rate that could be achieved is \( O(n^{-\frac{2}{\lambda+\frac{2}{\lambda}}}) \), for all \( s \in (0, 1] \).

The last point agrees with the earlier observation by Cortes et al. (2010) that importance weighting correction can succeed when the weights are bounded and gives slower rates under weak moment assumption. As pointed out by Kpotufe and Martinet (2021), the slow rates is not only the consequence of importance weighting correction. In a minimax sense, such situations are hard irrespective of the learning approach. To determine whether IW correction leads to the optimal rates or just affects constants, further investigations are needed.

### 3.2 Importance Weighting Correction under Target Shift.

To provide the learning guarantees for W-KRR under target shift, the condition similar to the Assumption 3 is needed.

**Assumption 4.** Let \( w_Y = d\rho^W_Y / d\rho^Y_Y \). There exists positive constants \( W_Y \) and \( \sigma_Y \) such that for all \( m \geq 2 \)

\[
\int w_Y^{m-1}(y) d\rho^W_Y(y \| x) \leq \frac{1}{2} m! W_Y^2 \sigma_Y^{m-2}.
\]

Before providing the generalization bounds let us explain why IW correction is a reasonable approach. First consider the random variable \( \xi := y K_{\xi, w_Y}(y) \) on \( (Z, \rho^Y) \) with the values in the Hilbert space \( \mathcal{H} \). By the low of large numbers,
the term $S_{\lambda}^T M_{w,y}$ in (5) converges to

$$\frac{1}{n} \sum_{i=1}^{n} \xi(z_i) \rightarrow \int_{Z} y w_Y(y) K_z d\rho^{tr}(y, x)$$

as the number of samples goes to infinity. But the integral is just the integral operator acting on the testing regression function $L_f^{tr}$ (this can be easily verified by the decomposition of the measures and target shift assumption (2)). This shows that $S_{\lambda}^T M_{w,y}$ is a good approximation of $L_f^{tr}$. Second with a function $f \in H$, look at the random variable $\xi := w_Y(y) f(x) K_z$ on $(Z, \rho^{tr})$ with values in $H$. Again we have

$$S_{\lambda}^T M_{w,y} s_{\lambda} = \frac{1}{n} \sum_{i=1}^{n} \xi(z_i) \rightarrow Tf$$

meaning that $S_{\lambda}^T M_{w,y} s_{\lambda}$ is a good approximation of the covariance operator $T$. Thus $f_{\lambda}^{w,\lambda}$ should approximate $f_{\lambda} := (T + \lambda I)^{-1} L f_{\lambda}$ and one would expect good error analysis of $f_{\lambda}^{w,\lambda} - f_{\lambda}$ in the space $H$. This observation is made precise by the following theorem.

**Theorem 5 (IW-KRR under Target Shift).** Let $\rho^{tr}$ and $\rho^{s'}$ be the distributions on $X \times [-M, M]$ satisfying target shift assumption and Assumptions 1,2,4. Furthermore, let $n$ and $\lambda$ satisfy the constraints $\lambda \leq \|T\|$ and

$$\lambda = \left( \frac{8 E_4(\sqrt{W_Y} + \sigma_Y) \log \left( \frac{6}{\delta} \right)}{\sqrt{n}} \right)^{-\frac{1}{2r + 2}}, \quad \text{for } \delta \in (0, 1),$$

(9)

for $r \geq 0.5$, with probability greater than $1 - \delta$, it holds

$$\|f_{\lambda}^{w,\lambda} - f_{\lambda}\|_{\rho_X^{s'}} \leq C \left( \frac{8 E_4(\sqrt{W_Y} + \sigma_Y) \log \left( \frac{6}{\delta} \right)}{\sqrt{n}} \right)^{\frac{1}{2r + 2}}.$$

(10)

where $C = 3 (M + R)$.

Comparing the rates of convergence known for the uniformly weighted KRR in absence of target shift allows us to conclude that with an appropriate choice of the regularization parameter the IW-KRR under target shift is minimax optimal. For the IW-KRR under covariate shift, the same rates are achieved only for the bounded IW (when $q = 0$), while a weaker boundedness assumption on the weights results in slower rates. In particular, it means that the IW correction of target shift is less sensitive toward the large shift in the output space.

### 4 Effect of Using Incorrect Weights

In Section 3 we have analyzed the generalization properties of the importance weighted KRR and concluded that importance weighting adaptation is an effective strategy for both covariate and target shift correction whenever the regularizer is properly tuned (Theorem 4 and 5). In the following we study the performance of the weighted KRR in the case of a weighing function $v$ that does not match the ratio between test and train marginal distributions:

$$f_{\lambda,\gamma} := \min_{f \in H} \left\{ \frac{1}{n} \sum_{i=1}^{n} v(x_i, y_i) (f(x_i) - y_i)^2 + \lambda \|f\|^2_H \right\}.$$

(11)

For the convenience, we assume that $v = d\rho'/d\rho^{tr}$ for some measure $\rho' \ll \rho^{tr}$. Depending on the scenario to be considered, the weights are defined accordingly. In the case of covariate shift, it corresponds to the likelihood ratio in the input space $v_X(x) = d\rho'_{X}(x)/d\rho_X^{tr}(x)$, whereas for target shift, the weighting function is defined on the output space $v_Y(y) = d\rho'_{Y}(y)/d\rho_Y^{tr}(y)$.

