Analysis of Least Squares Regularized Regression in Reproducing Kernel Kreîn Spaces

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Abstract

In this paper, we study the asymptotical properties of least squares regularized regression with indefinite kernels in reproducing kernel Kreîn spaces (RKKS). The classical approximation analysis cannot be directly applied to study its asymptotical behavior under the framework of learning theory as this problem is in essence non-convex and outputs stationary points. By introducing a bounded hyper-sphere constraint to such non-convex regularized risk minimization problem, we theoretically demonstrate that this problem has a globally optimal solution with a closed form on the sphere, which makes our approximation analysis feasible in RKKS. Accordingly, we modify traditional error decomposition techniques, prove convergence results for the introduced hypothesis error based on matrix perturbation theory, and derive learning rates of such regularized regression problem in RKKS. Under some conditions, the derived learning rates in RKKS are the same as that in reproducing kernel Hilbert spaces (RKHS), which is actually the first work on approximation analysis of regularized learning algorithms in RKKS.

Key words: learning theory, approximation analysis, regularized kernel regression, Kreîn spaces

1 Introduction

The aim of this paper is to study learning rates of the regularized risk minimization problem in a reproducing kernel Kreîn space (RKKS) [1], [2], [3], which are vector spaces with an indefinite bilinear form [4], [5]. This problem stems from indefinite (real, symmetric, but not positive definite) kernel-based algorithms [6], [2], [3] in machine learning due to intrinsic and extrinsic factors. Here, intrinsic means that we often meet some indefinite kernels such as tanh kernel [7], TL1 kernel [8], and log kernel [9]. Meanwhile, extrinsic indicates that some positive definite (PD) kernels degenerate to indefinite ones in some cases. An intuitive example is that a linear combination of PD kernels [10] may result in an indefinite one. Polynomial kernels on the unit sphere are not always PD [11]. We refer to a survey [12] for details.

Nevertheless, in learning theory, the asymptotical behavior of these regularized indefinite kernel learning based algorithms in RKKS has not been fully investigated. Let $X$ be a compact metric space and $Y \subseteq \mathbb{R}$, we assume that a sample set $z = \{(x_i, y_i)\}_{i=1}^m \in Z^m$ is drawn from a non-degenerate Borel probability measure $\rho$ on $X \times Y$. In the context of statistical learning theory, the target function of $\rho$ is defined by $f_\rho(x) = \int_Y y d\rho(y|x), x \in X$, where $\rho(\cdot|x)$ is the conditional distribution of $\rho$ at $x \in X$. The goal of a supervised learning task defined with a bounded, symmetric, and indefinite kernel function $k : X \times X \to \mathbb{R}$ and its associated RKKS $\mathcal{H}_k$ is to find a hypothesis $f : X \to Y$ such that $f(x)$ is a good approximation of the label $y \in Y$ corresponding to...
where the considered constraint set is defined as $B$. Hence the empirical risk minimization problem in RKKS [1], [2] is defined as

$$f_{x,\lambda} := \arg\min_{f \in \mathcal{H}_K \cap \mathcal{C}(f, X)} \left\{ \frac{1}{m} \sum_{i=1}^{m} \ell(f(x_i), y_i) + \lambda(f, f)_{\mathcal{H}_K} \right\},$$

(1)

where $\mathcal{C}(f, X)$ denotes a constraint set on $f$ in RKKS. The convex loss $\ell$ quantifies the merit of the evaluation $f(x)$ at $x \in X$. The regularizer is given by the inner product $\langle f, f \rangle_{\mathcal{H}_K}$ associated with a (reproducing) indefinite kernel in RKKS [1], [2], [13]. This regularization mechanism aims to understand the learning behavior in RKKS and avoid the inconsistency when using various regularizers spanned by different spaces, see [2], [14] for details. In learning theory, the parameter $\lambda$ depends on the sample size $\lambda := \lambda(m)$ with $\lim_{m \to \infty} \lambda(m) = 0$. Mathematically, we assume $\lambda = m^{-\gamma}$ with $\gamma \in (0, 1]$.

For classical learning problems in the reproducing kernel Hilbert space (RKHS) $\mathcal{H}$, there has been a large number of literature on approximation analysis and generalization error under the regularization scheme $\langle f, f \rangle_{\mathcal{H}_K}$, see [15], [16], [17] and references therein. However, analysis in RKHS cannot be directly applied to the above regularized risk minimization problems in RKKS due to the following two reasons. First, approximation analysis in RKHS requires a globally optimal solution yielded by learning algorithms. Since the optimization problem in RKKS is in essence non-convex, most indefinite kernel learning based algorithms just output stationary points [5], [2]. In this case, traditional concentration estimates in RKHS are invalid due to an unattainable optimal solution. Second, in Krein spaces, the inner product $\langle f, f \rangle_{\mathcal{H}_K}$ might be negative, which would fail to quantify complexity of a hypothesis. In this case, the excess error in RKKS can not be bounded by the sample error and the regularization error when using the classical error decomposition technique [18], which is not suitable for our analysis in RKKS.

