Sharp Generalization of Transductive Learning: A Transductive Local Rademacher Complexity Approach

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Abstract

We introduce a new tool, Transductive Local Rademacher Complexity (TLRC), to analyze the generalization performance of transductive learning methods and motivate new transductive learning algorithms. Our work extends the idea of the popular Local Rademacher Complexity (LRC) [1] to the transductive setting with considerable changes compared to the analysis of typical LRC methods in the inductive setting. While LRC has been widely used as a powerful tool in the analysis of inductive models with sharp generalization bounds for classification and minimax rates for nonparametric regression, it remains an open problem whether a localized version of Rademacher complexity based tool can be designed and applied to transductive learning and gain sharp bounds under proper conditions.

We give a confirmative answer to this open problem by TLRC. Similar to the development of LRC [2], we build TLRC by starting from a sharp concentration inequality for independent variables with variance information. The prediction function class of a transductive learning model is then divided into pieces with a sub-root function being the upper bound for the Rademacher complexity of each piece, and the variance of all the functions in each piece is limited. A carefully designed variance operator is used to ensure that the bound for the test loss on unlabeled test data in the transductive setting enjoys a remarkable similarity to that of the classical LRC bound in the inductive setting. That is, with high probability, for all $f \in \mathcal{F}$,

$$\textsf{Test Loss of } f \le \textsf{Training Loss of } f + \textsf{Fixed Point of the Sub-Root Function},$$

where scaling factors on the RHS are omitted and $\mathcal{F}$ is a class of prediction functions associated with a transductive learning method. We use the new TLRC tool to analyze the Transductive Kernel Learning (TKL) model, where the labels of test data are generated by a kernel function. The result of TKL lays the foundation for generalization bounds for two types of transductive learning tasks, Graph Transductive Learning (GTL) and Transductive Nonparametric Kernel Regression (TNKR). When the target function is low-dimensional or approximately low-dimensional, we design low rank methods for both GTL and TNKR, which enjoy particularly sharper generalization bounds by TLRC which cannot be achieved by existing learning theory methods, to the best of our knowledge. It is noted that GTL is similar to linear Graph Neural Network (GNN) such as [3], and it is expected that TLRC opens the door for analyzing existing models and designing new transductive models based on GNN. The proof of generalization bounds using TLRC involves several new techniques, such as building low-dimensional subspaces in Reproducing Kernel Hilbert Space (RKHS) for transductive learning, which are of independent interest.

1 Introduction

We study transductive learning in this paper, where the learner has access to both labeled training data and unlabeled test data, and the task is to predict the labels of the test data.

Obtaining a tight generalization bound for transductive learning is an important problem in statistical learning theory. Tools for inductive learning, such as Rademacher complexity and VC dimension, have been used for transductive learning, including empirical risk minimization, transductive regression, and transductive classification [4–7]. On the other hand, it is important to employ localized version of Rademacher complexity, such as Local Rademacher Complexity (LRC) [1], to obtain sharper generation bound for transductive learning, such as [8]. Given the fact that LRC is capable of achieving various minimax rates for M-estimators in tasks such as nonparametric regression in the inductive regime, we propose to solve the following interesting and important question for LRC based transductive learning: under the condition that $m \ge Cn$ for some constant $C \in (0,1)$, can we have a sharp LRC based generation bound for test loss of transductive learning as well as a sharp excess risk?

We give a confirmative answer to this question by presenting a new tool, Transductive Local Rademacher Complexity (TLRC), which renders particularly sharp bound for transductive learning. We obtain particularly sharp bounds when the target function is low-dimensional or approximately low-dimensional. We design new transductive learning algorithms and demonstrate their sharp generalization bounds by TLRC for Graph Transductive Learning (GTL) and Transductive Nonparametric Kernel Regression (TNKR).

1.1 Summary of Main Results

Our main results are summarized as follows. This summary also features a high-level description of the ideas we developed to obtain the detailed technical results in Section 3.

1. In Section 3.1-Section 3.3, we develop the basic concentration inequality of independent random variables which specify the training data for transductive learning, and then design a novel variance operator $\overline{\mathrm{Var}}\left[\cdot\right]$ to divide the prediction function class into pieces where the variance of functions in each piece is bounded. This procedure renders the basic TLCR bound for generic transductive learning:

$$\mathcal{U}(\ell_f) \le \mathcal{O}\left(\mathcal{L}^{(m)}_{\ell_f}(\overline{\mathbf{Z}(\mathbf{d})})\right) + \mathcal{O}(r_u^* + r_m^*) + \mathcal{O}\left(\frac{1}{m} + \frac{1}{u}\right), \qquad \text{(TLRC bounds in Theorem 3.2, 3.3)}$$

   which holds with high probability for any prediction function f in a function class. Here ℓ_f is the loss function applied to the prediction made by f. $\mathcal{U}$ and $\mathcal{L}^{(m)}$ denote the test loss and the training loss, r^* is the fixed point of a properly defined sub-root function which bounds our novel Transductive Rademacher Complexity of each piece of the function class. It is interesting to observe that the TLRC bound is very similar to the basic LRC bound [2, Theorem 3.3]. As a result, one expects that the established techniques developed for LRC can be adapted to transductive learning. This paper shows that such expectation can be fulfilled by applying the basic TLRC bound to the following transductive learning tasks.

2. We apply the basic TLRC bound to derive the generalization bound for Transductive Kernel Learning (TKL), where the labels of the test data are generated by a positive definite kernel. The generalization bound for TKL is then used to derive bounds for two transductive learning tasks, Graph Transductive Learning (GTL) and Transductive Nonparametric Kernel Regression (TNKR). Sharp generalization bounds are obtained for both tasks when the target function is low-dimensional.

   In particular, for GTL, when the target label vector lies on the subspace spanned by the top-r_0 eigenvectors of the matrix $\mathbf{L}$ which encodes the graph information, such as the normalized graph Laplacian, then a test loss of $\mathcal{O}(r_0/m)$ is achieved with m being the size of training data. Such sharp bound, when $r_0 \ll m$, is obtained by a novel Low-Rank GTL algorithm to be introduced in Section 3.6, which is not achievable by most existing theoretical tools for transductive learning that render bounds of $\mathcal{O}(m^{-1/2})$ or $\tilde{\mathcal{O}}(m^{-1/2})$, such as [7, 9].

Our proofs are deferred to the appendix, which are equipped with new techniques designed for TLRC and the potential future works in this direction. For example, although there is no given positive definite kernel function in the GTL task, the sharp bound of $\mathcal{O}(r_0/m)$ is still proved using a new technique which builds a positive definite kernel such that the prediction functions are in a r_0-dimensional subspace of the RKHS associated with that kernel.

We further note that when the target function is not on a low-dimensional subspace of the RKHS, Corollary 3.7 in Section 3.5.1 shows that TLRC can still obtain bounds of $\mathcal{O}(m^{-1/2})$ or even sharper in the interpolation regime where the training loss is almost 0. To see this, one can verify that (17) of Corollary 3.7 leads to a test loss of $\mathcal{O}\left(n^{-2\alpha/(2\alpha+1)}\right)$ is achieved by letting $Q \asymp n^{-1/(2\alpha+1)}$ when $\widehat{\lambda}_q \asymp q^{-2\alpha}$ for some constant $\alpha > 1/2$.

Comparison with LRC based Transductive Learning Bound in [8]. Let $\widehat{f}$ be the empirical minimizer on the training data, the excess bound by the LRC method in [8, Corollary 13-14] is presented below,

$$\text{Excess Risk of } \widehat{f} \le \mathcal{O}\left(\frac{n}{u} r_m^* + \frac{n}{m} r_u^* + \frac{1}{m} + \frac{1}{u}\right). \tag{1}$$

Here r_u^*, r_m^* are the fixed points of sub-root functions for empirical processes involving test loss and training loss respectively, m, u are the size of training data and test data, and $n = u + m$. Under our assumption specified in Assumption 1, that is, $m \ge Cn$ for some constant $C \in (0,1)$, we obtain

$$\text{Excess Risk of } \widehat{f} \le \mathcal{O}\left(r^* + \frac{1}{u} + \frac{1}{m}\right), \quad \text{(Theorem 3.4)}$$

where r^* is the fixed point of an empirical process involving both training and testing data, when the transductive learning is realizable.

1.2 Notations

We use bold letters for matrices and vectors, and regular lower letter for scalars throughout this paper. The bold letter with a single superscript indicates the corresponding column of a matrix, e.g. $\mathbf{A}_i$ is the i-th column of matrix $\mathbf{A}$, and the bold letter with subscripts indicates the corresponding element of a matrix or vector. We put an arrow on top of a letter with subscript if it denotes a vector, e.g., $\vec{\mathbf{x}}_i$ denotes the i-th training feature. We also use $\mathbf{Z}(i)$ to denote the i-th element of a vector $\mathbf{Z}$. $\mathrm{Span}(\mathbf{A})$ is the column space of matrix $\mathbf{A}$. $\|\cdot\|_F$ and $\|\cdot\|_p$ denote the Frobenius norm and the vector ℓ^p-norm or the matrix p-norm. $\mathrm{Var}[\cdot]$ denotes the variance of a random variable. $\mathbf{I}_n$ is a $n \times n$ identity matrix. $\mathbb{I}_{\{E\}}$ is an indicator function which takes the value of 1 if event E happens, or 0 otherwise. The complement of a set A is denoted by $\overline{A}$, and $|A|$ is the cardinality of the set A. $\mathrm{tr}(\cdot)$ is the trace of a matrix. We denote the unit sphere in d-dimensional Euclidean space by $\mathbb{S}^{d-1} \coloneqq \{\mathbf{x} \colon \mathbf{x} \in \mathbb{R}^d, \|\mathbf{x}\|_2 = 1\}$. Let $L^2(\mathcal{X}, \mu^{(P)})$ denote the space of square-integrable functions on $\mathbb{S}^{d-1}$ with probability measure $\mu^{(P)}$, and the inner product $\langle \cdot, \cdot \rangle_{\mu^{(P)}}$ and $\|\cdot\|_{\mu^{(P)}}^2$ are defined as $\langle f, g \rangle_{L^2} \coloneqq \int_{\mathbb{S}^{d-1}} f(x) g(x) \mathrm{d}\mu^{(P)}(x)$ and $\|f\|_{L^2}^2 \coloneqq \int_{\mathbb{S}^{d-1}} f^2(x) \mathrm{d}\mu^{(P)}(x) < \infty$. $\mathbb{P}_{\mathcal{A}}$ is the orthogonal projection onto a linear space $\mathcal{A}$, and $\mathcal{A}^\perp$ is the linear subspace orthogonal to $\mathcal{A}$. $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ and $\|\cdot\|_{\mathcal{H}}$ denote the inner product and the norm in the Hilbert space $\mathcal{H}$. we write $a = \mathcal{O}(b)$ if there exists a constant $C > 0$ such that $a \le Cb$, and $\tilde{\mathcal{O}}$ indicates there are specific requirements in the constants of the $\mathcal{O}$ notation. $a \asymp b$ denotes that there exists constants $c_1, c_2 > 0$ such that $c_1 b \le a \le c_2 b$. $\binom{m}{k}$ for $1 \le k \le m$ is the combinatory number of selecting k different objects from m objects. $\mathbb{R}^+$ is the set of all nonnegative real numbers, and $\mathbb{N}$ is the set of all the natural numbers. We use the convention that $\sum_{i=p}^{q} = 0$ if $p > q$ or $q = 0$. $[m : n]$ denotes all the natural numbers between m and n inclusively, and we abbreviate $[1 : n]$ as $[n]$.

2 Problem Setup of Transductive Learning

We consider a set $\mathbf{S}_{m+u} \coloneqq \left\{(\overrightarrow{\mathbf{x}}_i, y_i)\right\}_{i=1}^{m+u}$, where y_i is the label for the point $\overrightarrow{\mathbf{x}}_i$. Let $n = m + u$, $\left\{\overrightarrow{\mathbf{x}}_i\right\}_{i=1}^{n} \subseteq \mathcal{X} \subseteq \mathbb{R}^d$, $\{y_i\}_{i=1}^{n} \subseteq \mathcal{Y} \subseteq \mathbb{R}^+$ where $\mathcal{X}, \mathcal{Y}$ are the input and output spaces, and $\mathcal{X}$ is a compact subset. We consider the case that $\mathcal{Y}$ is a bounded set, and without loss of generality we let $\mathcal{Y} = [-1, 1]$. The learner is provided with the (unlabeled) full sample $\mathbf{X}_n \coloneqq \left\{\overrightarrow{\mathbf{x}}_i\right\}_{i=1}^{n}$. Under the standard setting of transductive learning [7,8], the training features $\mathbf{X}_m$ of size m are sampled uniformly from $\mathbf{X}_n$ without replacement. Because we are interested in bounding the empirical process $\mathcal{U}_h - \mathcal{L}_h^{(m)}$, we specify the sampling process of the test features $\mathbf{X}_u \coloneqq \mathbf{X}_n \setminus \mathbf{X}_m$. If $\mathbf{X}_u$ of size u are sampled uniformly from $\mathbf{X}_n$ without replacement, then by symmetry $\mathbf{X}_m$ are sampled uniformly from $\mathbf{X}_n$ without replacement.

Let $\mathbf{d} = [d_1, \ldots, d_u] \in \mathbb{N}^u$ be a random vector, and $\{d_i\}_{i=1}^{u}$ are u independent random variables such that d_i takes values in $[i : n]$ uniformly at random. Algorithm 1, which is adapted from [7] and deferred to the next subsection, specifies how to obtain $\mathbf{Z}_{\mathbf{d}} = [\mathbf{Z}_{\mathbf{d}}(1), \ldots, \mathbf{Z}_{\mathbf{d}}(u)]^\top \in \mathbb{N}^u$ as the first u elements of a uniformly distributed permutation of $[n]$, so that $\mathbf{Z}_{\mathbf{d}}$ are the indices of u test features sampled uniformly from $\mathbf{X}_n$ without replacement. Let $\mathbf{Z}$ be a vector, we use $\{\mathbf{Z}\}$ denote a set containing all the elements of the vector $\mathbf{Z}$ regardless of the orders of these elements in $\mathbf{Z}$. Let $\overline{\mathbf{Z}_{\mathbf{d}}} = [n] \setminus \{\mathbf{Z}_{\mathbf{d}}\}$ be indices not in $\{\mathbf{Z}_{\mathbf{d}}\}$. It has been verified in [7] that the u points $\mathbf{X}_u \coloneqq \left\{\overrightarrow{\mathbf{x}}_i\right\}_{i \in \mathbf{Z}_{\mathbf{d}}}$ are selected from $\mathbf{X}_n$ uniformly at random among all subsets of size u, and they serves as the test features. As a result, $\mathbf{X}_m = \mathbf{X}_n \setminus \mathbf{X}_u = \left\{\overrightarrow{\mathbf{x}}_i\right\}_{i \in \overline{\mathbf{Z}_{\mathbf{d}}}}$ are m training features sampled from $\mathbf{X}_n$ without replacement. The training features together with their labels, $\{y_i\}_{i \in \overline{\mathbf{Z}_{\mathbf{d}}}}$, are given to the learner as a training set. We denote the labeled training set by $\mathbf{S}_m \coloneqq \left\{\left(\overrightarrow{\mathbf{x}}_i, y_i\right)\right\}_{i \in \overline{\mathbf{Z}_{\mathbf{d}}}}$. $\mathbf{X}_u$ is also called the test set. The learner's goal is to predict the labels of the test points in $\mathbf{X}_u$ based on $\mathbf{S}_m \bigcup \mathbf{X}_u$.

Assumption 1 (Main Assumption)**.** There exist a constant $C \in (0, 1)$ such that $m \ge Cn$.

This paper studies the sharp generalization bounds of transductive learning algorithms. We also assume all the points in the full sample $\mathbf{X}_n$ are distinct. Given a prediction function f defined on $\mathcal{X}$, we define the following loss functions. We consider the loss function $\ell(f(\mathbf{x}), y) \coloneqq (f(\mathbf{x}) - y)^2$ throughout this paper. For simplicity of notations, we let $g(i) = g(\overrightarrow{\mathbf{x}}_i, y_i)$ or $g(i) = g(\overrightarrow{\mathbf{x}}_i)$ for a function g defined on $\mathcal{X} \times \mathcal{Y}$ or $\mathcal{X}$. we write $\ell \circ f$ as ℓ_f and let $\ell_f(i) = \ell(f(\overrightarrow{\mathbf{x}}_i), y_i)$. Let $\mathcal{H}$ be a class of functions defined on $\mathcal{X} \times \mathcal{Y}$. We define the training loss associated with h as $\mathcal{L}_h^{(m)}(\overline{\mathbf{Z}_{\mathbf{d}}}) \coloneqq \frac{1}{m} \sum\limits_{i \in \overline{\mathbf{Z}_{\mathbf{d}}}} h(i)$, and the test loss and average loss are defined as $\mathcal{U}_h(\mathbf{Z}_{\mathbf{d}}) \coloneqq \frac{1}{u} \sum\limits_{i \in \mathbf{Z}_{\mathbf{d}}} h(i)$ and $\mathcal{L}_n(h) \coloneqq \frac{1}{n} \sum\limits_{i=1}^{n} h(i)$. When $h = \ell_f$, $\mathcal{L}_h^{(m)}(\overline{\mathbf{Z}_{\mathbf{d}}})$ and $\mathcal{U}_h(\mathbf{Z}_{\mathbf{d}})$ are the training loss and test loss of the prediction function f.

2.1 Sampling Uniformly Distributed Permutations

A sampling strategy in [7] is adopted to sample u points from the full sample $\mathbf{X}_n$ uniformly at random among all subsets of size u, which is described in Algorithm 1. Let $\mathbf{Z_d}$ be the vector returned by Algorithm 1. Then $\{\mathbf{Z_d}\}$ is the set of the indices of the test features, and $\overline{\mathbf{Z_d}}$ is the set of the indices of the training features.

Algorithm 1 The RANDPERM Algorithm in [7], which obtains $\mathbf{Z_d} \in \mathbb{N}^u$ as the first u elements of a uniformly distributed permutation of $[n]$ by sampling independent random variables $d_1, \ldots, d_u$.