#### 4.1 Learning Guarantees of W-KRR under Covariate Shift

In order to provide guarantees for the finite data scenario we need a set of assumptions on $v$ and $\rho'_{X}$ that are similar to Assumptions 2 and 3.

**Assumption 5.** Let $\rho'_{X}(A) = \int_{A} v_X(x) d\rho'_{X}(x)$. For some $s' \in (0, 1]$ we assume that

$$E' := 1 \vee \sup_{\lambda \in (0, 1]} \sqrt{N'(\lambda)} \lambda^{s'} < \infty,$$

where $N'(\lambda) = \text{Tr} [T_{\rho'_{X}} (T_{\rho'_{X}} + \lambda)^{-1}]$.

**Assumption 6.** Let $v_X(x) = d\rho'_{X}(x)/d\rho_X^{tr}(x)$. For some $q' \in [0, 1]$ there exist positive constants $V_X$ and $\gamma_X$ depending on $q'$ such that for all $m \geq 2$

$$\left( \int_{X} v_X^{m-1} d\rho'_{X}(x) \right)^{q'} \leq \frac{1}{m} V_X^{m-2} \gamma_X^{2}.$$

(12)

Now we are ready to state our main results for the weighted kernel ridge regression under covariate shift.

**Theorem 6 (W-KRR under Covariate Shift).** Let $\rho^{tr}$ and $\rho'$ be the distributions on $X \times [-M, M]$ satisfying the covariate shift assumption and Assumptions 1,2,5. Let $q' \in [0, 1]$ and $s' \in [0, 1]$. Furthermore, let $n$ and $\lambda$ satisfy the constraints $\lambda \leq \|T_{\rho'_{X}}\|$ and

$$\lambda = \left( \frac{8 E' \sqrt{V_X + \gamma_X} \log \left( \frac{6}{\delta} \right)}{\sqrt{n}} \right)^{-\frac{1}{2r + 2 + q' (1 - s')}},$$

(13)

for $\delta \in (0, 1)$. Then, for $r \geq 0.5$, with probability greater than $1 - \delta$, it holds

$$\|f_{\lambda,\gamma} - f_{\lambda}\|_{\rho_X^{s'}} \leq C \left( \frac{8 E'(\sqrt{V_X + \gamma_X}) \log \left( \frac{6}{\delta} \right)}{\sqrt{n}} \right)^{\frac{1}{2r + 2 + q' (1 - s')}} + 4\|f_{\lambda,\gamma} - f_{\lambda}\|_{\rho_X^{s'}}.$$

(14)
With the right choice of the regularization parameter, both Assumption 7.
whenever universal kernels are used. As it is apparent from the theorem 6, a good choice of the weighted correction is applied.

This explains why uniform weights are often the best choice with better control of large values.

The above theorem provides convergence result in high probability for the weighted kernel ridge regression in an attainable case. Let us first discuss the case when importance weighted correction is applied.

As it is apparent from the theorem 6, a good choice of the weighting function heavily depends on the approximation to the "wrong" projection. In the standard learning scenario, when we do not distinguish training and testing measures, the usual empirical risk minimizer is concentrated around the projection of regression function on $H$ (and therefore to the regression function itself). Under covariate shift, when IW adaptation is not applied, the weighted algorithm provides a good approximation to the projection under the induced measure, not the testing one. This situation is illustrated in Figure 1. The role of importance weights in this case is clear; it avoids the approximation to the "wrong" projection.

The situation is drastically different when $f_{\rho^*,\gamma} \in H$ or when $f_{\rho^*,\gamma}$ is well approximated by the elements of $H$ (Figure 1b). With the right choice of the regularization parameter, both $f_{z,\lambda}^{IW}$ and $f_{z,\lambda}$ provide a good approximation to the regression function. Therefore, choosing weights that produce algorithms with small variances in this case is preferable. This explains why uniform weights are often the best choice whenever universal kernels are used.

4.2 Learning Guarantees of W-KRR under Target Shift

As we already discussed the rationale behind the IW correction in covariate shift is to eliminate the bias related to the mismatch between the projections of the regression function. Under target shift the main emphasis of the risk correction is to eliminate the difference between the regression function and the function $\phi(x)/\psi(x)$ induced by the candidate distribution $\rho$, where

$\phi(x) = \int_y yv(y)d\rho^\psi(y|x)$, $\psi(x) = \int_y w(y)d\rho^\psi(y|x)$.

The theorem below provides the learning guarantees of W-KRR under the target shift.

**Theorem 7.** Let $\rho^\psi$ and $\rho^\phi$ be the distributions on $X \times [-M,M]$, where $M > 0$ is some constant, satisfying target shift condition and Assumptions 1,2,7. Furthermore, let $n$ and $\lambda$ satisfy the constraints $\lambda \leq \lVert T \rVert$ and

$\lambda = \left( \frac{8DE_x(\sqrt{V_Y + \gamma_Y}) \log (\frac{1}{\delta})}{\sqrt{n}} \right)^{\frac{1}{s+2}}$ (15)

for $\delta \in (0,1)$, $s \in (0,1]$ and $D = \max \{1,1/\inf \psi(x)\}$

Then, for $r \geq 0.5$, with probability greater than $1 - \delta$, it holds

$\|f_{z,\lambda} - f_H\|_H^2 \leq C\left( \frac{8DE_x(\sqrt{V_Y + \gamma_Y}) \log (\frac{1}{\delta})}{\sqrt{n}} \right)^{\frac{1}{s+2}}$

$+ 4 \left( \frac{\phi}{\psi} - f_{\rho^*,\gamma} \right)_{\rho^\psi}$ (16)

where $C = 6D(M + R)$.

In the case of uniform weights (when $\rho = \rho^{\psi}$) the bias term of the bound (16) corresponds to the $L_2$ distance between the training and testing regression functions $\|f_{\rho^*,\gamma} - f_{\rho^*}^\psi\|_{\rho^\psi}$ where

$f_{\rho^*} = \int yd\rho^\phi(y|x)$.

Note that unlike the covariate shift case, there is no straightforward way to eliminate this bias even when the model is wellspecifies (see Figure 2).
5 Simulations

We use simulations to justify the theoretical results of previous sections. The points we made in Theorems can be summarized as follows:

1. We can safely forget about the covariate shift for high capacity models.
2. Under covariate shift, IW correction is beneficial for low capacity models.
3. Under target shift importance weighting correction is beneficial regardless of the model capacity.

We consider a simple one-dimensional regression problem with the testing regression function being \( f(x) = x^3 \).

**Experimental setup - Covariate Shift** We assume that \( x \sim \mathcal{N}(0.8, 0.5) \) at training time and \( x \sim \mathcal{N}(0, 0.35) \) at testing time. Output \( y \) assumed to be corrupted by homoscedastic Gaussian noise with mean \( \mu = 0 \) and standard deviation \( \sigma = 0.3 \). The regression function together with the training and test points generated in one random replication is shown on the left panel of Figure 3(a). The training and test sets consist of 200 data points each.

**Experimental setup - Target Shift** We assume that \( y \sim \mathcal{N}(0, 0.5) \) at training time and \( y \sim \mathcal{N}(1.5, 0.3) \) at testing time. The input is generated by \( x = (y + \varepsilon)^{1/3} \), with \( \varepsilon \sim \mathcal{N}(0, 0.3) \).

In the simulation we use the KRR with the polynomial kernel. For “misspecified” the degree of the kernel is two, while “wellspecified” corresponds to the cubic degree kernel. Left panel of Figure 3 shows the boxplot of the performances of all approaches, measured by the mean square error (MSE). Under covariate shift (a) the weighted models, as well as the unweighted misspecified model, perform equally well. Under target shift (b) deviation from the IW strategy leads to the larger test MSE regardless of the model capacity.

We do not report numerical experiments on the real data in this paper as exhaustive experimental results on KRR can already be found in [Gretton et al. 2009, Zhang et al. 2013].

6 Conclusion

We presented a series of theoretical results for importance weighting both in the covariate and target shift scenarios, in the context of nonparametric regression over a reproducing kernel Hilbert space. For the moderate covariate shift scenarios (when IW is bounded) we show that the kernel least squares corrected by the importance weights is optimal for both types of shifts and matches the learning rates of KRR without covariate shift. By considering the general reweighting KRR we quantify the exact bias terms associated to the different shifts. A main takeaway message was that the IW correction is the only reasonable approach to addressing the distributional shift in the output space. Deviation from the IW correction strategy leads to the irreducible bias term related to the mismatch between training and testing regression functions. For covariate shift the deviation from IW correction is possible by considering large models e.g. KRR with some universal kernel. In practice, however, full KRR is rarely an option. The main contributions that enabled scalability are based on low-rank approximations (Nyström approximation, random feature approximation), of the nonparametric kernel-based model. Under covariate shift we have two competing issues. We would like to fit exact (full-rank) kernel ridge regression in order to avoid IW correction. On the other hand, for the low-rank approximations we need IW correction to avoid the bias related to the mismatch between the projections of the regression function under different measures. Giving the precise trade-off between the model capacity and the deviation from the importance weighting strategy is a prominent future direction.