$\mathbf{Z_d} \leftarrow$ RANDPERM(u)
input: u
initialize: $\mathbf{I} = [n]$, $\mathbf{d}, \mathbf{Z_d} \in \mathbb{N}^u$ are initialized as zero vectors.
for $i = 1, \ldots, u$ **do**
  Sample d_i uniformly from $[i : n]$.
  $\mathbf{d}(i) = d_i$, $\mathbf{Z_d}(i) = \mathbf{I}(d_i)$.
  Swap the values of $\mathbf{I}(i)$ and $\mathbf{I}(d_i)$.
end for
return $\mathbf{Z_d}$

2.2 Basic Definitions

We define basic functions and the novel variance operator for TLRC. Let $\mathbf{d}' = [d'_1, \ldots, d'_m]$ be independent copies of $\mathbf{d}$, and $\mathbf{d}^{(i)} = [d_1, \ldots, d_{i-1}, d'_i, d_{i+1}, \ldots, d_m]$. Note that $\mathbb{E}_{\mathbf{d}}\left[\mathcal{U}_h(\mathbf{Z_d})\right] = \mathcal{L}_n(h)$. We define

$$g(\mathbf{d}) \coloneqq \sup_{h \in \mathcal{H}} \left(\mathcal{U}_h(\mathbf{Z_d}) - \mathcal{L}_h^{(m)}(\overline{\mathbf{Z_d}})\right), \tag{2}$$

where $\mathcal{L}_h^{(m)}(\overline{\mathbf{Z_d}}) \coloneqq \frac{1}{m} \sum\limits_{i \in [n] \setminus \{\mathbf{Z_d}\}} h(i)$ is the training loss. The Transductive Rademacher Complexity is then defined below.

Definition 2.1. Let $\{\sigma_i\}_{i=1}^n$ be n i.i.d. random variables such that $\Pr[\sigma_i = 1] = \Pr[\sigma_i = -1] = \frac{1}{2}$. Define $R_{u,\mathbf{d}} h \coloneqq \frac{1}{u} \sum\limits_{i \in \mathbf{Z_d}} \sigma_i h(i)$ and $R_{m,\mathbf{d}} h \coloneqq \frac{1}{m} \sum\limits_{i \in \overline{\mathbf{Z_d}}} \sigma_i h(i)$. Two types of Transductive Rademacher Complexity (TRC) of the function class $\mathcal{H}$ is defined as

$$\mathfrak{R}_u(\mathcal{H}) \coloneqq \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{h \in \mathcal{H}} R_{u,\mathbf{d}} h\right] = \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\frac{1}{u} \sup_{h \in \mathcal{H}} \sum_{i \in \mathbf{Z_d}} \sigma_i h(i)\right], \tag{3}$$

$$\mathfrak{R}_m(\mathcal{H}) \coloneqq \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{h \in \mathcal{H}} R_{m,\mathbf{d}} h\right] = \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\frac{1}{m} \sup_{h \in \mathcal{H}} \sum_{i \in \overline{\mathbf{Z_d}}} \sigma_i h(i)\right]. \tag{4}$$

For simplicity of notations, TRC is also denoted by $\mathbb{E}\left[\sup_{h \in \mathcal{H}} R_{u,\mathbf{d}} h\right]$ or $\mathbb{E}\left[\sup_{h \in \mathcal{H}} R_{m,\mathbf{d}} h\right]$ if the expectation over $\mathbf{d}, \boldsymbol{\sigma}$ is clear in the context.

We remark that the proposed TRC is fundamentally different from the transductive version of the Rademacher complexity in [7, Definition 1] in the sense that our TRC is operated only on the random training set, while the counterpart in [7, Definition 1] operates on the entire full sample.

In addition, the Rademacher variables used in our TRC are the same as the inductive Rademacher variables. In this sense, our TRC is closer to the Rademacher complexity and its localized variants in the inductive setting. We define the sub-root function below.

Definition 2.2 (Sub-root function, [1, Definition 3.1])**.** A function $\psi\colon [0,\infty) \to [0,\infty)$ is sub-root if it is nonnegative, nondecreasing and if $\frac{\psi(r)}{\sqrt{r}}$ is nonincreasing for $r > 0$.

3 Detailed Technical Results

3.1 A Concentration Inequality for Functions of Independent Random Variables

Theorem 3.1 (Concentration Inequality for Functions of Independent Random Variables)**.** Let $\mathcal{H}$ be a class of functions defined on $\mathcal{X} \times \mathcal{Y}$ and for any $h \in \mathcal{H}$, $0 \le h(i) \le H_0$ for all $i \in [n]$ with a positive number H_0. Assume that there is a positive number $r > 0$ such that $\sup_{h\in\mathcal{H}} \mathcal{L}_n(h) \le r$. Then for every $x > 0$, with probability at least $1 - e^{-x}$ over $\mathbf{d}$,

$$\begin{aligned} g(\mathbf{d}) &= \sup_{h\in\mathcal{H}} \left(\mathcal{U}_h(\mathbf{Z}_\mathbf{d}) - \mathcal{L}_h^{(m)}(\overline{\mathbf{Z}_\mathbf{d}})\right) \\ &\le \inf_{\alpha>0} \left(\left(2 + \frac{2}{\alpha}\right)(\mathfrak{R}_u(\mathcal{H}) + \mathfrak{R}_m(\mathcal{H})) + \frac{2(2+\alpha)H_0 x}{C^2 u}\right) + \sqrt{\frac{8H_0 r x}{C^3 u}}. \end{aligned} \tag{5}$$

$\mathfrak{R}_u(\mathcal{H}), \mathfrak{R}_m(\mathcal{H})$ are the two types of Transductive Rademacher Complexity of the function class $\mathcal{H}$ defined in (3) and (4).

3.2 The First Bound by Transductive Local Rademacher Complexity

Using Theorem 3.1 and the division and bound technique introduced in Section 1.1, we have the very basic bound for TLRC involving the fixed point of a sub-root function.

Theorem 3.2. Let $\mathcal{H}$ be a class of functions with ranges in $[0, H_0]$. Let ψ_u be a sub-root function and let r_u^* be the fixed point of ψ. Let ψ_u be another sub-root function and let r_m^* be the fixed point of ψ. Assume that for all $r \ge \max\{r_u^*, r_m^*\}$,

$$\psi_u(r) \ge \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{h\colon \mathcal{L}_n(h)\le r} R_{u,\mathbf{d}} h\right], \quad \psi_m(r) \ge \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{h\colon \mathcal{L}_n(h)\le r} R_{m,\mathbf{d}} h\right]. \tag{6}$$

Then for every $x > 0$, with probability at least $1 - \exp(-x)$,

$$\mathcal{U}_h(\mathbf{Z}_\mathbf{d}) \le \left(1 + \frac{1}{C}\right)\mathcal{L}_h^{(m)}(\overline{\mathbf{Z}_\mathbf{d}}) + 6400\,(r_u^* + r_m^*) + \frac{128 H_0 x}{C^3 u} + \frac{12 H_0 x}{C^2 u}, \quad \forall h \in \mathcal{H}. \tag{7}$$

3.3 TLRC Bound for Generic Transductive Learning

We apply Theorem 3.2 to the transductive learning task introduced in Section 2. We consider the function class $\mathcal{H} = \ell \circ \mathcal{F} := \{\ell \circ f \colon f \in \mathcal{F}\}$ in Theorem 3.2, and any $h \in \mathcal{H}$ can be written as $h = \ell \circ f$, which is the loss function expressed by $h(\mathbf{x}, y) = \ell(f(\mathbf{x}), y)$.

Theorem 3.3. Let $\mathcal{F}$ be a class of functions and for any $f \in \mathcal{F}$, $0 \le \ell_f(i) \le H_0$ for all $i \in [n]$. Let ψ_u, ψ_m be a sub-root functions and let r_u^* be the fixed point of ψ_u and r_m^* be the fixed point of ψ_m.

Assume that for all $r \geq r^* := r_u^* + r_m^*$,

$$\psi_u(r) \geq \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{f\colon f\in\mathcal{F},\mathcal{L}_n(\ell_f)\leq r} R_{u,\mathbf{d}}\ell_f\right], \quad \psi_m(r) \geq \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{f\colon f\in\mathcal{F},\mathcal{L}_n(\ell_f)\leq r} R_{m,\mathbf{d}}\ell_f\right]. \tag{8}$$

Then for every $x > 0$, with probability at least $1 - \exp(-x)$,

$$\mathcal{U}_{\ell_f}(\mathbf{Z_d}) \leq \left(1 + \frac{1}{C}\right)\mathcal{L}_{\ell_f}^{(m)}(\overline{\mathbf{Z_d}}) + c_1 r^* + \frac{c_2 x}{u}, \quad \forall f \in \mathcal{F}, \tag{9}$$

where $c_1 = 6400$, $c_2 = (128H_0 + 12H_0C)/C^3$.

Theorem 3.4. Under the conditions of Theorem 3.3, let $\widehat{f} := \arg\min_{f\in\mathcal{F}} \mathcal{L}_{\ell_f}^{(m)}(\overline{\mathbf{Z_d}})$ be the empirical minizer on the test data, and $f_u^* := \arg\min_{f\in\mathcal{F}} \mathcal{U}_{\ell_f}(\mathbf{Z_d})$ be the oracle minimizer on the test data. Assume there exists $f_n^* \in \mathcal{F}$ such that $\mathcal{L}_n(\ell_{f_n^*}) = 0$, that is, the transductive learning is realizable. Then for every $x > 0$, with probability at least $1 - 2\exp(-x)$, the excess risk $\mathcal{U}_{\ell_{\widehat{f}}}(\mathbf{Z_d}) - \mathcal{U}_{\ell_{f_u^*}}(\mathbf{Z_d})$ satisfies

$$\mathcal{U}_{\ell_{\widehat{f}}}(\mathbf{Z_d}) - \mathcal{U}_{\ell_{f_u^*}}(\mathbf{Z_d}) \leq \mathcal{O}\left(r^* + \frac{1}{u} + \frac{1}{m}\right). \tag{10}$$

Proof. Under the realizable transductive learning assumption, we have $\mathcal{U}_{\ell_{f_u^*}}(\mathbf{Z_d}) = 0$. Moreover, by Lemma B.9 we have

$$\mathcal{L}_{\ell_{\widehat{f}}}^{(m)}(\overline{\mathbf{Z_d}}) \leq \mathcal{L}_{f_n^*}^{(m)}(\overline{\mathbf{Z_d}}) \leq 2\mathcal{L}_n(\ell_{f_n^*}) + \frac{6H_0 x}{m} \tag{11}$$

with probability at least $1 - \exp(-x)$. It then follows by (9) in Theorem 3.3, (11), and $\mathcal{L}_n(\ell_{f_n^*}) = 0$ that (10) holds. □

3.4 TLRC Bound for Transductive Kernel Learning

3.4.1 Background in RKHS and Kernel Learning

Let $\mathcal{H}_K$ be the Reproducing Kernel Hilbert Space (RKHS) associated with K, where $K\colon \mathcal{X}\times\mathcal{X} \to \mathbb{R}$ is a positive definite kernel defined on the compact set $\mathcal{X}\times\mathcal{X}$. Let $\mathcal{H}_{\mathbf{X}_n} := \overline{\left\{\sum_{i=1}^n K(\cdot, \overrightarrow{\mathbf{x}}_i)\alpha_i \,\middle|\, \{\alpha_i\}_{i=1}^n \subseteq \mathbb{R}\right\}}$ be the usual RKHS spanned by $\left\{K(\cdot, \overrightarrow{\mathbf{x}}_i)\right\}_{i=1}^n$ on the full sample $\mathbf{X}_n = \left\{\overrightarrow{\mathbf{x}}_i\right\}_{i=1}^n$. Let the gram matrix of K over the full sample be $\mathbf{K} \in \mathbb{R}^{n\times n}, \mathbf{K}_{ij} = K(\overrightarrow{\mathbf{x}}_i, \overrightarrow{\mathbf{x}}_j)$ for $i, j \in [n]$, and $\mathbf{K}_n := \frac{1}{n}\mathbf{K}$. Throughout this paper, we assume that K is strictly positive definite, so that $\mathbf{K}$ is always positive definite with fixed $\mathbf{X}_n$. When $\mathbf{X}_n$ are sampled at random, we assume $\mathbf{K}$ is positive definite with probability 1. Such strictly positive kernel widely exists in machine learning, such as the Neural Tangent Kernel (NTK) [10,11].

Let $\widehat{\lambda}_1 \geq \widehat{\lambda}_2 \ldots \geq \widehat{\lambda}_n > 0$ be the eigenvalues of $\mathbf{K}_n$, and $\max_{\mathbf{x}\in\mathcal{X}} K(\mathbf{x},\mathbf{x}) = \tau_0^2 < \infty$. We then have $\widehat{\lambda}_1 \leq \operatorname{tr}(\mathbf{K}_n) \leq \tau_0^2$. For the task of transductive nonparametric kernel regression to be introduced in Section 3.7, the full sample $\mathbf{X}_n = \left\{\overrightarrow{\mathbf{x}}_i\right\}_{i=1}^n$ are drawn i.i.d. according to an underlying data distribution P, and P is the distribution of $\overrightarrow{\mathbf{x}}_i$ with probability measure $\mu^{(P)}$. The operator $T_n\colon \mathcal{H}_K \to \mathcal{H}_K$ is important for our analysis which is defined by $T_n g := \frac{1}{n}\sum_{i=1}^n K(\cdot, \overrightarrow{\mathbf{x}}_i) g(\overrightarrow{\mathbf{x}}_i)$ for all $g \in \mathcal{H}_K$. The first n eigenvalues of T_n are $\left\{\widehat{\lambda}_i\right\}_{i=1}^n$, and all the other eigenvalues are

0. By spectral theorem, all the normalized eigenfunctions, denoted by $\left\{\Phi^{(k)}\right\}_{k=1}^{n}$ with $\Phi^{(k)} = 1/\sqrt{n\widehat{\lambda}_k} \cdot \sum_{j=1}^{n} K(\cdot, \overrightarrow{\mathbf{x}}_j) \left[\mathbf{U}_k\right]_j$, is an orthonormal basis of $\mathcal{H}_{\mathbf{X}_n}$. Since $\mathcal{H}_{\mathbf{X}_n} \subseteq \mathcal{H}_K$, we can complete $\left\{\Phi^{(k)}\right\}_{k=1}^{n}$ so that $\left\{\Phi^{(k)}\right\}_{k\geq 1}$ is an orthonormal basis of the RKHS $\mathcal{H}_K$.

When K is also continuous on the compact set $\mathcal{X} \times \mathcal{X}$, the integral operator $T_K \colon L^2(\mathcal{X}, \mu) \to L^2(\mathcal{X}, \mu^{(P)}), (T_K f)(\mathbf{x}) := \int_{\mathcal{X}} K(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') \mathrm{d}\mu^{(P)}(\mathbf{x}')$ is a positive, self-adjoint, and compact operator on $\mathcal{X}$. By the spectral theorem, there is a countable orthonormal basis $\{e_j\}_{j\geq 1} \subseteq L^2(\mathcal{X}, \mu)$ and $\{\lambda_j\}_{j\geq 1}$ with $\lambda_1 \geq \lambda_2 \geq \ldots > 0$ such that λ_j is the eigenvalue with e_j being the corresponding eigenfunction. That is, $Te_j = \lambda_j e_j, j \geq 1$. It is well known that $\left\{v_j = \sqrt{\lambda_j} e_j\right\}_{j\ \geq 1}$ is an orthonormal basis of $\mathcal{H}_K$. Let $\left\{\mu^{(\ell)}\right\}_{\ell \geq 1}$ be the distinct eigenvalues of the integral operator L_K associated with T_K, and let m_ℓ be the be the sum of multiplicity of the eigenvalue $\left\{\mu^{(\ell')}\right\}_{\ell'=1}^{\ell}$. That is, $m_{\ell'} - m_{\ell'-1}$ is the multiplicity of $\mu^{(\ell')}$, and $\lambda_j = \mu^{(\ell)}$ for $j \in (m_{\ell-1}, m_\ell]$. For a positive number μ, define $\mathcal{H}_K(\mu) := \{f \in \mathcal{H}_K \mid \|f\|_{\mathcal{H}} \leq \mu\}$ be the closed ball in $\mathcal{H}_K$ centered at 0 with radius μ. For some positive constant μ, the ball in $\mathcal{H}_K$ centered at 0 with radius μ is defined by $\mathcal{H}_K(\mu) := \left\{f \in \mathcal{H}_K \colon \|f\|_{\mathcal{H}_K} \leq \mu\right\}$.

3.5 The Task of Transductive Kernel Learning

We consider the problem of learning the unknown target function $f^* \in \mathcal{H}_K(\mu)$. We let $y_i = f^*(\overrightarrow{\mathbf{x}}_i)$ where the target function $f^* \in \mathcal{H}_K(\mu)$ and f^* satisfies Assumption 2.

It is noted that [7] considers the function class where the output of any function in that class on the full sample $\mathbf{X}_n$ can be expressed by $\mathbf{K}\boldsymbol{\alpha}$ for some vector $\boldsymbol{\alpha} \in \mathbb{R}^n$. Formally, [7] considers the function class $\mathcal{H}_{\mathbf{X}_n}(v)$ for kernel transductive learning, where $\mathcal{H}_{\mathbf{X}_n}(\mu) := \left\{f \in \mathcal{H}_{\mathbf{X}_n} \colon \|f\|_{\mathcal{H}_K} \leq \mu\right\}$ is the ball in $\mathcal{H}_{\mathbf{X}_n}$ centered at 0 with radius μ. Let $\mathcal{H}_{\mathbf{X}_n, r_0}$ for $r_0 \in [n]$ be a linear subspace of $\mathcal{H}_{\mathbf{X}_n}$ spanned by $\left\{\Phi^{(k)}\right\}_{k=1}^{r_0}$, that is, $\mathcal{H}_{\mathbf{X}_n, r_0} := \mathrm{Span}\left(\left\{\Phi^{(k)}\right\}_{k=1}^{r_0}\right)$. We let $\mathcal{H}_{\mathbf{X}_n, r_0}(\mu) := \left\{f \in \mathcal{H}_{\mathbf{X}_n, r_0} \colon \|f\|_{\mathcal{H}_K} \leq \mu\right\}$. It can be verified that $\mathcal{H}_{\mathbf{X}_n, r_0}(\mu)$ is convex and symmetric. The convex and symmtric set is deferred to Definition B.1.

Assumption 2 (Assumption about the Target Function f^*)**.** We introduce the following assumptions with $r_0 \in [n]$. For any $\delta \in (0, 1)$, with probability $1 - \delta$ over the full sample $\mathbf{X}_n$, the following inequality holds:

$$\sum_{q=r_0+1}^{n} \left\langle f^*, \Phi^{(q)} \right\rangle_{\mathcal{H}_K}^2 \leq \zeta_{n,\delta}, \tag{12}$$

where $\zeta_{n,\delta} \geq 0$, and the LHS is 0 with $r_0 = n$.