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Importance Weighting Correction of Regularized Least-Squares for Covariate and Target Shifts

7 Proofs

In this section we give the proofs of Theorem 6 (see Appendix 7.1) and Theorem 7 (see Appendix 7.2). First we need some preliminary propositions.

The following version of Bernstein inequality for Hilbert space valued random variables is from [Caponnetto and De Vito, 2007, Proposition 2].

**Proposition 8.** Let \((Z, \rho)\) be a probability space and let \(\xi\) be a random variable on \(Z\) taking value in a real separable Hilbert space \(H\). Assume that there are two positive constants \(L\) and \(\sigma\) such that

\[
\mathbb{E} \left[ \| \xi - \mathbb{E}[\xi] \|_H^m \right] \leq \frac{1}{2} m! \sigma^2 L^{m-2}, \quad \forall m \geq 2
\]

then, for any \(\delta \in (0, 1]\)

\[
\left\| \frac{1}{n} \sum_{i=1}^{n} \xi(z_i) - \mathbb{E}[\xi] \right\|_H \leq \frac{2L \log(2/\delta)}{n} + \sqrt{\frac{2\sigma^2 \log(2/\delta)}{n}}
\]

with probability at least \(1 - \delta\).

We also need the following bound on the approximation error.

**Proposition 9.** Let \(f_H\) satisfies the Assumption \(2\) for some \(r > 0\), and

\[
f_\lambda = (T + \lambda)^{-1} L f_H.
\]

Then, the following estimate holds

\[
\| f_\lambda - f_H \|_{\rho_X^r} \leq \lambda^r \| L^{-r} f_H \|_{\rho_X^r} \quad \text{if} \; r \leq 1.
\]

Furthermore, for \(r > 0.5\)

\[
\| f_\lambda \|_H \leq \kappa^{-\frac{1}{2} + r} \| L^{-r} f_H \|_{\rho_X^r} \leq \| L^{-r} f_H \|_{\rho_X^r}.
\]
Proof. By the identity $A(A+\lambda I)^{-1} = I - \lambda(A+\lambda I)^{-1}$ valid for $\lambda > 0$ and any bounded self-adjoint positive operator, we have

$$(I - (T + \lambda)^{-T}) f_H = \lambda (T + \lambda)^{-1} f_H = \lambda^r \left( \lambda^{1-r} (T + \lambda)^{-(1-r)} \right) (T + \lambda)^{-r} f_H.$$  

From the equality above by taking the norm we have

$$\|f_H - f_H\|_{\rho_X^S} \leq \lambda \left\| \lambda^{1-r} (T + \lambda)^{-(1-r)} \right\| \left\| (T + \lambda)^{-r} \right\| \left\| f_H \right\|_{\rho_X^S}.$$  

Note that $\left\| \lambda^{1-r} (T + \lambda)^{-(1-r)} \right\| \leq 1$, $\left\| (T + \lambda)^{-r} \right\| \leq \left\| (T + \lambda)^{-1} \right\|^{-r} \leq 1$ and $\left\| f_H \right\|_{\rho_X^S} \leq R$ by Assumption 8.

Regarding the second estimate, if $r > 1/2$, since $\|T\| \leq 1$, we obtain,

$$\|f_H\|_H = \|(T + \lambda)^{-1} f_H\|_H$$

$$= \|(T + \lambda)^{-1} T T^r - \frac{1}{2} L^{\frac{1}{2}} \| f_H \|_H$$

$$\leq \|T\|^{r - \frac{1}{2}} \|L^{\frac{1}{2}} f_H\|_{\rho_X^S} \leq \|L^{\frac{1}{2}} f_H\|_{\rho_X^S}.$$  

The next result can be found in [Rudi and Rosasco, 2017, Proposition. 8]

**Proposition 10.** For any $\lambda > 0$ and any two bounded self-adjoint positive linear operators $A, B$ defined on separable Hilbert space $\mathcal{H}$, the following is true

$$\left\| (A + \lambda I)^{-1/2} B^{1/2} \right\| \leq \left\| (A + \lambda I)^{-1/2} (B + \lambda)^{1/2} \right\| \leq (1 - \mu)^{-1/2}$$

with

$$\mu = \mu_{\max} \left[ (B + \lambda I)^{-1/2} (B - A)(B + \lambda I)^{-1/2} \right].$$

### 7.1 Appendix - Bound for Covariate shift

Now we are ready to proof the main theorem on the generalization bound of W-KRR under covariate shift. In our analysis we decompose the excess risk as follows

$$f_{z,\lambda} - f_H = (T_x + \lambda)^{-1} \{ (g_x - g) + (T_{\rho_x}^* - T_x) f_\lambda \}$$

$$+ (T_x + \lambda)^{-1} T_{\rho_x}^* (f_H - f_H)$$

$$+ \left( (T_x + \lambda)^{-1} (T - T_{\rho_x}^*) + I \right) (f_\lambda - f_H)$$

where $T_x = S_x^T M_x S_x$, $g_x = S_x^T M_x y$ and $g = L_{\rho_x} f_H$. Here $v = (v_X(x_1), \ldots, v_X(x_n))$. Let us bound the $L^2(X, \rho_X^S)$ norm for each of the terms in the decomposition.

**I term.** Let us further decompose the first term as follows that

$$I \text{ term} = (T_x + \lambda)^{-1} \{ (g_x - g) + (T_{\rho_x}^* - T_x) f_\lambda \}$$

$$= (T_{\rho_x}^* + \lambda)^{-\frac{1}{2}} \left\{ 1 - (T_{\rho_x}^* + \lambda)^{-\frac{1}{2}} (T_{\rho_x}^* - T_x) (T_{\rho_x}^* + \lambda)^{-\frac{1}{2}} \right\}^{-1}$$

$$\left\{ (T_{\rho_x}^* + \lambda)^{-\frac{1}{2}} (g_x - g) + (T_{\rho_x}^* + \lambda)^{-\frac{1}{2}} (T_{\rho_x}^* - T_x) f_\lambda \right\}.$$  

Assuming that $\|T_{\rho_x}^* + \lambda\|^{-\frac{1}{2}} (T_{\rho_x}^* - T_x) (T_{\rho_x}^* + \lambda)^{-\frac{1}{2}} < 1$, we get

$$\|I \text{ term}\|_{\rho_X^S} \leq S_0 \frac{S_2 + S_3}{1 - S_1},$$
with an appropriate choice of the random variables $\xi$ with $\|\xi\|_2 = 1$, where it can be straightforwardly verified, the constants $\mu = \mu_{\text{max}} ((T + \lambda I)^{-1/2}(T - T_{\rho_X})(T + \lambda I)^{-1/2})$.

To find an upper bound for $S_i$, $i = 1, 2, 3$, notice that the following common representation holds

$$S_i = \left\| \frac{1}{n} \sum_{k=1}^{n} \xi_k - E[\xi_k] \right\|_H, \quad i = 1, 2, 3,$$

with an appropriate choice of the random variables $\xi$ and the norm $\| \cdot \|_H$. Indeed, in order to let the equality above hold, $\xi_1 : X \to \text{HS}(H)$ is defined by

$$\xi_1(x)[\cdot] = (T_{\rho_X} + \lambda)^{-\frac{1}{2}} v_X(x) K_x \langle K_x, \cdot \rangle_H (T_{\rho_X} + \lambda)^{-\frac{1}{2}}.$$

Moreover, $\xi_2 : Z \to H$ is defined by

$$\xi(x, y) = (T_{\rho_X} + \lambda)^{-\frac{1}{2}} v_X(x) K_x y.$$

Finally, $\xi_3 : X \to H$ is defined by

$$\xi(x) = (T_{\rho_X} + \lambda)^{-\frac{1}{2}} v_X(x) K_x f_\lambda(x).$$

Application of Proposition 10 to each of $S_i$, $i = 1, 2, 3$, yields to the following bounds with probability at least $1 - \delta / 3$

$$S_i \leq \frac{2L_i \log(6/\delta)}{n} + \sigma_i \sqrt{\frac{2\log(6/\delta)}{n}}$$

where, as it can be straightforwardly verified, the constants $L_i$ and $\sigma_i$ are given by the expressions

$$L_1 = \frac{V_X}{\lambda}, \quad \sigma_1 = 2\gamma_X \sqrt{\frac{N'(\lambda)^p}{\lambda^{1+q}}},$$

$$L_2 = \frac{M V_X}{\sqrt{\lambda}}, \quad \sigma_2 = 2M \gamma_X \sqrt{\frac{N'(\lambda)^p}{\lambda^{1+q}}},$$

$$L_3 = \frac{2\|f_\lambda\|_H V_X}{\sqrt{\lambda}}, \quad \sigma_3 = 2\|f_\lambda\|_H \gamma_X \sqrt{\frac{N'(\lambda)^p}{\lambda^{1+q}}},$$

with $p = 1 - q$. Let us demonstrate it for $S_2$. First, notice that

$$E\|\xi_2 - E\xi_2\|_H^m \leq E\|\xi_2 - \xi\|_H^m \leq 2^{m-1} E\xi_2 E\xi_2' (\|\xi_2\|_H^m + \|\xi\|_H^m) \leq 2^m E\|\xi_2\|_H^m.$$
where $\xi'$ is an independent copy of $\xi_2$. Second,

$$E\|\xi_2\|^2_H = E\langle \xi_2, \xi_2 \rangle_H^{m/2} \leq \int (T_{\rho_X'} + \lambda)^{-\frac{1}{2}} v_X(x) K_{xy} (T_{\rho_X'} + \lambda)^{-\frac{1}{2}} v_X(y) \| T_{\rho_X'} + \lambda \|^2_H \| T_{\rho_X'} + \lambda \|^2_H \| \rho_X' \| \rho_X' \| \rho_X' \| \rho_X' \|