We define

$$\mathcal{H}_{\mathbf{X}_n, r_0, \delta}(\mu) := \left\{ f \in \mathcal{H}_{\mathbf{X}_n}(\mu) \colon \Pr\left[\sum_{q=r_0+1}^{n} \left\langle f, \Phi^{(q)} \right\rangle_{\mathcal{H}_K}^2 \leq \zeta_{n,\delta}\right] \geq 1 - \delta \right\} \tag{13}$$

as the class of all the target functions $f^* \in \mathcal{H}_{\mathbf{X}_n}(v)$ which satisfies (12).

3.5.1 Results

We first demonstrate that a low-dimensional target function in $\mathcal{H}_K$ satisfies Assumption 2 by the following theorem, then introduce generalization bounds for TKL by TLRC.

Theorem 3.5. Suppose K is a continuous and positive definite kernel on $\mathcal{X} \times \mathcal{X}$, and the target function $f^* \in \mathcal{H}_K(\mu)$ is spanned by eigenfunctions $\{v_j\}_{j=1}^{m_{k_0}}$ in the first k_0 eigenspaces of T_k with $k_0 \geq 1$. That is,

$$f^* = \sum_{j=1}^{m_{k_0}} \beta_j v_j, \quad \sum_{j=1}^{m_{k_0}} \beta_j^2 \leq \mu^2. \tag{14}$$

Then with probability at least $1-\delta$ over the full sample $\mathbf{X}_n$, $\zeta_{n,\delta}$ can be chosen as

$$\zeta_{n,\delta} = \frac{8\mu^2 \tau_0^4 \log \frac{2}{\delta}}{\left(\lambda_{m_{k_0}} - \lambda_{m_{k_0}+1}\right)^2 n}. \tag{15}$$

In other words, $f^* \in \mathcal{H}_{\mathbf{X}_n, r_0, \delta}(\mu)$ with $\zeta_{n,\delta}$ set by (15) and $r_0 = m_{k_0}$.

Theorem 3.6. Suppose K is a positive definite kernel on $\mathcal{X} \times \mathcal{X}$ which may not be continuous. Let $\ell_f = (f - f^*)^2$, $f^* \in \mathcal{H}_{\mathbf{X}_n, r_0, \delta}(\mu)$ with $r_0 \in [n]$. Then for every $x > 0$, $\delta \in (0, 1/2)$, and any $K_0 > 1$, with probability at least $1 - \delta - \exp(-x)$,

$$\mathcal{U}_{\ell_f}(\mathbf{Z_d}) \leq \left(1 + \frac{1}{C}\right) \mathcal{L}_{\ell_f}^{(m)}(\overline{\mathbf{Z_d}}) + \frac{c_2 x}{u} + c_1 \min_{0 \leq Q \leq r_0} r(u, m, Q, r_0, \delta), \quad \forall f \in \mathcal{H}_{\mathbf{X}_n, r_0}(\mu). \tag{16}$$

Here

$$\begin{aligned} r(u, m, Q, r_0, \delta) &\coloneqq c_3 Q \left(\frac{1}{u} + \frac{1}{m}\right) \\ &+ c_4 \left(\sqrt{\frac{\zeta_{n, r_0, \delta} Q}{2u}} + \mu \sqrt{\frac{\sum_{q=Q+1}^{r_0} \widehat{\lambda}_q}{u}} + \sqrt{\frac{\zeta_{n, r_0, \delta} Q}{2m}} + \mu \sqrt{\frac{\sum_{q=Q+1}^{r_0} \widehat{\lambda}_q}{m}} \right), \end{aligned}$$

$c_1 = 3200$, $c_2 = (128 H_0 + 12 H_0 C)/C^3$, $c_3 = 128 \tau_0^2 \mu^2$, $c_4 = 16 \tau_0 \mu$, and $\zeta_{n, r_0, \delta} \coloneqq \widehat{\lambda}_{r_0+1} \zeta_{n,\delta}$.

An immediate application of Theorem 3.6 with $r_0 = n$ leads to the following corollary, which shows the bound for a target function which may not satisfy Assumption 2.

Corollary 3.7. Suppose K is a positive definite kernel on $\mathcal{X} \times \mathcal{X}$ which may not be continuous. Let $\ell_f = (f - f^*)^2$ with $f^* \in \mathcal{H}_{\mathbf{X}_n}(\mu)$. Then for every $x > 0$ and any $K_0 > 1$, with probability at least $1 - \exp(-x)$,

$$\begin{aligned} \mathcal{U}_{\ell_f}(\mathbf{Z_d}) &\leq \left(1 + \frac{1}{C}\right) \mathcal{L}_{\ell_f}^{(m)}(\overline{\mathbf{Z_d}}) + \frac{c_2 x}{u} \\ &+ c_1 \min_{0 \leq Q \leq n} \left(c_3 Q \left(\frac{1}{u} + \frac{1}{m}\right) + c_4 \mu \sqrt{\frac{\sum_{q=Q+1}^{n} \widehat{\lambda}_q}{u}} + c_4 \mu \sqrt{\frac{\sum_{q=Q+1}^{n} \widehat{\lambda}_q}{m}} \right) \end{aligned} \tag{17}$$

holds for all $f \in \mathcal{H}_{\mathbf{X}_n}(\mu)$, where c_1, c_2, c_3, c_4 are positive constants in Theorem 3.6.

3.6 Application to Graph Transductive Learning

Let $\mathbf{L} \in \mathbb{R}^{n \times n}$ be a positive definite matrix which encodes the graph information over the full sample, for example, $\mathbf{L}$ can be a graph laplaican or its normalized variants. Let the eigendecomposition of $\mathbf{L}_n = \frac{1}{n}\mathbf{L}$ be $\mathbf{L}_n = \mathbf{U}^{(\mathbf{L})}\mathbf{\Sigma}^{(\mathbf{L})}\mathbf{U}^{(\mathbf{L})^\top}$ where $\mathbf{U}^{(\mathbf{L})}$ is a $n \times n$ orthogonal matrix, and $\mathbf{\Sigma}^{(\mathbf{L})}$ is a diagonal matrix with its diagonal elements $\left\{\widehat{\lambda}_i^{(\mathbf{L})}\right\}_{i=1}^n$ being eigenvalues of $\mathbf{L}_n$ and sorted in a non-increasing order. The following convex optimization problem is solved for Graph Transductive Learning with $\mathbf{L}$:

$$\mathbf{v}^* = \underset{\mathbf{v} \in \mathbb{R}^n \colon \mathbf{v}^\top \mathbf{L} \mathbf{v} \le \mu^2}{\arg\min} \mathcal{L}^{(m)}(\mathbf{v}), \quad \mathcal{L}^{(m)}(\mathbf{v}) := \frac{1}{2m} \left\| [\mathbf{L}\mathbf{v} - \mathbf{y}]_{\overline{\mathbf{Z_d}}} \right\|_2^2, \tag{18}$$

where μ is a positive constant number. $[\mathbf{t}]_{\overline{\mathbf{Z_d}}} \in \mathbb{R}^m$ for a vector $\mathbf{t} \in \mathbb{R}^n$ denotes a subvector of $\mathbf{t}$ formed by rows of $\mathbf{t}$ indexed by $\overline{\mathbf{Z_d}}(1), \ldots, \overline{\mathbf{Z_d}}(m)$. That is, the i-th row of $[\mathbf{t}]_{\overline{\mathbf{Z_d}}}$ is the $\mathbf{t}_{\overline{\mathbf{Z_d}}(i)}$. We are interested in the test loss $\mathcal{U}(\ell_{f_{\mathbf{v}^*}})$ of the prediction function $f_{\mathbf{v}^*}$ with $f_{\mathbf{v}^*}(\overset{\rightharpoonup}{\mathbf{x}}_i) = [\mathbf{L}\mathbf{v}^*]_i$ and $\ell_{f_{\mathbf{v}^*}}(i) = \left(f_{\mathbf{v}^*}(\overset{\rightharpoonup}{\mathbf{x}}_i) - y_i\right)^2$ for $i \in [n]$. We note that problem (18) is very similar to the optimization problem of transductive learning by multi-layer linear Graph Neural Network (GNN), such as Simple Graph Convolution (SGC) [3], where the following problem is solved: $\min_{\Theta \in \mathbb{R}^d} \frac{1}{2m} \left\| \left[\tilde{\mathbf{S}}^k \mathbf{X} \Theta - \mathbf{y}\right]_{\overline{\mathbf{Z_d}}} \right\|_2^2$. Here $\tilde{\mathbf{S}} \in \mathbb{R}^{n \times n}$ is positive definite, and $\mathbf{X} \in \mathbb{R}^{n \times d}$ denotes the node features, k is the number of layers. If $d \ge n$ with $\mathrm{rank}(\mathbf{X}) = d$, then the above problem is equivalent to (18) with $\mathbf{L} = \tilde{\mathbf{S}}^k$.

The following theorem offers the upper bound for $\mathcal{U}(\ell_{f_{\mathbf{v}^*}})$ by applying Corollary 3.7.

Theorem 3.8. Suppose $\mathbf{L}$ is positive definite, $\mathbf{v}^*$ is an optimal solution to (18), and a positive number μ satisfies

$$\sum_{i=1}^n \frac{\left[{\mathbf{U}^{(\mathbf{L})}}^\top \mathbf{y}\right]_i^2}{n \widehat{\lambda}_i^{(\mathbf{L})}} \le \mu^2. \tag{19}$$

Then for every $x > 0$, with probability at least $1 - 2\exp(-x)$,

$$\begin{aligned}\mathcal{U}_{\ell_{f_{\mathbf{v}^*}}}(\mathbf{Z_d}) \le{}& \frac{6\left(1 + \frac{1}{C}\right) H_0 x}{m} + \frac{c_2 x}{u} \\ &+ c_1 \min_{0 \le Q \le n} \left(c_3 Q \left(\frac{1}{u} + \frac{1}{m}\right) + c_4 \mu \sqrt{\frac{\sum\limits_{q=Q+1}^{r_0} \widehat{\lambda}_q}{u}} + c_4 \mu \sqrt{\frac{\sum\limits_{q=Q+1}^{r_0} \widehat{\lambda}_q}{m}} \right),\end{aligned} \tag{20}$$

where c_1, c_2, c_3, c_4 are the same as those in Theorem 3.6, $H_0 = 4\mu^2\tau_0^2$, and $\tau_0^2 = \max_{i \in [n]} \mathbf{L}_{ii}$.

We further consider the case that the target labels $\mathbf{y}$ lies on a low dimensional subspace, that is, $\mathbf{y}$ lies on the subspace spanned to the top r_0 eigenvectors of $\mathbf{L}$. In this case, the Low-Rank Graph

Transductive Learning (LR-GTL) problem below is solved:

$$\mathbf{v}^{*(r_0)} = \underset{\mathbf{v}\in\mathbb{R}^n:\, \mathbf{v}^\top \mathbf{L}^k \mathbf{v} \le \mu^2}{\arg\min} \frac{1}{2m} \left\| \left[\mathbf{L}^{(r_0)} \mathbf{v} - \mathbf{y} \right]_{\overline{\mathbf{Z_d}}} \right\|_2^2, \tag{21}$$

where $\mathbf{L}^{(r_0)}$ is the rank-r_0 approximation to $\mathbf{K}$. That is, $\mathbf{L}^{(r_0)} = \mathbf{U}^{(\mathbf{L})} \mathbf{\Sigma}^{(\mathbf{L},r_0)} \mathbf{U}^\top$, $\mathbf{\Sigma}_{ii}^{(\mathbf{L},r_0)} = n\widehat{\lambda}_i^{(\mathbf{L})}$ for $i \in [r_0]$, and $\mathbf{\Sigma}_{ii}^{(\mathbf{L},r_0)} = 0$ otherwise. We take $\mathbf{v}^{*(r_0)}$ as the optimal solution to (21) with the minimum ℓ^2-norm, so that $\mathbf{v}^{*(r_0)} \in \operatorname{Span}\left(\mathbf{U}^{(\mathbf{L},r_0)}\right)$. The following theorem, which can be proved by applying Theorem 3.6, shows a sharper bound for the test loss than (20) in Theorem 3.8, when r_0 is small.

Theorem 3.9. Suppose $\mathbf{L}$ is positive definite, $\mathbf{y} \in \operatorname{Span}\left(\mathbf{U}^{(\mathbf{L},r_0)}\right)$ for some $r_0 \in [n]$, and a positive number μ satisfies

$$\sum_{i=1}^{r_0} \frac{\left[{\mathbf{U}^{(\mathbf{L},r_0)}}^\top \mathbf{y} \right]_i^2}{n\widehat{\lambda}_i^{(\mathbf{L})}} \le \mu^2. \tag{22}$$

Then for every $x > 0$, with probability at least $1 - 2\exp(-x)$,

$$\mathcal{U}_{\ell_{f_{\mathbf{v}^{*(r_0)}}}}(\mathbf{Z_d}) \le \frac{6\left(1 + \frac{1}{C}\right) H_0 x + c_1 c_3 r_0}{m} + \frac{c_2 x + c_1 c_3 r_0}{u}, \tag{23}$$

where $c_2 = \left(128 H_0 + 12 H_0 C\right)/C^3$, $c_3 = 128\tau_0^2\mu^2$, $H_0 = 4\mu^2\tau_0^2$ and $\tau_0^2 = \max_{i\in[n]} \mathbf{L}_{ii}$.

It can be observed from (23) that a particularly sharp bound is achieved by LR-GTL, that is, $\mathcal{U}(\ell_{f_{\mathbf{v}^{*(r_0)}}}) \le \mathcal{O}(\frac{1}{m})$, if r_0 is bounded by a constant.

3.7 Application to Transductive Nonparametric Kernel Regression

The setting of the task of Transductive Nonparametric Kernel Regression (TNKR) is described first. In TNKR, the full sample $\mathbf{X}_n = \left\{ \overrightarrow{\mathbf{x}}_i \right\}_{i=1}^n$ are drawn i.i.d. according to an underlying data distribution P. The label y_i is given by $y_i = f^*(\overrightarrow{\mathbf{x}}_i) + \varepsilon_i$, where $f^* \in \mathcal{H}_{\mathbf{X}_n, r_0, \delta}(\mu_0)$ with $r_0 \in [n]$ and μ_0 is a positive constant. $\{\varepsilon_i\}_{i=1}^n$ are i.i.d. Gaussian random noise with mean 0 and finite variance σ^2, that is, $\varepsilon_i \sim \mathcal{N}(0,\sigma^2)$. We define $\mathbf{y} := [y_1, \ldots, y_n]$, $\boldsymbol{\varepsilon} := [\varepsilon_1, \ldots, \varepsilon_n]^\top$, and use $f^*(\mathbf{X}_n) := \left[f^*(\overrightarrow{\mathbf{x}}_1), \ldots, f^*(\overrightarrow{\mathbf{x}}_n) \right]^\top$ to denote the unknown clean target labels. Let the eigendecomposition of $\mathbf{K}_n$ be $\mathbf{K}_n = \mathbf{U}\mathbf{\Sigma}\mathbf{U}^\top$ where $\mathbf{U} \in \mathbb{R}^{n\times n}$ is an orthogonal matrix, and $\mathbf{\Sigma}$ is a diagonal matrix with its diagonal elements $\left\{ \widehat{\lambda}_i \right\}_{i=1}^n$ being eigenvalues of $\mathbf{K}_n$ and sorted in a non-increasing order. Let $\mathbf{U}^{(r_0)} \in \mathbb{R}^{n\times r_0}$ be the submatrix of $\mathbf{U}$ formed by the first r_0 columns of $\mathbf{U}$, so $\mathbf{U}^{(r_0)}$ contains the top r_0 eigenvectors of $\mathbf{K}$. We define $\boldsymbol{\varepsilon}^{(r_0)} := \mathbf{U}^{(r_0)} {\mathbf{U}^{(r_0)}}^\top \boldsymbol{\varepsilon}$.

We design the Low-Rank TNKR (LR-TNKR) algorithm as follows. Let $\bar{\mu} := \max\{\sqrt{2\mu_0^2 + \mu_1}, \mu_0\}$ where μ_1 is a positive constant. The following convex optimization problem is solved for TNKR:

$$\widehat{\mathbf{u}} = \underset{\mathbf{u}\in\mathbb{R}^n:\, \mathbf{u}^\top \mathbf{K} \mathbf{u} \le \bar{\mu}^2}{\arg\min} \frac{1}{2m} \left\| \left[\mathbf{K}^{(r_0)} \mathbf{u} - \mathbf{y} \right]_{\overline{\mathbf{Z_d}}} \right\|_2^2, \tag{24}$$

where $\mathbf{K}^{(r_0)}$ is the rank-r_0 approximation to $\mathbf{K}$, that is, $\mathbf{K}^{(r_0)} = \mathbf{U}\mathbf{\Sigma}^{(r_0)}\mathbf{U}^\top$ with $\mathbf{\Sigma}_{ii}^{(r_0)} = n\widehat{\lambda}_i$ for $i \in [r_0]$, and $\mathbf{\Sigma}_{ii}^{(r_0)} = 0$ otherwise. We take $\widehat{\mathbf{u}}$ as the solution to (24) with the minimum ℓ^2-norm, so that $\widehat{\mathbf{u}} \in \mathrm{Span}\left(\mathbf{U}^{(r_0)}\right)$. $\mathbf{K}^{(r_0)}\widehat{\mathbf{u}}$ is used to predict the labels of the test set, and the performance guarantee of the LR-TNKR algorithm is presented below.