\leq M^m \int (T_{\rho_X'} + \lambda)^{-1} T_{xy} (T_{\rho_X'} + \lambda)^{-1} T_{xy} \| T_{\rho_X'} + \lambda \|^2 H \| T_{\rho_X'} + \lambda \|^2 H \| \rho_X' \| \rho_X' \| \rho_X' \| \rho_X' \|

\leq M^m \int (T_{\rho_X'} + \lambda)^{-1} T_{xy} (T_{\rho_X'} + \lambda)^{-1} T_{xy} \| T_{\rho_X'} + \lambda \|^2 H \| T_{\rho_X'} + \lambda \|^2 H \| \rho_X' \| \rho_X' \| \rho_X' \| \rho_X' \|

\leq M^m \left( \sqrt{\frac{1}{\lambda}} \right)^{m-2} \left( \sqrt{\frac{1}{\lambda}} \right)^2 \mathcal{N}_p \mathcal{N}_p \gamma_X^2

\leq \frac{1}{2} m! \left( MV_X \sqrt{\frac{1}{\lambda}} \right)^{m-2} \left( MV_X \sqrt{\frac{1}{\lambda}} \right)^{\frac{2}{\lambda}} \mathcal{N}_p \mathcal{N}_p \gamma_X^2.

Now, choosing $n\lambda^{1+q} \geq 16(V_X + \gamma_X^2) \mathcal{N}_p \mathcal{N}_p \log^2 \left( \frac{6}{\delta} \right)$, we have with probability $1 - \frac{\delta}{3}$

$$S_1 \leq 4 \log \left( \frac{6}{\delta} \right) \left( \frac{V_X}{n\lambda} + \sqrt{\frac{\gamma_X^2 \mathcal{N}_p \mathcal{N}_p}{n\lambda^{1+q}}} \right)

\leq 4 \frac{V_X \mathcal{N}_p \mathcal{N}_p}{n\lambda^{1+q}} \log^2 \left( \frac{6}{\delta} \right) + \sqrt{\frac{\gamma_X^2 \mathcal{N}_p \mathcal{N}_p}{n\lambda^{1+q}}} \log^2 \left( \frac{6}{\delta} \right)

\leq \frac{3}{4}.

So, with probability at least $1 - \delta$

$$\|I\text{ term}\|_{\rho_X} \leq 16 \log \left( \frac{6}{\delta} \right) \left( \frac{M + \| f_\lambda \|_H}{\sqrt{1 - \mu}} \right) \left( \frac{V_X}{n\sqrt{\lambda}} + \gamma_X \sqrt{\frac{\mathcal{N}_p \mathcal{N}_p}{n\lambda^q}} \right)

= 16 \log \left( \frac{6}{\delta} \right) \left( \frac{M + \| R \|}{\sqrt{1 - \mu}} \right) \left( \frac{V_X}{n\sqrt{\lambda}} + \gamma_X \sqrt{\frac{\mathcal{N}_p \mathcal{N}_p \lambda^q}{n\lambda^{1+q}}} \right).

\text{II term. To bound the second term notice that}

$$\| (T_x + \lambda)^{-1} T_{\rho_X'} \| = \| (T_x + \lambda)^{-1} (T_{\rho_X'} + \lambda) (T_{\rho_X'} + \lambda)^{-1} T_{\rho_X'} \|

\leq \| (T_x + \lambda)^{-1} (T_{\rho_X'} + \lambda) \|

= \left\| (T_{\rho_X'} + \lambda)^{-\frac{1}{2}} \left( I - (T_{\rho_X'} + \lambda)^{-\frac{1}{2}} (T_{\rho_X'} + \lambda)^{-\frac{1}{2}} \right) \right\|^{-1} \left( T_{\rho_X'} + \lambda \right)^{-\frac{1}{2}}

\leq \frac{1}{1 - S_1} \leq 4,

\text{where the last inequality follows form (21). Thereof we have}

$$\|\text{II term}\|_{\rho_X} \leq \| (T_x + \lambda)^{-1} T_{\rho_X'} \| \| f'_{\mathcal{H}} - f_{\mathcal{H}} \|_{\rho_X} \leq 4 \| f'_{\mathcal{H}} - f_{\mathcal{H}} \|_{\rho_X}.
III term For the III term, by using the proposition 10 we can write

\[ \| (T_\lambda + \lambda)^{-1} (T - T_{\rho'_\lambda}) + I \| = \| (T_\lambda + \lambda)^{-1} (T_{\rho'_\lambda} + \lambda) (T_{\rho'_\lambda} + \lambda)^{-1} (T - T_{\rho'_\lambda}) + I \| \]
\[ \leq \| (T_\lambda + \lambda)^{-1} (T_{\rho'_\lambda} + \lambda) \| \| (T_{\rho'_\lambda} + \lambda)^{-1} (T - T_{\rho'_\lambda}) + I \| \]
\[ \leq 4 \| (T_{\rho'_\lambda} + \lambda)^{-1} (T + \lambda - (T_{\rho'_\lambda} + \lambda)) + I \| \]
\[ \leq 4 \| (T_{\rho'_\lambda} + \lambda)^{-1} (T + \lambda) \| \]
\[ \leq \frac{4}{1 - \mu}, \]

this leads us to the following bound for the last term

\[ \| \text{III term} \|_{\rho'_\lambda} \leq \frac{4}{1 - \mu} \| f_{\lambda} - f_{\mathcal{H}} \|_{\rho'_{\lambda}} \leq \frac{4}{1 - \mu} \lambda^r R, \]  

where the last inequality follows from the Proposition 9.

Considering (22), (23), (24) in the decomposition (17) we have, with probability at least \( 1 - \delta \)

\[ \| f_{\lambda, \lambda} - f_{\mathcal{H}} \|_{\rho'_{\lambda}} \leq 16 \log \left( \frac{6}{\delta} \right) \left( \frac{M + R}{\sqrt{1 - \mu}} \right) \left( \frac{V_X}{n \sqrt{\lambda}} + \frac{\gamma_X E' \rho}{\sqrt{n \lambda^{p+q}}} \right) + \frac{4}{1 - \mu} \lambda^r R + 4 \| f_{\mathcal{H}}^1 - f_H \|_{\rho'_{\lambda}} \]

By choosing \( \lambda \) as in (7) we finally get

\[ \| f_{\lambda, \lambda} - f_{\mathcal{H}} \|_{\rho'_{\lambda}} \leq 16 \log \left( \frac{6}{\delta} \right) \left( \frac{M + R}{\sqrt{1 - \mu}} \right) \left( \frac{V_X}{n \sqrt{\lambda}} + \frac{\gamma_X E' \rho}{\sqrt{n \lambda^{s' p+q}}} \right) + \frac{4}{1 - \mu} \lambda^r R + 4 \| f_{\mathcal{H}}^1 - f_H \|_{\rho'_{\lambda}} \]
\[ \leq 2D (M + R) \lambda^r \left( \frac{\gamma_X}{\sqrt{V_X}} + \frac{V_X}{s' \sqrt{n \lambda^{s' p+q}}} \right) + \frac{8 E'^2 \log \left( \frac{6}{\delta} \right)}{(V_X + \gamma_X)^2} + 4D \lambda^r R + 4 \| f_{\mathcal{H}}^1 - f_H \|_{\rho'_{\lambda}}, \quad \text{for} \quad s' \in (0, 1]. \]

Substituting the expression (13) for \( \lambda \) in the inequality above, concludes the proof of Theorem 6.

Let us note that the Theorem 4 follows from the Theorem 6 by taking \( \rho' = \rho'^{\alpha} \). In this case \( f_{\mathcal{H}}^1 = f_{\mathcal{H}}, E' = E_\alpha \) and \( s' = s \).

7.2 Appendix - Bound for Target shift

Let us decompose the excess risk as follows

\[ f_{\lambda, \lambda} - f_{\mathcal{H}} = (T_\lambda + \lambda)^{-1} \{ (g_\alpha - L \phi) + (LM_\phi - T_\alpha) f_{\lambda} \} \]
\[ + (T_\lambda + \lambda)^{-1} \{ L \phi - f_{\rho'_{\lambda}} \} + (T - L M_\phi) f_{\lambda} \]  

(25)

where \( T_\alpha = S_{T, \alpha}^T M_\alpha S_\alpha, g_\alpha = S_{T, \alpha}^T M_\alpha y \) and \( M_\phi f = f_\psi \) is a multiplication operator. Here \( v = (v_\gamma(y_1), \ldots, v_\gamma(y_n)). \)

I term Similarly to the first term of the previous proof we can show

\[ \| \text{I term} \|_{\rho'_{\lambda}} \leq \frac{1}{1 - \mu} \left( S_2' + S_3' \right) \]

where

\[ S_2' := \| (T + \lambda)^{-\frac{1}{2}} (g_\alpha - L \phi) \|_{\mathcal{H}}, \]
\[ S_3' := \| (T + \lambda)^{-\frac{1}{2}} (LM_\phi - T_\alpha) f_{\lambda} \|_{\mathcal{H}}, \]
\[ S_4' := \| (LM_\phi + \lambda)^{-\frac{1}{2}} (LM_\phi - T_\alpha) (LM_\phi + \lambda)^{-\frac{1}{2}} \|_{\text{HS}}, \]
and

\[ \mu = \mu_{\text{max}} \left( (T + \lambda I)^{-1/2} (T - LM\psi)(T + \lambda I)^{-1/2} \right). \]