Theorem 3.10. Suppose the target function is $f^* = \sum\limits_{j=1}^{m_{k_0}} \beta_j v_j$ with $\sum_{j=1}^{m_{k_0}} \beta_j^2 \le \mu_0^2$ for some constant integer $k_0 \ge 1$. Suppose K is a continuous and positive definite kernel on $\mathcal{X} \times \mathcal{X}$, and suppose $n \ge \max\left\{\frac{4r_0(\sigma+1)^2}{\mu_1 \lambda_{r_0}}, \frac{32\tau_0^4 \log\frac{2}{\delta}}{\lambda_{r_0}^2}\right\}$ for a positive constant μ_1 and $\delta \in (0, \frac{1}{4})$. Let $\ell_f = (f - f^*)^2$. Then for every $x > 0$, $\delta \in (0, \frac{1}{4})$, with probability at least $1 - 2\delta - 2\exp\left(\frac{-m_{k_0}}{2\sigma^2}\right) - 2\exp(-x)$,

$$\mathcal{U}(\ell_{f_{\widehat{\mathbf{u}}}}) \le \left(1 + \frac{1}{C}\right)\left(2 + \frac{6x}{C}\right)\left(2\zeta_{n,m_{k_0},\delta} + \frac{2m_{k_0}(\sigma+1)^2}{n}\right) + \frac{c_2 x}{u} + c_1 c_3 m_{k_0}\left(\frac{1}{u} + \frac{1}{m}\right) + c_1 c_4 \sqrt{\zeta_{n,m_{k_0},\delta} m_{k_0}}\left(\frac{1}{\sqrt{2u}} + \frac{1}{\sqrt{2m}}\right), \tag{25}$$

where $c_1 = 3200$, $c_2 = (128H_0 + 12H_0C)/C^3$, $c_3 = 128\tau_0^2\bar{\mu}^2$, $c_4 = 16\tau_0\bar{\mu}$, $H_0 = 4\bar{\mu}^2\tau_0^2$, and $\bar{\mu} = \max\left\{\sqrt{2\mu_0^2 + \mu_1}, \mu_0\right\}$ with μ_1 being a positive constant.

We remark that (25) is the among the first to offer a sharp bound for transductive learning in the kernel regression setting, which connects the generalization performance to the spectrum of the kernel and dimension of the target function. To see an immediate application, consider the case that K is a dot-product kernel [12, 13] such that $K(\mathbf{x}, \mathbf{x}')$ is a function of $\langle \mathbf{x}, \mathbf{x}' \rangle$, $\mathcal{X} = \mathbb{S}^{d-1}$ which is the unit sphere in $\mathbb{R}^d$, and $\mu^{(P)}$ is the spherical uniform measure on $\mathbb{S}^{d-1}$. Let $k_0 = 1$, then $m_{k_0} = d$, $f^* \in \mathcal{H}_{\mathbf{X}_n, m_1, \delta}$ which is the class of all the linear functions on the unit sphere, and $\zeta_{n,d,\delta} \in \mathcal{O}(1/n)$. It can be verified by (25) that the test loss satisfies $\mathcal{U}(\ell_{f_{\widehat{\mathbf{u}}}}) \le \mathcal{O}(\sqrt{d/(nu)} + \frac{d}{u} + \frac{d}{m})$ with high probability (we let $d \to \infty, d < \min\{u, m\}$ as $u, m \to \infty$).

We present the basic mathematical results required in our proofs in Section A, then present proofs in Section B.

A Mathematical Tools

We introduce the basic concentration inequality which we used to develop Let $X_1, X_2, \ldots, X_n$ are independent random variables taking values in a measurable space $\mathcal{X}$, and let X_1^n denote the vector of these n random variables. Let $f \colon \mathcal{X}^n \to \mathbb{R}$ be some measurable function. We are concerned with concentration of the random variable $Z = f(X_1, X_2, \ldots, X_n)$. Let $X_1', X_2', \ldots, X_n'$ denote independent copies of $X_1, X_2, \ldots, X_n$, and we write

$$Z^{(i)} = f(X_1, \ldots, X_{i-1}, X_i', X_{i+1}, \ldots, X_n).$$

Theorem A.1. ([14, Theorem 5]) Assume that there exist constants $a \geq 0$ and $b > 0$ such that

$$V_+ \coloneqq \mathbb{E}\left[\sum_{i=1}^{n} \left(Z - Z^{(i)}\right)^2 \mathbb{I}_{\left\{Z > Z^{(i)}\right\}} \mid X_1^n\right] \leq aZ + b.$$

Then, for all $t > 0$,

$$\Pr\left[Z > \mathbb{E}\left[Z\right] + t\right] \leq \exp\left(\frac{-t^2}{4a\mathbb{E}\left[Z\right] + 4b + 2at}\right) \tag{26}$$

Remark A.2. While $a > 0$ in the original Theorem 5 of [14], one can use the same proof of this theorem to show that (26) holds for $a = 0$ with $b > 0$.

B Proofs

B.1 The First Bound Local by Transductive Rademacher Complexity

For all $h \in \mathcal{H}$, we define

$$E(h, \mathbf{d}, \mathbf{d}^{(i)}) \coloneqq g(\mathbf{Z}_{\mathbf{d}}) - g(\mathbf{Z}_{\mathbf{d}^{(i)}})$$

as the change of the training loss if one element of $\mathbf{d}$ is changed. Then we have the following lemma showing the change of the training loss in this case.

Lemma B.1. There are four cases for the value of $E(h, \mathbf{d}, \mathbf{d}^{(i)})$ for $i \in [m]$.

Case 1: $E(h, \mathbf{d}, \mathbf{d}^{(i)}) = \left(\frac{1}{u} + \frac{1}{m}\right)\left(h(\mathbf{Z}_{\mathbf{d}}(i)) - h(\mathbf{Z}_{\mathbf{d}^{(i)}}(q(i)))\right)$,
if $d_i \neq d_i'$, $i \in [u-1], q(i) \leq u, p(i) > u$,

Case 2: $E(h, \mathbf{d}, \mathbf{d}^{(i)}) = \left(\frac{1}{u} + \frac{1}{m}\right)\left(h(\mathbf{Z}_{\mathbf{d}}(p(i))) - h(\mathbf{Z}_{\mathbf{d}^{(i)}}(i))\right)$,
if $d_i \neq d_i'$, $i \in [u-1], p(i) \leq u, q(i) > u$,

Case 3: $E(h, \mathbf{d}, \mathbf{d}^{(i)}) = \left(\frac{1}{u} + \frac{1}{m}\right)\left(h(\mathbf{Z}_{\mathbf{d}}(i)) - h(\mathbf{Z}_{\mathbf{d}^{(i)}}(i))\right)$,
if $d_i \neq d_i'$, $i \in [u], p(i) > u, q(i) > u$,

Case 4: $E(h, \mathbf{d}, \mathbf{d}^{(i)}) = 0$.

if $d_i = d'_i$ or $p(i), q(i) \le u$ for all $i \in [u]$.

Here

$$q(i) \coloneqq \min\left\{i' \in [i+1, u] \colon \mathbf{Z}_{\mathbf{d}^{(i)}}(i') = i\right\}, \tag{27}$$

$$p(i) \coloneqq \min\left\{i' \in [i+1, u] \colon \mathbf{Z}_{\mathbf{d}}(i') = i\right\}. \tag{28}$$

We use the convention that the min over a set returns $+\infty$ if the set is empty.

Proof. It can be checked by running Algorithm 1 that $\mathbf{Z}_{\mathbf{d}}$ and $\mathbf{Z}_{\mathbf{d}^{(i)}}$ can differ at most by one element. As a reminder, we let $\{\mathbf{Z}\}$ denote a set containing all the elements of a vector $\mathbf{Z}$ regardless of the orders of these elements in $\mathbf{Z}$.

If $\{\mathbf{Z}_{\mathbf{d}}\} = \{\mathbf{Z}_{\mathbf{d}^{(i)}}\}$, then Case 4 happens. This case can happen if $d'_i = d_i$, or $p(i), q(i) \le u$. When $p(i) \le u$, then $\mathbf{Z}_{\mathbf{d}^{(i)}}(p(i)) = \mathbf{Z}_{\mathbf{d}}(i)$. When $q(i) \le u$, then $\mathbf{Z}_{\mathbf{d}}(q(i)) = \mathbf{Z}_{\mathbf{d}^{(i)}}(i)$. As a result, when $p(i) \ne u+1$ and $q(i) \ne u+1$, for $\mathbf{Z}_{\mathbf{d}}$, the element $\mathbf{Z}_{\mathbf{d}^{(i)}}(i)$ would be picked up at a location $i' = q(i) \in (i, u]$. Similarly, for $\mathbf{Z}_{\mathbf{d}^{(i)}}$, the element $\mathbf{Z}_{\mathbf{d}}(i)$ would be picked up at a location $i' = p(i) \in (i, u]$.

Otherwise, when only one of $p(i)$ and $q(i)$ is not ∞, we have Case 2 and Case 1 respectively. If $d'_i \ne d_i$, and $\{\mathbf{Z}_{\mathbf{d}}\}$ $\{\mathbf{Z}_{\mathbf{d}^{(i)}}\}$ differs by only one element, then we must have Case 3. $\square$

Lemma B.2. Define $V_+ \coloneqq \mathbb{E}\left[\sum\limits_{i=1}^{u}\left(g(\mathbf{d}) - g(\mathbf{d}^{(i)})\right)^2 \mathbb{1}_{\left\{g(\mathbf{d}) > g(\mathbf{d}^{(i)})\right\}} \,\middle|\, \mathbf{d}\right]$, and let $\sup_{h \in \mathcal{H}} \mathcal{L}_n(h) \le r$, then

$$V_+ \le \frac{2H_0}{C^2 u} g(\mathbf{d}) + \frac{2H_0 r}{C^3 u}. \tag{29}$$

Proof. For a given $\mathbf{d}$, let the supremum in $g(\mathbf{d})$ is achieved by $h^* \in \mathcal{H}$, $g(\mathbf{d}) = \sup_{h \in \mathcal{H}}\left(\mathcal{U}_h(\mathbf{Z}_{\mathbf{d}}) - \mathcal{L}_n(h)\right) = \mathcal{U}_{h^*}(\mathbf{Z}_{\mathbf{d}}) - \mathcal{L}_{h^*}^{(m)}(\overline{\mathbf{Z}_{\mathbf{d}}})$. Note that if such superemum is not achievable, then there exists $h^* \in \mathcal{H}$ such that $g(\mathbf{d}) \le \mathcal{U}_{h^*}(\mathbf{Z}_{\mathbf{d}}) - \mathcal{L}_{h^*}^{(m)}(\overline{\mathbf{Z}_{\mathbf{d}}}) + \varepsilon$ for a infinitely small positive number ε, and we have the same results claimed in this lemma by letting $\varepsilon \to 0+$. Therefore, without loss of generality, we assume that the supremum is achievable.

We then

$$\begin{aligned}&\left(g(\mathbf{d}) - g(\mathbf{d}^{(i)})\right)\mathbb{1}_{\left\{g(\mathbf{d}) > g(\mathbf{d}^{(i)})\right\}} \\ &\qquad \le \left(\mathcal{U}_{h^*}(\mathbf{Z}_{\mathbf{d}}) - \mathcal{L}_{h^*}^{(m)}(\overline{\mathbf{Z}_{\mathbf{d}}}) + \mathcal{L}_{h^*}^{(m)}(\overline{\mathbf{Z}_{\mathbf{d}^{(i)}}}) - \mathcal{U}_{h^*}(\mathbf{Z}_{\mathbf{d}^{(i)}})\right)\mathbb{1}_{\left\{g(\mathbf{d}) > g(\mathbf{d}^{(i)})\right\}}.\end{aligned}$$

When $g(\mathbf{d}) > g(\mathbf{d}^{(i)})$, it follows by the above inequality that $\mathcal{U}_{h^*}(\mathbf{Z}_{\mathbf{d}}) - \mathcal{L}_{h^*}^{(m)}(\overline{\mathbf{Z}_{\mathbf{d}}}) + \mathcal{L}_{h^*}^{(m)}(\overline{\mathbf{Z}_{\mathbf{d}^{(i)}}}) - \mathcal{U}_{h^*}(\mathbf{Z}_{\mathbf{d}^{(i)}}) > 0$.

We consider the four cases in Lemma B.1. Define

$$\mathcal{A}_1 \coloneqq \left\{i \in [u] \colon E(h, \mathbf{d}, \mathbf{d}^{(i)}) \text{ satisfies Case 1 or Case 3 or Case 4}\right\}.$$

According to Lemma B.1, we have $\left(g(\mathbf{d}) - g(\mathbf{d}^{(i)})\right)\mathbb{1}_{\left\{g(\mathbf{d}) > g(\mathbf{d}^{(i)})\right\}} \le \frac{1}{m} h^*(\mathbf{Z}_{\mathbf{d}}(i))$ for all $i \in \mathcal{A}_1$. Also, $\left(g(\mathbf{d}) - g(\mathbf{d}^{(i)})\right)\mathbb{1}_{\left\{g(\mathbf{d}) > g(\mathbf{d}^{(i)})\right\}} \le \frac{1}{m} h^*(\mathbf{Z}_{\mathbf{d}}(p(i)))$ for all $i \in \overline{\mathcal{A}_1}$.

As a result,

$$
\begin{aligned}
&\sum_{i=1}^{u}\left(g(\mathbf{d})-g(\mathbf{d}^{(i)})\right)^2 \mathbb{1}_{\left\{g(\mathbf{d})>g(\mathbf{d}^{(i)})\right\}} \\
&= \sum_{i\in\mathcal{A}_1}\left(g(\mathbf{d})-g(\mathbf{d}^{(i)})\right)^2 \mathbb{1}_{\left\{g(\mathbf{d})>g(\mathbf{d}^{(i)})\right\}} + \sum_{i\in\overline{\mathcal{A}_1}}\left(g(\mathbf{d})-g(\mathbf{d}^{(i)})\right)^2 \mathbb{1}_{\left\{g(\mathbf{d})>g(\mathbf{d}^{(i)})\right\}} \\
&\le \left(\frac{1}{u}+\frac{1}{m}\right)^2 \sum_{i\in\mathcal{A}_1}(h^*(\mathbf{Z_d}(i)))^2 + \left(\frac{1}{u}+\frac{1}{m}\right)^2 \sum_{i\in\overline{\mathcal{A}_1}}(h^*(\mathbf{Z_d}(p(i))))^2 \\
&\overset{①}{\le} \left(\frac{1}{u}+\frac{1}{m}\right)^2 \sum_{i=1}^{u}(h^*(\mathbf{Z_d}(i)))^2 + \left(\frac{1}{u}+\frac{1}{m}\right)^2 \sum_{i=1}^{u}(h^*(\mathbf{Z_d}(i)))^2 \\
&\le 2H_0\left(\frac{1}{u}+\frac{1}{m}\right)^2 \sum_{i=1}^{u}h^*(\mathbf{Z_d}(i)) \\
&= 2H_0u\left(\frac{1}{u}+\frac{1}{m}\right)^2 \mathcal{U}_{h^*}(\mathbf{Z_d}) \\
&= 2H_0u\left(\frac{1}{u}+\frac{1}{m}\right)^2 \left(\mathcal{U}_{h^*}(\mathbf{Z_d})-\mathcal{L}_{h^*}^{(m)}(\overline{\mathbf{Z_d}})\right) + 2H_0u\left(\frac{1}{u}+\frac{1}{m}\right)^2 \mathcal{L}_{h^*}^{(m)}(\overline{\mathbf{Z_d}}) \\
&\le 2H_0u\left(\frac{1}{u}+\frac{1}{m}\right)^2 \left(\mathcal{U}_{h^*}(\mathbf{Z_d})-\mathcal{L}_{h^*}^{(m)}(\overline{\mathbf{Z_d}})\right) + u\left(\frac{1}{u}+\frac{1}{m}\right)^2\cdot\frac{2H_0n}{m}\mathcal{L}_n(h) \\
&\le \frac{2H_0}{C^2u}\left(\mathcal{U}_{h^*}(\mathbf{Z_d})-\mathcal{L}_{h^*}^{(m)}(\overline{\mathbf{Z_d}})\right) + \frac{2H_0}{C^3u}\mathcal{L}_n(h).
\end{aligned} \tag{30}
$$

Here ① follows from the property that all the elements in

$$\mathcal{P} \coloneqq \{p(i) \colon i\in[u-1], p(i)\le u\}$$

are distinct. To see this, suppose there are $i,j\in[u-1]$, $i\neq j$, such that $p(i)=p(j)$. According to the definition of p in (28), $\mathbf{Z_d}(p(i))=i=\mathbf{Z_d}(p(j))=j$. This conatriction shows that all the elements in $\mathcal{P}$ are distinct.

It follows by (30) that

$$
\begin{aligned}
V_+ \coloneqq \mathbb{E}_{\mathbf{d}'}&\left[\sum_{i=1}^{m}\left(g(\mathbf{d})-g(\mathbf{d}^{(i)})\right)^2 \mathbb{1}_{\left\{g(\mathbf{d})>g(\mathbf{d}^{(i)})\right\}}\,\middle|\,\mathbf{d}\right] \\
&\le \frac{2H_0}{C^2u}g(\mathbf{d}) + \frac{2H_0r}{C^3u},
\end{aligned}
$$

where the last inequality is due to the definition of $g(\mathbf{d})$ and $r\ge\sup_{h\in\mathcal{H}}\mathcal{L}_n(h)$.