One can easily show that \( \mu \leq 1 - \inf \psi, \) therefore

\[ \| \text{I term} \|_{\rho_X^\psi} \leq D \left( S'_2 + S'_3 \right). \]

The following constants for \( S'_1, S'_2, S'_3 \) can be straightforwardly verified,

\[ L'_1 = 2 \frac{V_Y}{\lambda}, \quad \sigma'_1 = 2 \sqrt{\frac{\lambda}{\lambda} \gamma_Y}, \]
\[ L'_2 = 2 \frac{MV_Y}{\sqrt{\lambda}}, \quad \sigma'_2 = 2 \frac{M}{\sqrt{\lambda} \gamma_Y}, \]
\[ L'_3 = 2 \frac{\| f_X \|_{\mathcal{H}} V_Y}{\sqrt{\lambda}}, \quad \sigma'_3 = 2 \frac{\| f_X \|_{\mathcal{H}} \gamma_Y \sqrt{\lambda}}{\lambda}. \]

Now, choosing \( n\lambda \geq (V_Y + \gamma_Y^2)|\mathcal{N}(\lambda)|D^2 \) with probability at least \( 1 - \delta/3, \) we get

\[ S'_1 = \left\| (LM\psi + \lambda)^{-\frac{1}{2}} (LM\psi - T_{\lambda}) (LM\psi + \lambda)^{-\frac{1}{2}} \right\|_{\text{HS}} \]
\[ \leq D \left\| (T + \lambda)^{-\frac{1}{2}} (LM\psi - T_{\lambda}) (T + \lambda)^{-\frac{1}{2}} \right\|_{\text{HS}} \]
\[ \leq 4 \log \left( \frac{6}{\delta} \right) \left( \frac{V_Y}{n\lambda(1 - \mu)} + 2 \sqrt{\frac{\gamma_Y^2 |\mathcal{N}(\lambda)|}{n\lambda(1 - \mu)^2}} \right) \]
\[ \leq \frac{3}{4}. \]

So, with probability at least \( 1 - \delta, \) we have

\[ \| \text{I term} \|_{\rho_X^\psi} \leq 16 \log \left( \frac{6}{\delta} \right) D (M + R) \lambda^r \left( \frac{V_Y \lambda^{r+s-0.5}}{n\lambda^{2r+s}} + \gamma \frac{E_s}{\sqrt{n\lambda^{2r+s}}} \right). \] (26)

**II term** For the second term notice that

\[ \text{II term} = (T_{\lambda} + \lambda)^{-1} \left\{ L(\phi - f_{\rho^*}) + (T - LM\psi) f_{\lambda} \right\} = (T_{\lambda} + \lambda)^{-1} LM\psi \left\{ \left( \frac{\phi}{\psi} - f_{\rho^*} \right) + \frac{1 - \psi}{\psi} (f_{\lambda} - f_{\mathcal{H}}) \right\}. \]

The argument used to bound the second term of the previous section allows us to conclude that \( \| (T_{\lambda} + \lambda)^{-1} LM\psi \| \leq 4, \) therefore

\[ \| \text{II term} \|_{\rho_X^\psi} \leq 4 \left\| \frac{\phi}{\psi} - f_{\rho^*} \right\|_{\rho_X^\psi} + 5D \| f_{\lambda} - f_{\mathcal{H}} \|_{\rho_X^\psi}. \] (27)

Considering (26) and (27) in the decomposition (25) and using the proposition [9] we have with probability at least \( 1 - \delta \)

\[ \| f_{\lambda} - f_{\mathcal{H}} \|_{\rho_X^\psi} \leq 16 \log \left( \frac{6}{\delta} \right) D (M + R) \lambda^r \left( \frac{V_Y \lambda^{r+s-0.5}}{n\lambda^{2r+s}} + \gamma \frac{E_s}{\sqrt{n\lambda^{2r+s}}} \right) + 6D \lambda^r R \] (28)
\[ + 4 \left\| \frac{\phi}{\psi} - f_{\rho^*} \right\|_{\rho_X^\psi}. \] (29)

By choosing \( \lambda \) as in (15) we have

\[ \| f_{\lambda} - f_{\mathcal{H}} \|_{\rho_X^\psi} \leq 6D(M + R) \lambda^r + 4 \left\| \frac{\phi}{\psi} - f_{\rho^*} \right\|_{\rho_X^\psi}. \]

Substituting the expression (15) for \( \lambda \) in the inequality above, concludes the proof of Theorem [7]. Theorem [5] follows from the Theorem [7] by taking \( \rho^* = \rho_{\rho^*}. \) In this case \( D = 1 \) and the bias term \( \left\| \frac{\phi}{\psi} - f_{\rho^*} \right\|_{\rho_X^\psi} \) vanishes.