□

Proof of Theorem 3.1 . We first estimate the upper bound for $\mathbb{E}_{\mathbf{d}}[g(\mathbf{d})]$. We have

$$
\begin{aligned}
\mathbb{E}_{\mathbf{d}}[g(\mathbf{d})] &= \mathbb{E}_{\mathbf{d}}\left[\sup_{h\in\mathcal{H}}\left(\mathcal{U}_h(\mathbf{Z_d})-\mathcal{L}_h^{(m)}(\overline{\mathbf{Z_d}})\right)\right] \\
&= \mathbb{E}_{\mathbf{d}}\left[\sup_{h\in\mathcal{H}}\left(\mathcal{U}_h(\mathbf{Z_d})-\mathcal{L}_n(h)+\mathcal{L}_n(h)-\mathcal{L}_h^{(m)}(\overline{\mathbf{Z_d}})\right)\right]
\end{aligned}
$$

$$\leq \underbrace{\mathbb{E}_{\mathbf{d}}\left[\sup_{h\in\mathcal{H}}\left(\mathcal{U}_h(\mathbf{Z}_{\mathbf{d}})-\mathcal{L}_n(h)\right)\right]}_{E_1}+\underbrace{\mathbb{E}_{\mathbf{d}}\left[\sup_{h\in\mathcal{H}}\left(\mathcal{L}_n(h)-\mathcal{L}_h^{(m)}(\overline{\mathbf{Z}_{\mathbf{d}}})\right)\right]}_{E_2}. \tag{31}$$

We now bound E_1. Let $\mathbf{d}'=[d_1',\ldots,d_m']$ be independent copies of $\mathbf{d}$, we then have

$$\begin{aligned}
E_1 &= \mathbb{E}_{\mathbf{d}}\left[\sup_{h\in\mathcal{H}}\left(\mathcal{U}_h(\mathbf{Z}_{\mathbf{d}})-\mathbb{E}_{\mathbf{d}'}\left[\mathcal{U}_h(\mathbf{Z}_{\mathbf{d}'})\right]\right)\right]\\
&\overset{①}{\leq} \mathbb{E}_{\mathbf{d}}\left[\mathbb{E}_{\mathbf{d}'}\left[\sup_{h\in\mathcal{H}}\left(\mathcal{U}_h(\mathbf{Z}_{\mathbf{d}})-\mathcal{U}_h(\mathbf{Z}_{\mathbf{d}'})\right)\right]\right]\\
&\leq \mathbb{E}_{\mathbf{d},\mathbf{d}'}\left[\frac{1}{u}\sup_{h\in\mathcal{H}}\left(\sum_{i=1}^{u}h(\mathbf{Z}_{\mathbf{d}}(i))-\sum_{i=1}^{u}h(\mathbf{Z}_{\mathbf{d}'}(i))\right)\right]\\
&= \mathbb{E}_{\mathbf{d},\mathbf{d}'}\left[\frac{1}{u}\sup_{h\in\mathcal{H}}\left(\sum_{i=1}^{u}\frac{1}{2}\left(h(\mathbf{Z}_{\mathbf{d}}(i))-h(\mathbf{Z}_{\mathbf{d}'}(i))\right)+\frac{-1}{2}\left(h(\mathbf{Z}_{\mathbf{d}}(i))-h(\mathbf{Z}_{\mathbf{d}'}(i))\right)\right)\right]\\
&= \mathbb{E}_{\mathbf{d},\mathbf{d}'}\left[\frac{1}{u}\sup_{h\in\mathcal{H}}\left(\sum_{i=1}^{u}\sigma_{\mathbf{Z}_{\mathbf{d}}(i)}\left(h(\mathbf{Z}_{\mathbf{d}}(i))-h(\mathbf{Z}_{\mathbf{d}'}(i))\right)\right)\right]\\
&\overset{②}{\leq} 2\mathfrak{R}_u(\mathcal{H}),
\end{aligned} \tag{32}$$

where ① is due to the Jensen's inequality, and ② is due to the definition of the Rademacher variables $\{\sigma_i\}_{i=1}^n$. Note that ② also indicates that the established symmetrization inequality of inductive Rademacher complexity also holds for our transductive setting.

By a similar argument, we have $E_2 \leq 2\mathfrak{R}_m(\mathcal{H})$.

Now let $Z=g(\mathbf{d})$, $a=\frac{2H_0}{C^2u}$, $b=\frac{2H_0r}{C^3u}$ in Theorem A.1. It follows by Lemma B.2 again that $V_+\leq aZ+b$. It then follows by Theorem A.1 that that for all $x>0$,

$$\begin{aligned}
&\Pr\left[g(\mathbf{d})\leq \mathbb{E}\left[g(\mathbf{d})\right]+\inf_{\alpha>0}\left(\frac{2}{\alpha}\left(\mathfrak{R}_u(\mathcal{H})+\mathfrak{R}_m(\mathcal{H})\right)+\frac{2(2+\alpha)H_0x}{C^2u}\right)+\sqrt{\frac{8H_0rx}{C^3u}}\right]\\
&\geq 1-\exp(-x).
\end{aligned} \tag{33}$$

□

For $r>0$, define the function class

$$\mathcal{H}_r=\left\{\frac{r}{w(h)}h\colon h\in\mathcal{H}\right\}, \tag{34}$$

where $w(h)\coloneqq \min\left\{r\lambda^k\colon k\geq 0, r\lambda^k\geq \mathcal{L}_n(h)\right\}$ with $\lambda>1$.

Define

$$U_r^+\coloneqq \sup_{s\in\mathcal{H}_r}\left(\mathcal{U}_s(\mathbf{Z}_{\mathbf{d}})-\mathcal{L}_s^{(m)}(\overline{\mathbf{Z}_{\mathbf{d}}})\right). \tag{35}$$

Lemma B.3. Fix $\lambda>1$ and $r>0$. If $U_r^+\leq \frac{r}{\lambda}$, then

$$\mathcal{U}_h(\mathbf{Z}_{\mathbf{d}})\leq\left(1+\frac{1}{C}\right)\mathcal{L}_h^{(m)}(\overline{\mathbf{Z}_{\mathbf{d}}})+\frac{r}{\lambda},\quad \forall h\in\mathcal{H}. \tag{36}$$

Proof. If $\mathcal{L}_n(h) \le r$, then $w(h) = r$ and $s = \frac{r}{w(h)} h = h$. Therefore, $U_r^+ \le \frac{r}{\lambda} \Rightarrow \mathcal{U}_s(\mathbf{Z_d}) - \mathcal{L}_s^{(m)}(\overline{\mathbf{Z_d}}) \le \frac{r}{\lambda}$ and (36) holds.

If $\mathcal{L}_n(h) > r$, then $w(h) = r\lambda^k$ with $\mathcal{L}_n(h) \in (r\lambda^{k-1}, r\lambda^k]$. Again, it follows by $U_r^+ \le \frac{r}{\lambda}$ that

$$\mathcal{U}_s(\mathbf{Z_d}) - \mathcal{L}_s^{(m)}(\overline{\mathbf{Z_d}}) \le \frac{r}{\lambda}, s = \frac{h}{\lambda^k},$$

and we have

$$\mathcal{U}_h(\mathbf{Z_d}) - \mathcal{L}_h^{(m)}(\overline{\mathbf{Z_d}}) \le r\lambda^{k-1} \le \mathcal{L}_n(h) = \frac{m}{n}\mathcal{L}_h^{(m)}(\overline{\mathbf{Z_d}}) + \frac{u}{n}\mathcal{U}_h(\mathbf{Z_d}).$$

It follows by the above inequality that

$$\mathcal{U}_h(\mathbf{Z_d}) \le \frac{1+m/n}{1-u/n}\mathcal{L}_h^{(m)}(\overline{\mathbf{Z_d}}) = \left(1+\frac{n}{m}\right)\mathcal{L}_h^{(m)}(\overline{\mathbf{Z_d}}) \le \left(1+\frac{1}{C}\right)\mathcal{L}_h^{(m)}(\overline{\mathbf{Z_d}}),$$

which indicates (36). □

Proof of Theorem 3.2. Let r be chosen such that $r \ge r^*$. Let $s = \frac{r}{w(h)} h \in \mathcal{H}_r$, then we have $\mathcal{L}_n(s) \le r$. To see this, if $\mathcal{L}_n(h) \le r$, then $w(h) = r$ and $s = h$, so $\mathcal{L}_n(s) = \mathcal{L}_n(h) \le r$. Otherwise, if $\mathcal{L}_n(h) > r$, then $s = \frac{h}{\lambda^k}$ where k is such that $\mathcal{L}_n(h) \in (r\lambda^{k-1}, r\lambda^k]$. It follows that $\mathcal{L}_n(s) = \frac{\mathcal{L}_n(h)}{\lambda^k} \le \frac{r\lambda^k}{\lambda^k} \le r$. It follows that $\mathcal{L}_n(s) \le r$ for all $s \in \mathcal{H}_r$.

Applying Theorem 3.1 to the function class $\mathcal{H}_r$, then for all $x > 0$, with probability at least $1 - e^{-x}$,

$$U_r^+ \le 4\left(\mathfrak{R}_u(\mathcal{H}_r) + \mathfrak{R}_m(\mathcal{H}_r)\right) + \frac{6H_0 x}{C^2 u} + \sqrt{\frac{8H_0 r x}{C^3 u}}. \tag{37}$$

Define the function class $\mathcal{H}(x,y) \coloneqq \{h \in \mathcal{H} \colon x \le \mathcal{L}_n(h) \le y\}$. Let T be the smallest integer such that $r\lambda^{T+1} \ge H_0$. Then we have

$$\begin{aligned}
\mathfrak{R}_u(\mathcal{H}_r) &\le \mathbb{E}\left[\sup_{h \in \mathcal{H}(0,r)} R_{u,\mathbf{d}} h\right] + \mathbb{E}\left[\sup_{h \in \mathcal{H}(r,H_0)} \frac{r}{w(h)} R_{u,\mathbf{d}} h\right] \\
&\le \mathbb{E}\left[\sup_{h \in \mathcal{H}(0,r)} R_{u,\mathbf{d}} h\right] + \sum_{t=0}^{T} \mathbb{E}\left[\sup_{h \in \mathcal{H}(r\lambda^t, r\lambda^{t+1})} \frac{r}{w(h)} R_{u,\mathbf{d}} h\right] \\
&\overset{①}{\le} \psi_u(r) + \sum_{t=0}^{T} \lambda^{-t}\psi_u(r\lambda^{t+1}) \\
&\overset{②}{\le} \psi_u(r)\left(1 + \lambda^{1/2}\sum_{t=0}^{T}\lambda^{-t/2}\right).
\end{aligned} \tag{38}$$

Here ① is due to $w(h) \ge r\lambda^t$ and $\mathbb{E}\left[\sup_{h\colon \mathcal{L}_n(h) \le r\lambda^{t+1}} R_{u,\mathbf{d}} h\right] \le \psi_u(r\lambda^{t+1})$. ② is due to the fact that the sub-root function ψ satisfies $\psi_u(\alpha r) \le \psi_u(r)$ for if $\alpha > 1$.

Setting $\lambda = 4$ on the RHS of (38), we have

$$\mathfrak{R}_u(\mathcal{H}_r) \le 5\psi_u(r) \le 5\sqrt{r r_u^*}. \tag{39}$$

The last inequality follows from $\psi_u(r) \le \sqrt{\frac{r}{r_u^*}}\psi(r_u^*) = \sqrt{rr_u^*}$ because $r \ge r_u^*$.

Following a similar argument, we also have

$$\mathfrak{R}_m(\mathcal{H}_r) \le 5\sqrt{rr_m^*} \tag{40}$$

It follows by (37), (39), and (40) that

$$\begin{aligned} U_r^+ &\le 20\sqrt{rr_u^*} + 20\sqrt{rr_m^*} + \frac{6H_0x}{C^2u} + \sqrt{\frac{8H_0rx}{C^3u}} \\ &= \sqrt{r}\left(20\left(\sqrt{r_u^*} + \sqrt{r_m^*}\right) + \sqrt{\frac{8H_0x}{C^3u}}\right) + \frac{6H_0x}{C^2u}. \end{aligned} \tag{41}$$

Let r_0 be the largest solution to $\sqrt{r}\left(20\left(\sqrt{r_u^*} + \sqrt{r_m^*}\right) + \sqrt{\frac{8H_0x}{C^3u}}\right) + \frac{6H_0x}{C^2u} = \frac{r}{\lambda}$, we have

$$r_0 \le r_1 \coloneqq 2\lambda\left(\lambda\left(20\left(\sqrt{r_u^*} + \sqrt{r_m^*}\right) + \sqrt{\frac{8H_0x}{C^3u}}\right)^2 + \frac{6H_0x}{C^2u}\right). \tag{42}$$

Then $r_1 \ge r^*$. Setting $r = r_1$ in (41), we have

$$U_{r_1}^+ \le \frac{r_1}{\lambda} = 2\lambda\left(20\left(\sqrt{r_u^*} + \sqrt{r_m^*}\right) + \sqrt{\frac{8H_0x}{C^3u}}\right)^2 + \frac{12H_0x}{C^2u}.$$

It follows by Lemma B.3 that

$$\begin{aligned} \mathcal{U}_h(\mathbf{Z_d}) &\le \left(1 + \frac{1}{C}\right)\mathcal{L}_h^{(m)}(\overline{\mathbf{Z_d}}) + \frac{r_1}{\lambda} \\ &= \left(1 + \frac{1}{C}\right)\mathcal{L}_h^{(m)}(\overline{\mathbf{Z_d}}) + 2\lambda\left(20\left(\sqrt{r_u^*} + \sqrt{r_m^*}\right) + \sqrt{\frac{8H_0x}{C^3u}}\right)^2 + \frac{12H_0x}{C^2u}, \end{aligned}$$

Then (7) follows by noting that $\left(20\left(\sqrt{r_u^*} + \sqrt{r_m^*}\right) + \sqrt{\frac{8H_0x}{C^3u}}\right)^2 \le 800(r_u^* + r_m^*) + \frac{16H_0x}{C^3u}$ and setting $\lambda = 4$.

□

B.2 TLRC Bound for Generic Transductive Learning

Proof of Theorem 3.3. We apply Theorem 3.2 with $\mathcal{H} = \ell \circ \mathcal{F}$, $B = L_0$. Then (9) follows by Theorem 3.2. □

B.3 TLRC Bound for Kernel Transductive Learning

Proof of Theorem 3.5. We note that $\left\{\Phi^{(k)}\right\}_{k\ge 1}$ is an orthonormal basis of the RKHS $\mathcal{H}_K$, so $v_j = \sum_{k\ge 1}\left\langle v_j, \Phi^{(k)}\right\rangle \Phi^{(k)}$. As a result, let $r_0 = m_{k_0}$, then with probability at least $1-\delta$,

$$\begin{aligned}
\sum_{q=r_0+1}^{n}\left\langle f^*, \Phi^{(q)}\right\rangle_{\mathcal{H}_K}^2 &= \sum_{q=r_0+1}^{n}\left\langle \sum_{j=1}^{m_{k_0}}\beta_j v_j, \Phi^{(q)}\right\rangle_{\mathcal{H}_K}^2 \\
&= \sum_{q=r_0+1}^{n}\sum_{j=1}^{m_{k_0}}\beta_j^2\left\langle v_j, \Phi^{(k)}\right\rangle^2 \\
&\le \mu^2\sum_{q=r_0+1}^{n}\sum_{j=1}^{m_{k_0}}\left\langle v_j, \Phi^{(k)}\right\rangle^2 \le \frac{8\mu^2\tau_0^4\log\frac{2}{\delta}}{\left(\lambda_{m_{k_0}}-\lambda_{m_{k_0}+1}\right)^2 n}.
\end{aligned}$$

Here the last inequality follows by Lemma B.12. □

Before presenting the proof of Theorem 3.6, we introduce the definition about convex and symmetric sets below, as well as Lemma B.4 and Lemma B.5 which lay the foundation of the proof of Theorem 3.6.

Definition B.1. A set X is convex if $\alpha X + (1-\alpha)X \subseteq X$ for all $\alpha \in [0,1]$. X is symmetric if $-X \subseteq X$.

Lemma B.4. Let τ be a contraction, that is, $|\tau(x)-\tau(y)| \le L|x-y|$ for $L>0$. Then the following contraction property holds:

$$\mathfrak{R}_u(\tau\circ\mathcal{H}) \le L\mathfrak{R}_u(\mathcal{F}), \quad \mathfrak{R}_m(\tau\circ\mathcal{H}) \le L\mathfrak{R}_m(\mathcal{F}), \tag{43}$$

Proof. The proof follows the standard proof for contraction property of Rademacher complexity in [15]. □

Lemma B.5. For every $r>0$ and $r_0\in[n]$,

$$\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{f\colon f\in\mathcal{H}_{\mathbf{X}_n,r_0}(\mu),\mathcal{L}_n(f^2)\le r} R_{u,\mathbf{d}}f\right] \le \tilde{\varphi}_u(r), \tag{44}$$

where

$$\tilde{\varphi}_u(r) \coloneqq \min_{Q\colon 0\le Q\le r_0}\left(\sqrt{\frac{rQ}{u}} + \mu\sqrt{\frac{\sum_{q=Q+1}^{r_0}\widehat{\lambda}_q}{u}}\right). \tag{45}$$

Similarly, for every $r>0$ and $r_0\in[n]$,

$$\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{f\colon f\in\mathcal{H}_{\mathbf{X}_n,r_0}(\mu),\mathcal{L}_n(f^2)\le r} R_{m,\mathbf{d}}f\right] \le \tilde{\varphi}_m(r), \tag{46}$$

where

$$\tilde{\varphi}_m(r) \coloneqq \min_{Q\colon 0 \le Q \le r_0} \left(\sqrt{\frac{rQ}{m}} + \mu \sqrt{\frac{\sum_{q=Q+1}^{r_0} \widehat{\lambda}_q}{m}} \right). \tag{47}$$

Proof. We have

$$R_{u,\mathbf{d}} f = \frac{1}{u} \sum_{i=1}^{u} \sigma_{\mathbf{Z_d}(i)} f(\vec{\mathbf{x}}_{\mathbf{Z_d}(i)}) = \left\langle f, \frac{1}{u} \sum_{i=1}^{u} \sigma_{\mathbf{Z_d}(i)} K(\cdot, \vec{\mathbf{x}}_{\mathbf{Z_d}(i)}) \right\rangle_{\mathcal{H}_K}. \tag{48}$$

Because $\{\Phi^{(k)}\}_{k\ge1}$ is an orthonormal basis of $\mathcal{H}_K$, for any $0 \le Q \le r_0$, we further express the first term on the RHS of (48) as

$$\left\langle f, \frac{1}{u} \sum_{i=1}^{u} \sigma_{\mathbf{Z_d}(i)} K(\cdot, \vec{\mathbf{x}}_{\mathbf{Z_d}(i)}) \right\rangle_{\mathcal{H}_K} = \left\langle \sum_{q=1}^{Q} \sqrt{\widehat{\lambda}_q} \left\langle f, \Phi_q \right\rangle_{\mathcal{H}_K} \Phi_q, v(\mathbf{d}, \boldsymbol{\sigma}) \right\rangle_{\mathcal{H}_K} + \left\langle \bar{f}, \bar{v}^{(Q)}(\mathbf{d}, \boldsymbol{\sigma}) \right\rangle_{\mathcal{H}_K}, \tag{49}$$

where

$$\begin{aligned}
\bar{f} &= f - \sum_{q=1}^{Q} \left\langle f, \Phi_q \right\rangle_{\mathcal{H}_K} \Phi_q, \\
v^{(Q)}(\mathbf{d}, \boldsymbol{\sigma}) &\coloneqq \frac{1}{u} \sum_{q=1}^{Q} \frac{1}{\sqrt{\widehat{\lambda}_q}} \left\langle \sum_{i=1}^{u} \sigma_{\mathbf{Z_d}(i)} K(\cdot, \vec{\mathbf{x}}_{\mathbf{Z_d}(i)}), \Phi_q \right\rangle_{\mathcal{H}_K} \Phi_q, \\
\bar{v}^{(Q)}(\mathbf{d}, \boldsymbol{\sigma}) &\coloneqq \frac{1}{u} \sum_{q=Q+1}^{r_0} \left\langle \sum_{i=1}^{u} \sigma_{\mathbf{Z_d}(i)} K(\cdot, \vec{\mathbf{x}}_{\mathbf{Z_d}(i)}), \Phi_q \right\rangle_{\mathcal{H}_K} \Phi_q.
\end{aligned}$$

We have

$$\left\langle T_n f, f \right\rangle_{\mathcal{H}_K} = \left\langle \frac{1}{n} \sum_{i=1}^{n} K(\cdot, \vec{\mathbf{x}}_{\mathbf{Z_d}(i)}) f(\vec{\mathbf{x}}_{\mathbf{Z_d}(i)}), f \right\rangle_{\mathcal{H}_K} = \mathcal{L}_n f^2.$$

As a result,

$$\left\| \sum_{q=1}^{Q} \sqrt{\widehat{\lambda}_q} \left\langle f, \Phi_q \right\rangle \Phi_q \right\|_{\mathcal{H}_K}^2 = \sum_{q=1}^{Q} \widehat{\lambda}_q \left\langle f, \Phi_q \right\rangle_{\mathcal{H}_K}^2 \le \sum_{q=1}^{n} \widehat{\lambda}_q \left\langle f, \Phi_q \right\rangle_{\mathcal{H}_K}^2 = \left\langle T_n f, f \right\rangle_{\mathcal{H}_K} = \mathcal{L}_n f^2 \le r, \tag{50}$$

which holds for all f such that $\mathcal{L}_n(f^2) \le r$.

Combining (48) and (49), we have

$$\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}} \left[\sup_{f\colon f \in \mathcal{H}_{\mathbf{X}_n, r_0}(\mu), \mathcal{L}_n(f^2) \le r} \left\langle f, \frac{1}{m} \sum_{i=1}^{m} \sigma_{\mathbf{Z_d}(i)} K(\cdot, \vec{\mathbf{x}}_{\mathbf{Z_d}(i)}) \right\rangle \right]$$

$$
\begin{aligned}
&\overset{①}{\leq} \sup_{f\colon f\in\mathcal{H}_{\mathbf{X}_n, r_0}(\mu), \mathcal{L}_n(f^2)\le r} \left\| \sum_{q=1}^{Q} \sqrt{\widehat{\lambda}_q} \left\langle f, \Phi_q \right\rangle_{\mathcal{H}_K} \Phi_q \right\|_{\mathcal{H}_K} \cdot \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}} \left[\left\| v^{(Q)}(\mathbf{d},\boldsymbol{\sigma}) \right\|_{\mathcal{H}_K} \right] \\
&\quad + \left\| \bar{f} \right\|_{\mathcal{H}_K} \cdot \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}} \left[\left\| \bar{v}^{(Q)}(\mathbf{d},\boldsymbol{\sigma}) \right\|_{\mathcal{H}_K} \right] \\
&\le \sqrt{r} \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}} \left[\left\| v^{(Q)}(\mathbf{d},\boldsymbol{\sigma}) \right\|_{\mathcal{H}_K} \right] + \mu \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}} \left[\left\| \bar{v}^{(Q)}(\mathbf{d},\boldsymbol{\sigma}) \right\|_{\mathcal{H}_K} \right].
\end{aligned} \tag{51}
$$

where ① is due to the Cauchy-Schwarz inequality.

We have

$$
\begin{aligned}
\frac{1}{u} \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}} \left[\left\langle \sum_{i=1}^{u} \sigma_{\mathbf{Z}_{\mathbf{d}}(i)} K(\cdot, \overrightarrow{\mathbf{x}}_{\mathbf{Z}_{\mathbf{d}}(i)}), \Phi_q \right\rangle_{\mathcal{H}_K}^2 \right] &\overset{①}{=} \frac{1}{u} \mathbb{E}_{\mathbf{d}} \left[\sum_{i=1}^{u} \left\langle K(\cdot, \overrightarrow{\mathbf{x}}_{\mathbf{Z}_{\mathbf{d}}(i)}), \Phi_q \right\rangle_{\mathcal{H}_K}^2 \right] \\
&= \frac{1}{u} \mathbb{E}_{\mathbf{d}} \left[\sum_{i=1}^{u} \Phi_q(\overrightarrow{\mathbf{x}}_{\mathbf{Z}_{\mathbf{d}}(i)})^2 \right] \\
&= \frac{1}{u} \cdot \frac{u}{n} \sum_{i=1}^{n} \Phi_q^2(\overrightarrow{\mathbf{x}}_i) \\
&= \left\langle T_n \Phi_q, \Phi_q \right\rangle = \widehat{\lambda}_q.
\end{aligned} \tag{52}
$$

Here ① is due to the fact that $\mathbb{E}\left[\sigma_i\right] = 0$ for all $i \in [n]$. ② follows by the fact that $\left\{ \Phi_q^2(\overrightarrow{\mathbf{x}}_{\mathbf{Z}_{\mathbf{d}}(i)}) \right\}_{i=1}^{m}$ follows a distribution of uniform draw of distinct u elements from $\left\{ \Phi_q(\overrightarrow{\mathbf{x}}_j) \right\}_{j=1}^{n}$ without replacement, so $\mathbb{E}_{\mathbf{d}} \left[\sum\limits_{i=1}^{u} \Phi_q^2(\overrightarrow{\mathbf{x}}_{\mathbf{Z}_{\mathbf{d}}(i)}) \right] = \frac{u}{n} \sum\limits_{i=1}^{n} \Phi_q^2(\overrightarrow{\mathbf{x}}_i)$.

It follows by (52) that

$$
\begin{aligned}
\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}} \left[\left\| v^{(Q)}(\mathbf{d},\boldsymbol{\sigma}) \right\|_{\mathcal{H}_K} \right] &= \frac{1}{\sqrt{u}} \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}} \left[\sqrt{ \frac{1}{u} \sum_{q=1}^{Q} \frac{1}{\widehat{\lambda}_q} \left\langle \sum_{i=1}^{u} \sigma_{\mathbf{Z}_{\mathbf{d}}(i)} K(\cdot, \overrightarrow{\mathbf{x}}_{\mathbf{Z}_{\mathbf{d}}(i)}), \Phi_q \right\rangle_{\mathcal{H}_K}^2 } \right] \\
&\overset{①}{\leq} \frac{1}{\sqrt{u}} \sqrt{ \frac{1}{u} \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}} \left[\sum_{q=1}^{Q} \frac{1}{\widehat{\lambda}_q} \left\langle \sum_{i=1}^{u} \sigma_{\mathbf{Z}_{\mathbf{d}}(i)} K(\cdot, \overrightarrow{\mathbf{x}}_{\mathbf{Z}_{\mathbf{d}}(i)}), \Phi_q \right\rangle_{\mathcal{H}_K}^2 \right] } \\
&\overset{②}{=} \sqrt{\frac{Q}{u}},
\end{aligned} \tag{53}
$$

where ① is due to the Jensen's inequality, ② is due to the fact that $\mathbb{E}\left[\sigma_i\right] = 0$ for all $i \in [n]$. Similarly, we have

$$
\begin{aligned}
\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}} \left[\left\| \bar{v}^{(Q)}(\mathbf{d},\boldsymbol{\sigma}) \right\|_{\mathcal{H}_K} \right] &= \frac{1}{\sqrt{u}} \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}} \left[\sqrt{ \frac{1}{u} \sum_{q=Q+1}^{r_0} \left\langle \sum_{i=1}^{u} \sigma_{\mathbf{Z}_{\mathbf{d}}(i)} K(\cdot, \overrightarrow{\mathbf{x}}_{\mathbf{Z}_{\mathbf{d}}(i)}), \Phi_q \right\rangle_{\mathcal{H}_K}^2 } \right] \\
&\le \frac{1}{\sqrt{u}} \sqrt{ \frac{1}{u} \mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}} \left[\sum_{q=Q+1}^{r_0} \left\langle \sum_{i=1}^{u} \sigma_{\mathbf{Z}_{\mathbf{d}}(i)} K(\cdot, \overrightarrow{\mathbf{x}}_{\mathbf{Z}_{\mathbf{d}}(i)}), \Phi_q \right\rangle_{\mathcal{H}_K}^2 \right] }
\end{aligned}
$$

$$= \sqrt{\frac{\sum_{q=Q+1}^{r_0} \widehat{\lambda}_q}{u}}. \tag{54}$$

It follows by (51), (53), and (54) that

$$\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{f\colon f\in\mathcal{H}_{\mathbf{X}_n,r_0},\mathcal{L}_n(f^2)\le r}\left\langle f, \frac{1}{u}\sum_{i=1}^{u}\sigma_{\mathbf{Z}_{\mathbf{d}}(i)}K(\cdot,\overset{\rightharpoonup}{\mathbf{x}}_{\mathbf{Z}_{\mathbf{d}}(i)})\right\rangle\right] \le \min_{Q\colon 0\le Q\le r_0}\left(\sqrt{\frac{rQ}{u}} + \mu\sqrt{\frac{\sum_{q=Q+1}^{r_0}\widehat{\lambda}_q}{u}}\right), \tag{55}$$

which completes the proof of (44). (46) can be proved by a similar argument. □

Proof of Theorem 3.6. We apply Theorem 3.3 and consider the function class

$$\ell \circ \mathcal{H}_{\mathbf{X}_n,r_0}(v) = \left\{\ell_f = (f-f^*)^2 \mid f \in \mathcal{H}_{\mathbf{X}_n,r_0}(v)\right\}.$$

Because $f, f^* \in \mathcal{H}_{\mathbf{X}_n}(v)$, we have $|f(\mathbf{x}_i) - f^*(\mathbf{x}_i)| \le 2\mu\tau_0$ for all $i \in [n]$. We let $H_0 = 4\mu^2\tau_0^2 \ge \max_{i\in[n]}\left(f(\mathbf{x}_i) - f^*(\mathbf{x}_i)\right)^2$.

Let f^{*,r_0} be the orthogonal projection of f^* onto $\mathcal{H}_{\mathbf{X}_n,r_0}$, that is, $f^{*,r_0} := \mathbb{P}_{\mathcal{H}_{\mathbf{X}_n,r_0}}(f^*)$, and $\bar{f}^{*,r_0} := f^* - f^{*,r_0}$. If $\mathcal{L}_n(f-f^*)^2 \le r$ for some $r > 0$, by Cauchy-Schwarz inequality we have

$$\begin{aligned}\mathcal{L}_n\left(f - f^{*,r_0}\right)^2 &\le 2\mathcal{L}_n\left(f-f^*\right)^2 + 2\mathcal{L}_n\left(\bar{f}^{*,r_0}\right)^2 \\ &\le 2r + 2\mathcal{L}_n\left(\bar{f}^{*,r_0}\right)^2.\end{aligned} \tag{56}$$

We have

$$\left\langle T_n\bar{f}^{*,r_0}, \bar{f}^{*,r_0}\right\rangle = \left\langle \frac{1}{n}\sum_{i=1}^{n}K(\cdot,\overset{\rightharpoonup}{\mathbf{x}}_i)\bar{f}^{*,r_0}(\overset{\rightharpoonup}{\mathbf{x}}_i), \bar{f}^{*,r_0}\right\rangle_{\mathcal{H}_K} = \mathcal{L}_n\left(\bar{f}^{*,r_0}\right)^2. \tag{57}$$

On the other hand, with probability $1-\delta$,

$$\begin{aligned}\left\langle T_n\bar{f}^{*,r_0}, \bar{f}^{*,r_0}\right\rangle &= \left\langle T_n\sum_{q=r_0+1}^{n}\left\langle \bar{f}^{*,r_0}, \Phi^{(q)}\right\rangle\Phi^{(q)}, \sum_{q=r_0+1}^{n}\left\langle \bar{f}^{*,r_0}, \Phi^{(q)}\right\rangle\Phi^{(q)}\right\rangle_{\mathcal{H}_K} \\ &= \sum_{q=r_0+1}^{n}\widehat{\lambda}_q\left\langle \bar{f}^{*,r_0}, \Phi^{(q)}\right\rangle^2 \\ &\le \widehat{\lambda}_{r_0+1}\sum_{q=r_0+1}^{n}\left\langle f^*, \Phi^{(q)}\right\rangle^2 \\ &\overset{①}{\le} \widehat{\lambda}_{r_0+1}\zeta_{n,\delta} := \zeta_{n,r_0,\delta}.\end{aligned} \tag{58}$$

where ① is due to Assumption 2. It follows by (56)- (58) that

$$\mathcal{L}_n\left(f - f^{*,r_0}\right)^2 \le 2r + 2\zeta_{n,r_0,\delta}. \tag{59}$$

Furthermore,

$$\left|(f_1(\mathbf{x}) - f^*(\mathbf{x}))^2 - (f_2(\mathbf{x}) - f^*(\mathbf{x}))^2\right| \le 4\mu\tau_0 \left|f_1(\mathbf{x}) - f_2(\mathbf{x})\right|.$$

Therefore, for $r > 0$ we have

$$\begin{aligned}
&\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{f\colon f\in\mathcal{H}_{\mathbf{X}_{n},r_0}(\mu),\mathcal{L}_n(f-f^*)^2\le r} R_{u,\mathbf{d}}\left(f-f^*\right)^2\right] \\
&\overset{①}{\le} 4\mu\tau_0\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{f\colon f\in\mathcal{H}_{\mathbf{X}_{n},r_0}(\mu),\mathcal{L}_n(f-f^*)^2\le r} R_{u,\mathbf{d}}(f-f^*)\right] \\
&= 4\tau_0\mu\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{f\colon f\in\mathcal{H}_{\mathbf{X}_{n},r_0}(\mu),\mathcal{L}_n(f-f^*)^2\le r} R_{u,\mathbf{d}} f\right] \\
&\le 4\tau_0\mu\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{f\colon f\in\mathcal{H}_{\mathbf{X}_{n},r_0}(\mu),\mathcal{L}_n(f-f^{*,r_0})^2\le 2r+2\zeta_{n,r_0,\delta}} R_{u,\mathbf{d}}\left(f-f^{*,r_0}\right)\right] \\
&\overset{②}{\le} 8\tau_0\mu\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{h\colon h\in\mathcal{H}_{\mathbf{X}_{n},r_0}(\mu),\mathcal{L}_n(h^2)\le\frac{r}{2}+\frac{\zeta_{n,r_0,\delta}}{2}} R_{u,\mathbf{d}} h\right] \\
&\overset{③}{\le} 8\tau_0\mu\tilde{\varphi}_u\left(\frac{r}{2}+\frac{\zeta_{n,r_0,\delta}}{2}\right).
\end{aligned} \tag{60}$$

Here ① is due to the contraction property in Lemma B.4. ② follows by letting $h = \frac{1}{2}\left(f - f^{*,r_0}\right)$. It can be verified that $h \in \mathcal{H}_{\mathbf{X}_{n},r_0}$ because $f^{*,r_0}, f \in \mathcal{H}_{\mathbf{X}_{n},r_0}(\mu)$ and $\mathcal{H}_{\mathbf{X}_{n},r_0}(\mu)$ is symmetric and convex. $\tilde{\varphi}_u$ in ③ is defined in (45) in Lemma B.5.

It follows by (60) that

$$\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{f\colon f\in\mathcal{H}_{\mathbf{X}_{n},r_0}(\mu),\mathcal{L}_n(\ell_f)\le r} R_{u,\mathbf{d}}\ell_f\right] \le \varphi_u(r) \coloneqq 8\tau_0\mu\tilde{\varphi}_u\left(\frac{r}{2}+\frac{\zeta_{n,r_0,\delta}}{2}\right),$$

and φ_u is a sub-root function by checking that $\varphi_u(r)/\sqrt{r}$ is nonincreasing.

By a similar argument, we have

$$\mathbb{E}_{\mathbf{d},\boldsymbol{\sigma}}\left[\sup_{f\colon f\in\mathcal{H}_{\mathbf{X}_{n},r_0}(\mu),\mathcal{L}_n(\ell_f)\le r} R_{m,\mathbf{d}}\ell_f\right] \le \varphi_m(r) \coloneqq 8\tau_0\mu\tilde{\varphi}_m\left(\frac{r}{2}+\frac{\zeta_{n,r_0,\delta}}{2}\right).$$

It can be verified that φ_m is also a sub-root function. Let r_u^*, r_m^* be the fixed point of φ_u and φ_m respectively. We define $\varphi(r) \coloneqq \varphi_u(r) + \varphi_m(r)$, then φ is also a sub-root function, and $r^* = r_u^* + r_m^*$ is the fixed point of φ.

Let $0 \le r \le r^*$ .Then it follows by [1, Lemma 3.2] that $0 \le r \le \varphi(r)$. Therefore, by the definition of $\tilde{\varphi}_u$ in (45) and $\tilde{\varphi}_m$ in (47), for every $0 \le Q \le r_0$, we have

$$\frac{r}{8\tau_0\mu} \le \sqrt{\frac{rQ}{2u}} + \sqrt{\frac{rQ}{2m}} + \sqrt{\frac{\zeta_{n,r_0,\delta}Q}{2u}} + \mu\sqrt{\frac{\sum\limits_{q=Q+1}^{r_0}\widehat{\lambda}_q}{u}} + \sqrt{\frac{\zeta_{n,r_0,\delta}Q}{2m}} + \mu\sqrt{\frac{\sum\limits_{q=Q+1}^{r_0}\widehat{\lambda}_q}{m}}.$$

Solving the above quadratic inequality for r, we have

$$\begin{aligned} r &\le 128\tau_0^2\mu^2 Q\left(\frac{1}{u}+\frac{1}{m}\right) \\ &+ 16\tau_0\mu\left(\sqrt{\frac{\zeta_{n,r_0,\delta}Q}{2u}} + \mu\sqrt{\frac{\sum\limits_{q=Q+1}^{r_0}\widehat{\lambda}_q}{u}} + \sqrt{\frac{\zeta_{n,r_0,\delta}Q}{2m}} + \mu\sqrt{\frac{\sum\limits_{q=Q+1}^{r_0}\widehat{\lambda}_q}{m}}\right) := r(u,m,Q,r_0,\delta). \end{aligned} \tag{61}$$

(61) holds for every $0 \le Q \le r_0$, so we have

$$r \le \min_{0\le Q\le r_0} r(u,m,Q,r_0,\delta). \tag{62}$$

Finally, it follows by Theorem 3.3 and (62) that

$$\mathcal{U}_{\ell_f}(\mathbf{Z_d}) \le \left(1+\frac{1}{C}\right)\mathcal{L}_{\ell_f}^{(m)}(\mathbf{Z_d}) + \frac{c_2 x}{u} + c_1 \min_{0\le Q\le r_0} r(u,m,Q,r_0,\delta),$$

which indicates (16). $\square$

Proof of Corollary 3.7. Let $r_0 = n$, then it can be verified by definition that any $f^* \in \mathcal{H}_{\mathbf{X}_n}(\mu)$ is in the function class $\mathcal{H}_{\mathbf{X}_n,r_0,0}(\mu)$ with $\zeta_{n,n,0} = 0$. Then (17) follow by applying Theorem 3.6. $\square$

B.4 Application to Graph Transductive Learning

Proof of Theorem 3.8. Let $\phi(i) \in \mathbb{R}^n$ and $\phi(i)^\top$ is the i-th row of $\mathbf{U}^{(\mathbf{L})}\mathbf{\Sigma}^{(\mathbf{L})^{\frac{1}{2}}} = \mathbf{L}^{\frac{1}{2}}$ for all $i \in [n]$. Then $[\mathbf{L}]_{ij} = \langle\phi(i),\phi(j)\rangle$, where $\phi(i)$ is the feature map of $\vec{\mathbf{x}}_i$. We define a PSD kernel

$$K(\mathbf{x},\mathbf{x}') = \left\langle\tilde{\phi}(\mathbf{x}),\tilde{\phi}(\mathbf{x}')\right\rangle, \quad \forall \mathbf{x},\mathbf{x}' \in \mathbb{R}^d, \tag{63}$$

where

$$\tilde{\phi}(\mathbf{x}) := \begin{cases} \phi(i) & \mathbf{x} = \vec{\mathbf{x}}_i \\ \mathbf{0} & \text{otherwise.} \end{cases}$$

Let

$$\tilde{\mathbf{v}}^* = \operatorname*{arg\,min}_{\mathbf{v}\in\mathbb{R}^n} \mathcal{L}_n(\mathbf{v}), \quad \mathcal{L}_n(\mathbf{v}) := \frac{1}{n}\|\mathbf{L}\mathbf{v}-\mathbf{y}\|_2^2,$$

and $\mathcal{L}^{(m)}(\tilde{\mathbf{v}}^*) = \frac{1}{m}\left\|[\mathbf{L}\tilde{\mathbf{v}}^* - \mathbf{y}]_{\mathbf{Z_d}(1:m)}\right\|_2^2$. Let $f_{\mathbf{v}} \in \mathcal{H}_{\mathbf{X}_n}$ with $\mathbf{v} \in \mathbb{R}^n$ be defined by

$$f_{\mathbf{v}} \coloneqq \sum_{i=1}^{n} K(\cdot, \overset{\rightharpoonup}{\mathbf{x}}_i)\mathbf{v}_i.$$

Then $f_{\tilde{\mathbf{v}}^*}(\overset{\rightharpoonup}{\mathbf{x}}_i) = y_i$ because $\mathbf{L}\tilde{\mathbf{v}}^* = \mathbf{y}$ due to the positive definiteness of $\mathbf{L}$. It follows by the given condition (22) that $\|f_{\tilde{\mathbf{v}}^*}\|_{\mathcal{H}_K} = \sqrt{(\tilde{\mathbf{v}}^*)^\top \mathbf{L}\tilde{\mathbf{v}}^*} \le \mu$.

It follows from $\mathbf{v}^\top\mathbf{L}\mathbf{v} \le \mu^2$ that $\|f_{\mathbf{v}}\|_{\mathcal{H}_K} \le \mu$. It then follows by Corollary 3.7 that for every $x > 0$, with probability at least $1 - \exp(-x)$,

$$\begin{aligned}\mathcal{U}_{\ell_{f_{\mathbf{v}}}} &\le \left(1 + \frac{1}{C}\right)\mathcal{L}^{(m)}_{\ell_{f_{\mathbf{v}}}}(\overline{\mathbf{Z}_{\mathbf{d}}}) + \frac{c_2 x}{u} \\ &\quad + c_1 \min_{0 \le Q \le n}\left(c_3 Q\left(\frac{1}{u} + \frac{1}{m}\right) + c_4\mu\sqrt{\frac{\sum\limits_{q=Q+1}^{n}\widehat{\lambda}_q}{u}} + c_4\mu\sqrt{\frac{\sum\limits_{q=Q+1}^{n}\widehat{\lambda}_q}{m}}\right).\end{aligned} \tag{64}$$

Here we set $H_0 = 4\mu^2\tau_0^2$, and $\tau_0^2 = \max_{i\in[n]} \mathbf{L}_{ii}$, and c_1, c_2, c_3, c_4 are the same as those in Theorem 3.6. We note that (64) holds for $\mathbf{v} = \mathbf{v}^*$.

We now bound $\mathcal{L}^{(m)}_{\ell_{f_{\mathbf{v}^*}}}(\mathbf{Z_d})$. It follows by Lemma B.9 that for every $x > 0$ with probability at least $1 - \exp(-x)$,

$$\begin{aligned}0 \le \mathcal{L}^{(m)}_{\ell_{f_{\mathbf{v}^*}}}(\overline{\mathbf{Z}_{\mathbf{d}}}) &\overset{①}{\le} \mathcal{L}^{(m)}(\tilde{\mathbf{v}}^*) \\ &\overset{②}{\le} 2\mathcal{L}_n(\tilde{\mathbf{v}}^*) + \frac{6H_0 x}{m} = \frac{6H_0 x}{m}.\end{aligned} \tag{65}$$

Here ① follows by the optimality of $\mathbf{v}^*$. ② follows by Lemma B.9. (65) indeed indicates that the training loss $\mathcal{L}^{(m)}_{\ell_{f_{\mathbf{v}^*}}}(\overline{\mathbf{Z}_{\mathbf{d}}})$ vanishes with high probability. (20) then follows by (64) and (65).

□

Proof of Theorem 3.9. We follow almost the same proof strategy as that for Theorem 3.8. We first define the kernel

$$K(\mathbf{x}, \mathbf{x}') = \left\langle \tilde{\phi}(\mathbf{x}), \tilde{\phi}(\mathbf{x}')\right\rangle, \quad \forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^d,$$

with feature mapping $\tilde{\phi}$ being the same as that in the proof of Theorem 3.8.

Let

$$\tilde{\mathbf{v}}^* = \mathbf{L}^{-1}\mathbf{U}^{(\mathbf{L},r_0)}{\mathbf{U}^{(\mathbf{L},r_0)}}^\top\mathbf{y},$$

and $\mathcal{L}^{(m)}(\tilde{\mathbf{v}}^*) = \frac{1}{m}\left\|[\mathbf{L}\tilde{\mathbf{v}}^* - \mathbf{y}]_{\mathbf{Z_d}(1:m)}\right\|_2^2$. Let $f_{\mathbf{v}} \in \mathcal{H}_{\mathbf{X}_n}$ be defined by $f_{\mathbf{v}} \coloneqq \sum\limits_{i=1}^{n} K(\cdot, \overset{\rightharpoonup}{\mathbf{x}}_i)\mathbf{v}_i$. Then $f_{\tilde{\mathbf{v}}^*}(\overset{\rightharpoonup}{\mathbf{x}}_i) = y_i$ because $\mathbf{L}\tilde{\mathbf{v}}^* = \mathbf{y}$ due to the positive definiteness of $\mathbf{L}$ and $\mathbf{U}^{(\mathbf{L},r_0)}{\mathbf{U}^{(\mathbf{L},r_0)}}^\top\mathbf{y} = \mathbf{y}$. It follows by the given condition (22) that $\|f_{\tilde{\mathbf{v}}^*}\|_{\mathcal{H}_K} = (\tilde{\mathbf{v}}^*)^\top\mathbf{L}\tilde{\mathbf{v}}^* \le \mu$.

Because $\tilde{\mathbf{v}}^* \in \mathrm{Span}\left(\mathbf{U}^{(\mathbf{L},r_0)}\right)$, it can be verified that $f_{\tilde{\mathbf{v}}^*} \in \mathcal{H}_{\mathbf{X}_n, r_0, 0}(\mu)$ with $\zeta_{n,0} = 0$.

For $\mathbf{v}$ such that $\mathbf{v}^\top \mathbf{L}\mathbf{v} \le \mu^2$ and $\mathbf{v} \in \mathrm{Span}\left(\mathbf{U}^{(\mathbf{L},r_0)}\right)$, we have $f_{\mathbf{v}} \in \mathcal{H}_{\mathbf{X}_n,r_0}(\mu)$. Therefore, it follows by Theorem 3.6 that for every $x>0$, with probability at least $1-\exp(-x)$,

$$\mathcal{U}_{\ell_{f_{\mathbf{v}}}}(\mathbf{Z_d}) \le \left(1+\frac{1}{C}\right)\mathcal{L}^{(m)}_{\ell_{f_{\mathbf{v}}}}(\overline{\mathbf{Z_d}}) + \frac{c_2 x}{u} + c_1 c_3 r_0\left(\frac{1}{u}+\frac{1}{m}\right), \tag{66}$$

where Q is set to r_0 in Theorem 3.6. We note that (64) holds for $\mathbf{v} = \mathbf{v}^{*(r_0)}$.

We now bound $\mathcal{L}^{(m)}_{\ell_{f_{\mathbf{v}^{*(r_0)}}}}(\overline{\mathbf{Z_d}})$. It follows by Lemma B.9 that for every $x>0$ with probability at least $1-\exp(-x)$,

$$\begin{aligned} 0 \le \mathcal{L}^{(m)}_{\ell_{f_{\mathbf{v}^{*(r_0)}}}}(\overline{\mathbf{Z_d}}) &\overset{①}{\le} \mathcal{L}^{(m)}(\tilde{\mathbf{v}}^*) \\ &\overset{②}{\le} 2\mathcal{L}_n(\tilde{\mathbf{v}}^*) + \frac{6H_0 x}{m} = \frac{6H_0 x}{m}. \end{aligned} \tag{67}$$

Here ① follows by the optimality of $\mathbf{v}^{*(r_0)}$. ② follows by Lemma B.9, and $H_0 = 4\mu^2\tau_0$, $\tau_0^2 = \max_{i\in[n]} \mathbf{L}_{ii}$. (23) then follows by (66) and (67).

□

B.5 Application to Transductive Nonparametric Kernel Regression

Proof of Theorem 3.10. Let $r_0 = m_{k_0}$ in Theorem B.6. It follows by Theorem 3.5 that $f^* \in \mathcal{H}_{\mathbf{X}_n,m_{k_0},\delta}(\mu_0)$ and

$$\zeta_{n,\delta} = \frac{8\mu_0^2\tau_0^4 \log\frac{2}{\delta}}{\left(\lambda_{m_{k_0}} - \lambda_{m_{k_0}+1}\right)^2 n}. \tag{68}$$

Then it follows by (69) in Theorem B.6 and $\zeta_{n,r_0,\delta} = \widehat{\lambda}_{r_0+1}\zeta_{n,\delta} \le \tau_0^2 \zeta_{n,\delta}$ that

$$\begin{aligned} \mathcal{U}(\ell_{f_{\hat{\mathbf{u}}}}) \le{}& \left(1+\frac{1}{C}\right)\left(2+\frac{6x}{C}\right)\left(2\zeta_{n,m_{k_0},\delta} + \frac{2m_{k_0}(\sigma+1)^2}{n}\right) + \frac{c_2 x}{u} \\ &+ c_1 c_3 m_{k_0}\left(\frac{1}{u}+\frac{1}{m}\right) + c_1 c_4\sqrt{\zeta_{n,m_{k_0},\delta}\, m_{k_0}}\left(\frac{1}{\sqrt{2u}}+\frac{1}{\sqrt{2m}}\right). \end{aligned}$$

□

Theorem B.6. Suppose K is a continuous and positive definite kernel on $\mathcal{X}\times\mathcal{X}$, and suppose $n \ge \max\left\{\frac{4r_0(\sigma+1)^2}{\mu_1\lambda_{r_0}}, \frac{32\tau_0^4\log\frac{2}{\delta}}{\lambda_{r_0}^2}\right\}$ for a positive constant μ_1 and $\delta \in (0,\frac{1}{4})$. Let $\ell_f = (f-f^*)^2$. Suppose the target function satisfies $f^* \in \mathcal{H}_{\mathbf{X}_n,r_0,\delta}(\mu_0)$ with $r_0 \in [n]$ and μ_0 is a positive constant. Then for every $x>0$, with probability at least $1-2\delta-2\exp\left(\frac{-r_0}{2\sigma^2}\right)-2\exp(-x)$,

$$\begin{aligned} \mathcal{U}_{\ell_{f_{\hat{\mathbf{u}}}}}(\mathbf{Z_d}) \le{}& \left(1+\frac{1}{C}\right)\left(2+\frac{6x}{C}\right)\left(2\zeta_{n,r_0,\delta} + \frac{2r_0(\sigma+1)^2}{n}\right) + \frac{c_2 x}{u} \\ &+ c_1 c_3 r_0\left(\frac{1}{u}+\frac{1}{m}\right) + c_1 c_4\sqrt{\zeta_{n,r_0,\delta}\, r_0}\left(\frac{1}{\sqrt{2u}}+\frac{1}{\sqrt{2m}}\right), \end{aligned} \tag{69}$$

where $c_1 = 3200$, $c_2 = (128H_0 + 12H_0 C)/C^3$, $c_3 = 128\tau_0^2\bar{\mu}^2$, $c_4 = 16\tau_0\bar{\mu}$, $H_0 = 4\bar{\mu}^2\tau_0^2$, and

$\bar{\mu} = \max\left\{\sqrt{2\mu_0^2+\mu_1}, \mu_0\right\}$ with μ_1 being a positive constant.

Proof of Theorem B.6. Let $f_{\mathbf{u}} = \sum_{i=1}^n K(\cdot, \vec{\mathbf{x}}_i)\mathbf{u}_i$ for $\mathbf{u} \in \mathbb{R}^n$ and $\mathbf{u} \in \mathrm{Span}(\mathbf{U}^{(r_0)})$ such that

$$\|f_{\mathbf{u}}\|_{\mathcal{H}_k} = \sqrt{\mathbf{u}^\top \mathbf{K}\mathbf{u}} \le \bar{\mu}, \tag{70}$$

Then $f_{\mathbf{u}} \in \mathcal{H}_{\mathbf{X}_n, r_0}$. Since $f^* \in \mathcal{H}_{\mathbf{X}_n, r_0, \delta}(\mu_0)$, it follows by (16) in Theorem 3.6 that with probability at least $1-\delta-\exp(-x)$, for any f that satisfies (70), we have

$$\mathcal{U}(\ell_{f_{\mathbf{u}}}) \le \left(1+\frac{1}{C}\right)\mathcal{L}^{(m)}_{\ell_{f_{\mathbf{u}}}}(\mathbf{Z_d}) + \frac{c_2 x}{u} + c_1 c_3 r_0\left(\frac{1}{u}+\frac{1}{m}\right) + c_1 c_4\sqrt{\zeta_{n,r_0,\delta} r_0}\left(\frac{1}{\sqrt{2u}}+\frac{1}{\sqrt{2m}}\right), \tag{71}$$

where $\mathcal{L}^{(m)}_{\ell_{f_{\mathbf{u}}}}(\mathbf{Z_d}) = \frac{1}{m}\left\|[\mathbf{K}\mathbf{u} - f^*(\mathbf{X}_n)]_{\overline{\mathbf{Z_d}}}\right\|_2^2$. Note that (71) holds for $\mathbf{u} = \widehat{\mathbf{u}}$.

Let $\tilde{\mathbf{u}}^*$ be an optimal solution to the following surrogate TNKR problem:

$$\tilde{\mathbf{u}}^* = \operatorname*{arg\,min}_{\mathbf{u}\in\mathbb{R}^n} \frac{1}{2n}\left\|\mathbf{K}\mathbf{u} - \mathbf{U}^{(r_0)}{\mathbf{U}^{(r_0)}}^\top \mathbf{y}\right\|_2^2.$$

It follows by Lemma B.7 that with probability at least $1-2\delta-2\exp\left(\frac{-r_0}{2\sigma^2}\right)-\exp(-x)$,

$$\mathcal{L}^{(m)}_{\ell_{f_{\tilde{\mathbf{u}}^*}}}(\mathbf{Z_d}) \le \left(2+\frac{6x}{C}\right)\left(2\zeta_{n,r_0,\delta} + \frac{2r_0(\sigma+1)^2}{n}\right),$$

and $\|f_{\tilde{\mathbf{u}}^*}\|_{\mathcal{H}_K} = \sqrt{(\tilde{\mathbf{u}}^*)^\top \mathbf{K}\tilde{\mathbf{u}}^*} \le \bar{\mu}$ due to the given condition on n. Moreover, $\mathbf{K}\tilde{\mathbf{u}}^* = \mathbf{K}^{(r_0)}\tilde{\mathbf{u}}^*$. Therefore, by the optimality of $\widehat{\mathbf{u}}$, we have

$$\mathcal{L}^{(m)}_{\ell_{f_{\widehat{\mathbf{u}}}}}(\mathbf{Z_d}) \le \mathcal{L}^{(m)}_{\ell_{f_{\tilde{\mathbf{u}}^*}}}(\mathbf{Z_d}) \le \left(2+\frac{6x}{C}\right)\left(2\zeta_{n,r_0,\delta} + \frac{2r_0(\sigma+1)^2}{n}\right). \tag{72}$$

Then (69) follows by (71) and (72).

□

Lemma B.7. Let $\tilde{\mathbf{u}}^*$ be an optimal solution to the following surrogate TNKR problem (73), that is,

$$\tilde{\mathbf{u}}^* = \operatorname*{arg\,min}_{\mathbf{u}\in\mathbb{R}^n} \frac{1}{2n}\left\|\mathbf{K}\mathbf{u} - \mathbf{U}^{(r_0)}{\mathbf{U}^{(r_0)}}^\top \mathbf{y}\right\|_2^2. \tag{73}$$

Suppose $n > \frac{32\tau_0^4 \log\frac{2}{\delta}}{\lambda_{r_0}^2}$, then for any $x>0$, $\delta \in (0, \frac{1}{4})$, with probability at least $1-2\delta-2\exp\left(\frac{-r_0}{2\sigma^2}\right)-\exp(-x)$, the following inequalities hold:

$$\frac{1}{m}\left\|[\mathbf{K}\tilde{\mathbf{u}}^* - f^*(\mathbf{X}_n)]_{\mathbf{Z_d}(1:m)}\right\|_2^2 \le \left(2+\frac{6x}{C}\right)\left(2\zeta_{n,r_0,\delta} + \frac{2r_0(\sigma+1)^2}{n}\right), \tag{74}$$

$$(\tilde{\mathbf{u}}^*)^\top \mathbf{K}\tilde{\mathbf{u}}^* \le 2\mu_0^2 + \frac{4r_0(\sigma+1)^2}{n\lambda_{r_0}}, \tag{75}$$

where $\zeta_{n,r_0,\delta} = \widehat{\lambda}_{r_0+1}\zeta_{n,\delta}$.

Proof. It follows by Lemma B.8 that with high probability,

$$\frac{1}{n}\|\mathbf{K}\tilde{\mathbf{u}}^* - f^*(\mathbf{X}_n)\|_2^2 \le 2\zeta_{n,r_0,\delta} + \frac{2r_0(\sigma+1)^2}{n}. \tag{76}$$

Define $\mathbf{L}^{(\tilde{\mathbf{u}}^*)} \in \mathbb{R}^n$ with $\mathbf{L}_i^{(\tilde{\mathbf{u}}^*)} = [\mathbf{K}\tilde{\mathbf{u}}^* - f^*(\mathbf{X}_n)]_i^2$. It then follows by Lemma B.9 that with probability at least $1-\exp(-x)$,

$$\begin{aligned}\frac{1}{m}\left[\mathbf{L}_{\tilde{\mathbf{u}}^*}\right]_{\mathbf{Z_d}(1:m)} &\overset{①}{\le} \frac{2}{n}\left\|\mathbf{K}^{(r_0)} - f^*(\mathbf{X}_n)\right\|_2^2 + \frac{6H_0 x}{m} \\ &\overset{②}{\le} \left(2+\frac{6x}{C}\right)\left(2\zeta_{n,r_0,\delta} + \frac{2r_0(\sigma+1)^2}{n}\right)\end{aligned} \tag{77}$$

where ① follows by Lemma B.9 and $H_0 = \max_{i\in[n]} \mathbf{L}_i^{(\tilde{\mathbf{u}}^*)} \le 2n\zeta_{n,r_0,\delta} + 2r_0(\sigma+1)^2$ according to (76). ② follows by (76) the aforementioned bound for H_0, and $m \ge Cn$.

We also have $\tilde{\mathbf{u}}^* = \mathbf{K}^{-1}\mathbf{U}^{(r_0)}\mathbf{U}^{(r_0)\top}\mathbf{y}$, so that with probability at least $1-\delta$,

$$\begin{aligned}\left(\tilde{\mathbf{u}}^*\right)^\top \mathbf{K}\tilde{\mathbf{u}} &= \left(f^*(\mathbf{X}_n)+\boldsymbol{\varepsilon}\right)^\top \mathbf{U}^{(r_0)}\mathbf{U}^{(r_0)\top}\mathbf{K}^{-1}\mathbf{U}^{(r_0)}\mathbf{U}^{(r_0)\top}\left(f^*(\mathbf{X}_n)+\boldsymbol{\varepsilon}\right) \\ &\overset{①}{\le} 2\sum_{i=1}^{r_0}\frac{\left[\mathbf{U}^{(r_0)\top} f^*(\mathbf{X}_n)\right]_i^2}{n\widehat{\lambda}_i} + 2\sum_{i=1}^{r_0}\frac{\left[\mathbf{U}^{(r_0)\top}\boldsymbol{\varepsilon}\right]_i^2}{n\widehat{\lambda}_i} \\ &\overset{②}{\le} 2\mu_0^2 + 2\left\|\boldsymbol{\varepsilon}^{(r_0)}\right\|_2^2 \cdot \frac{1}{n\left(\lambda_{r_0} - \sqrt{\frac{8\tau_0^4\log\frac{2}{\delta}}{n}}\right)} \\ &\overset{③}{\le} 2\mu_0^2 + \frac{4r_0(\sigma+1)^2}{n\lambda_{r_0}}.\end{aligned} \tag{78}$$

Here ① follows by the Cauchy-Schwarz inequality. ② follows by Lemma B.11 and Lemma B.10. ③ follows by the bound for $\boldsymbol{\varepsilon}^{(r_0)} = \mathbf{U}^{(r_0)}\mathbf{U}^{(r_0)\top}\boldsymbol{\varepsilon}$ in (82) and $n > \frac{32\tau_0^4\log\frac{2}{\delta}}{\lambda_{r_0}^2}$.

□

Lemma B.8. Let $\tilde{\mathbf{u}}^*$ be an optimal solution to (73). For any $\delta \in (0,1)$, with probability at least $1-\delta-2\exp\left(-\frac{r_0}{2\sigma^2}\right)$,

$$\frac{1}{n}\|\mathbf{K}\tilde{\mathbf{u}}^* - f^*(\mathbf{X}_n)\|_2^2 \le 2\zeta_{n,r_0,\delta} + \frac{2r_0(\sigma+1)^2}{n}, \tag{79}$$

where $\zeta_{n,r_0,\delta} = \widehat{\lambda}_{r_0+1}\zeta_{n,\delta}$.

Proof. It can be verified that $\mathbf{K}^{(r_0)}\tilde{\mathbf{u}}^*$ is the orthogonal projection of $\mathbf{y}$ onto the column space of $\mathbf{U}^{(r_0)}$, that is,

$$\mathbf{K}\tilde{\mathbf{u}}^* = \mathbf{U}^{(r_0)}\mathbf{U}^{(r_0)\top} f^*(\mathbf{X}_n) + \mathbf{U}^{(r_0)}\mathbf{U}^{(r_0)\top}\boldsymbol{\varepsilon}.$$

As a result, we have

$$\mathbf{K}\tilde{\mathbf{u}}^* - f^*(\mathbf{X}_n) \overset{①}{=} \mathbf{U}^{(-r_0)}\mathbf{U}^{(-r_0)\top} f^*(\mathbf{X}_n) + \boldsymbol{\varepsilon}^{(r_0)},$$

where in ① $\mathbf{U}^{(-r_0)} \in \mathbb{R}^{n \times (n-r_0)}$ is the submatrix formed by all the columns of $\mathbf{U}$ except for the top r_0 columns in $\mathbf{U}^{(r_0)}$, and $\boldsymbol{\varepsilon}^{(r_0)} = \mathbf{U}^{(r_0)} {\mathbf{U}^{(r_0)}}^\top \boldsymbol{\varepsilon}$. It then follows by Cauchy-Schwarz inequality that

$$\left\|\mathbf{K}\tilde{\mathbf{u}}^* - f^*(\mathbf{X}_n)\right\|_2^2 \le 2\left\|\mathbf{U}^{(-r_0)} {\mathbf{U}^{(-r_0)}}^\top f^*(\mathbf{X}_n)\right\|_2^2 + 2\left\|\boldsymbol{\varepsilon}^{(r_0)}\right\|_2^2. \tag{80}$$

Note that

$$\begin{aligned}
&\mathbb{P}_{\mathcal{H}_{\mathbf{X}_n}}(f^*) = \sum_{k=1}^{n} \left\langle f^*, \Phi^{(k)} \right\rangle \Phi^{(k)}, \\
&\mathbb{P}_{\mathcal{H}_{\mathbf{X}_n, r_0}}(f^*) = \sum_{k=1}^{r_0} \left\langle f^*, \Phi^{(k)} \right\rangle \Phi^{(k)}, \\
&\mathbf{U}^{(-r_0)} {\mathbf{U}^{(-r_0)}}^\top \Phi^{(k)}(\mathbf{X}_n) = 0, \forall k \in [r_0].
\end{aligned}$$

As a result, define $\bar{f}^{*,r_0} := f^* - \mathbb{P}_{\mathcal{H}_{\mathbf{X}_n, r_0}}(f^*)$, we have that with probability at least $1-\delta$,

$$\frac{1}{n}\left\|\mathbf{U}^{(-r_0)} {\mathbf{U}^{(-r_0)}}^\top f^*(\mathbf{X}_n)\right\|_2^2 \le \frac{1}{n}\sum_{i=1}^{n}\left(\bar{f}^{*,r_0}(\vec{\mathbf{x}}_i)\right)^2 \overset{①}{\le} \zeta_{n,r_0,\delta}, \tag{81}$$

Here ① follows by (57)- (58) in the proof of Theorem 3.6, and $\zeta_{n,r_0,\delta} = \widehat{\lambda}_{r_0+1}\zeta_{n,\delta}$.

We consider the function $g(\boldsymbol{\varepsilon}) := \left\|\boldsymbol{\varepsilon}^{(r_0)}\right\|_2 = \left\|\mathbf{U}^{(r_0)} {\mathbf{U}^{(r_0)}}^\top \boldsymbol{\varepsilon}\right\|_2$ which is a Lipschitz continuous with the Lipschitz constant being 1. Due to the standard Gaussian concentration inequality for Lipschitz functions [16], for all $\bar{t} > 0$,

$$\Pr\left[\left|\left\|\boldsymbol{\varepsilon}^{(r_0)}\right\|_2 - \mathbb{E}\left[\left\|\boldsymbol{\varepsilon}^{(r_0)}\right\|_2\right]\right| > \bar{t}\right] \le 2e^{-\frac{\bar{t}^2}{2\sigma^2}}, \tag{82}$$

and $\mathbb{E}\left[\left\|\boldsymbol{\varepsilon}^{(r_0)}\right\|_2\right] \le \sqrt{\mathbb{E}\left[\left\|\boldsymbol{\varepsilon}^{(r_0)}\right\|_2^2\right]} = \sqrt{r_0}\sigma$. Therefore, $\Pr\left[\left\|\boldsymbol{\varepsilon}^{(r_0)}\right\|_2 - \sqrt{r_0}\sigma > \bar{t}\right] \le 2e^{-\frac{\bar{t}^2}{2\sigma^2}}$. Then (79) follows by setting $\bar{t} = \sqrt{r_0}$ in the above inequality, (80), (81), and (82).

□

We now provide the following lemma showing that the empirical loss $\mathcal{L}_h^{(m)}(\mathbf{Z}_\mathbf{d})$ is upper bounded by a constant factor of its expectation, $\mathbb{E}_d\left[\mathcal{L}_h^{(m)}(\mathbf{Z}_\mathbf{d})\right] = \mathcal{L}_n(h)$.

Lemma B.9. Given any function h defined on $\mathcal{X} \times \mathcal{Y}$ with $0 \le h(i) := h(\vec{\mathbf{x}}_i, y_i) \le H_0$ for all $i \in [n]$. Then for every $x > 0$,

$$\Pr\left[\mathcal{L}_h^{(m)}(\mathbf{Z}_\mathbf{d}) \le 2\mathcal{L}_n(h) + \frac{6H_0 x}{m}\right] \ge 1 - \exp(-x). \tag{83}$$

Proof. Given a function h, define $g(\mathbf{d}) = \mathcal{L}_h^{(m)}(\overline{\mathbf{Z}_\mathbf{d}})$, and let $\mathbf{d}' = [d_1', \ldots, d_m']$ be independent copies of $\mathbf{d} = [d_1, \ldots, d_m]$, and $\mathbf{d}^{(i)} := [d_1, \ldots, d_{i-1}, d_i', d_{i+1}, \ldots, d_m]$.

Let

$$V_+ := \mathbb{E}\left[\sum_{i=1}^{m}\left(g(\mathbf{d}) - g(\mathbf{d}^{(i)})\right)^2 \mathrm{I\!I}_{\left\{g(\mathbf{d}) > g(\mathbf{d}^{(i)})\right\}} \middle| \mathbf{d}\right].$$

It follows by Lemma B.1 and the argument in Lemma B.2 that

$$V_+ \le \frac{2H_0}{m} g(\mathbf{d}). \tag{84}$$

It follows by Theorem A.1 that

$$\Pr\left[g(\mathbf{d}) \le \mathbb{E}_{\mathbf{d}}\left[g(\mathbf{d})\right] + \inf_{\alpha>0}\left(\left(2+\frac{1}{\alpha}\right)\frac{2H_0 x}{m} + \alpha \mathbb{E}_{\mathbf{d}}\left[g(\mathbf{d})\right]\right)\right] \ge 1-\exp(-x),$$

which proves (83) with $\alpha = 1$.

□

Lemma B.10. [[17, Proposition 10]] Let $\delta \in (0,1)$, then with probability $1-\delta$ over the full sample $\mathbf{X}_n$, for all $j \in [n]$,

$$\left|\lambda_j - \widehat{\lambda}_j\right| \le \sqrt{\frac{8\tau_0^4 \log \frac{2}{\delta}}{n}}. \tag{85}$$

Lemma B.11 (In the proof of [18, Lemma 8])**.** For any $f \in \mathcal{H}_K(\mu_0)$, we have

$$\frac{1}{n}\sum_{i=1}^{n} \frac{\left[\mathbf{U}^\top f(\mathbf{X}_n)\right]_i^2}{\widehat{\lambda}_i} \le \mu_0^2, \tag{86}$$

where $\mathbf{K} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{U}^\top$ is the eigendecomposition of the gram matrix $\mathbf{K}$ of the kernel K on the full sample $\mathbf{X}_n$.

Lemma B.12. Let $\sup_{\mathbf{x}\in\mathcal{X}} K(\mathbf{x},\mathbf{x}) = \tau_0^2$. For any $\delta \in (0,1)$, with probability at least $1-\delta$ over the full sample $\mathbf{X}_n$,

$$\sum_{i>m_{k_0}} \sum_{j=1}^{m_{k_0}} \left\langle \Phi^{(i)}, v_j \right\rangle_{\mathcal{H}}^2 \le \frac{8\tau_0^4 \log \frac{2}{\delta}}{\left(\lambda_{m_{k_0}} - \lambda_{m_{k_0}+1}\right)^2 n}. \tag{87}$$

Proof. Define operator $T_n \colon \mathcal{H}_K \to \mathcal{H}_K$ by $T_n g = \frac{1}{n}\sum_{i=1}^{n} K(\cdot, \vec{\mathbf{x}}_i) g(\vec{\mathbf{x}}_i)$, and let $\left\{\Phi^{(k)}\right\}_{k\ge1}$ be an orthonormal basis of the RKHS $\mathcal{H}_K$.

Let P_N^T be an orthogonal projection operator which projects any input onto the subspace spanned by eigenfunctions corresponding to the top N eigenvalues of the operator T, and T is defined on the RKHS $\mathcal{H}$.

We now work on the following two orthogonal projection operators, $P_{m_{k_0}}^{T_{\mathcal{H}}}$ and $P_{m_{k_0}}^{T_n}$. Each of the two operators projects its input onto the space spanned by all the eigenfunctions of the corresponding operator, that is.

$$P_{m_{k_0}}^{T_{\mathcal{H}}} h = \sum_{j=1}^{m_{k_0}} \langle h, v_j\rangle_{\mathcal{H}} v_j, \quad P_{m_{k_0}}^{T_n} h = \sum_{j=1}^{m_{k_0}} \left\langle h, \Phi^{(j)}\right\rangle_{\mathcal{H}} \Phi^{(j)}. \tag{88}$$

The Hilbert-Schmidt norm of $P_{m_{k_0}}^{T_{\mathcal{H}}} - P_{m_{k_0}}^{T_n}$ is

$$\left\| P_{m_{k_0}}^{T_{\mathcal{H}}} - P_{m_{k_0}}^{T_n} \right\|_{\mathrm{HS}}^2 = \sum_{i\geq 1, j\geq 1} \left\langle \left(P_{m_{k_0}}^{T_{\mathcal{H}}} - P_{m_{k_0}}^{T_n} \right) \Phi^{(i)}, v_j \right\rangle_{\mathcal{H}}^2, \tag{89}$$

which is due to the fact that both $\left\{\Phi^{(j)}\right\}_{j\geq 1}$ and $\{v_j\}_{j\geq 1}$ are orthonormal bases of $\mathcal{H}$. It can be verified that

$$\left\langle \left(P_{m_{k_0}}^{T_{\mathcal{H}}} - P_{m_{k_0}}^{T_n} \right) \Phi^{(i)}, v_j \right\rangle_{\mathcal{H}} = \begin{cases} 0 & \text{if } i \in [m_{k_0}], j \in [m_{k_0}], \\ \left\langle \Phi^{(i)}, v_j \right\rangle_{\mathcal{H}} & \text{if } i \in [m_{k_0}], j > m_{k_0} \\ -\left\langle \Phi^{(i)}, v_j \right\rangle_{\mathcal{H}} & \text{if } i > m_{k_0}, j \in [m_{k_0}] \\ 0 & \text{if } i > m_{k_0}, j > m_{k_0}, \end{cases} \tag{90}$$

and similar results are obtained in the proof of [17, Theorem 12].

Because $T_{\mathcal{H}}$ and T_n are Hilbert-Schmidt operators, by [17, Theorem 7], for all $\delta \in (0,1)$, with probability at least $1-\delta$,

$$\| T_{\mathcal{H}} - T_n \|_{\mathrm{HS}} \leq \frac{2\sqrt{2}\tau_0^2 \sqrt{\log \frac{2}{\delta}}}{\sqrt{n}}. \tag{91}$$

When $n \geq \frac{128\tau_0^4 \log \frac{2}{\delta}}{\left(\lambda_{m_{k_0}} - \lambda_{m_{k_0}+1}\right)^2}$, $\| T_{\mathcal{H}} - T_n \|_{\mathrm{HS}} \leq \frac{\lambda_{m_{k_0}} - \lambda_{m_{k_0}+1}}{4}$. By [17, Proposition 6] (noting that the operator norm in Proposition 6 can be replaced by the Hilbert-Schmidt norm),

$$\begin{aligned} \left\| P_{m_{k_0}}^{T_{\mathcal{H}}} - P_{m_{k_0}}^{T_n} \right\|_{\mathrm{HS}}^2 &\leq \frac{4}{\left(\lambda_{m_{k_0}} - \lambda_{m_{k_0}+1}\right)^2} \| T_{\mathcal{H}} - T_n \|_{\mathrm{HS}}^2 \\ &\overset{(91)}{\leq} \frac{8\tau_0^4 \log \frac{2}{\delta}}{\left(\lambda_{m_{k_0}} - \lambda_{m_{k_0}+1}\right)^2 n}. \end{aligned} \tag{92}$$

It follows by (89), (90), and (92) that

$$\sum_{i > m_{k_0}} \sum_{j=1}^{m_{k_0}} \left\langle \Phi^{(i)}, v_j \right\rangle_{\mathcal{H}}^2 \leq \left\| P_{m_{k_0}}^{T_{\mathcal{H}}} - P_{m_{k_0}}^{T_n} \right\|_{\mathrm{HS}}^2 \leq \frac{8\tau_0^4 \log \frac{2}{\delta}}{\left(\lambda_{m_{k_0}} - \lambda_{m_{k_0}+1}\right)^2 n}. \tag{93}$$

□

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