To overcome the mentioned essential problems for analyzing the asymptotic properties in RKKS, we consider the least squares regularized regression problem given by the RKKS regularization scheme in Eq. (1)

$$f_{x,\lambda} := \arg\min_{f \in B(r)} \left\{ \frac{1}{m} \sum_{i=1}^{m} (f(x_i) - y_i)^2 + \lambda(f, f)_{\mathcal{H}_K} \right\},$$

(2)

where the considered constraint set is defined as $B(r) := \{ f \in \mathcal{H}_K : \frac{1}{m} \sum_{i=1}^{m} (f(x_i))^2 \leq r^2 \}$ is a bounded hyper-sphere, which is similarly given by [19], [3] to prohibit the objective function value in problem (2) approaches to $-\infty$. Adding this bounded constraint still preserves the specifics of learning in RKKS, i.e., there are still points in $B(r)$ with $\langle f, f \rangle_{\mathcal{H}_K} < 0$. The solution of problem (2) without any constraint is the result of a stabilization procedure [5], [2]. If a hyper-spherical equality constraint is added, Oglic and Gaertner [19] demonstrate that the learning problem can be expressed as the minimization of a quadratic form over a hypersphere of constant radius, and thus yields a globally optimal solution with promising generalization performance. This nice result motivates us to obtain the first-step to understand the learning behavior in RKKS.

To determine the radius $r$ of the spherical constraint, in practical algorithms, $r$ is often chosen by cross validation or hyper-parameter optimization [19]. In a theoretical sense, this spherical inequality constraint is naturally needed and common in classical approximation analysis in RKHS [16], [18], [17]. This is because, assuming the existence of $f_\rho$ implies that $f_\rho$ belongs to a ball of radius $r_{\rho,\mathcal{H}_K}$ [20]. The radius $r$ can be given by an iterative technique [16], [21], [22] that estimates the bound for $\|f_{x,\lambda}\|$ in some Hilbert spaces, and thus our analysis will employ this scheme to determine it. In our analysis, it can be lower bounded to avoid failing to zero. Besides, the upper bound of the selected radius varies with $m$ and thus it can consider a wide range of RKKS.

Formally, we study learning rates of least squares regularized regression in RKKS. The main purpose of this paper is to provide a detailed error analysis for problem (2), and then derive its
learning rates. To be specific, we demonstrate that the inequality constraint in problem (2) can be equivalently substituted by an equality constraint. In this case, albeit non-convex, problem (2) with a spherical equality constraint has a global minimum with a closed form as demonstrated by [19], see Section 3 for details. We start the analysis from the regularized algorithm (2) that has an analytical solution and obtain the first-step to understand the learning behavior in RKKS. To aid our proof, we introduce another \( \langle f, T f \rangle_{\mathcal{H}_K} \) regularization scheme with the empirical covariance operator \( T \) [23] in RKKS. By modifying the traditional error decomposition approach, the excess error can be bounded by the sample error, the regularization error, and the introduced hypothesis error. Then we attempt to bound the additional hypothesis error yielded by two such regularizers, which is based on matrix perturbation theory for non-Hermitian and non-diagonalizable matrices. The revised error decomposition technique and estimates for the hypothesis error are the main elements on novelty in our proof. Our analysis is able to bridge the gap between the least squares regularized regression problem in RKHS and RKKS. Under some conditions, the derived learning rates in RKKS is the same as that in RKHS (the best case). To the best of our knowledge, this is the first work to study learning rates of regularized risk minimization problems in RKKS.

The rest of the paper is organized as follows. We briefly review Kreın spaces and RKKS in Section 2. In Section 3, we present the least squares regularized regression model in RKKS and give a globally optimal solution. The main results on approximation analysis are given in Section 4. In Section 5, we give the framework of convergence analysis for the modified error decomposition technique, detail the estimates for the introduced hypothesis error, and derive the learning rates. In Section 6, we report numerical experiments to demonstrate our theoretical results and the conclusion is drawn in Section 7.

2 Preliminaries

In this section, we briefly review Kreın spaces and the reproducing kernel Kreın space (RKKS) [24]. Kreın spaces are indefinite inner product spaces endowed with a Hilbertian topology.

**Definition 1. (Kreın space [24])** An inner product space \( \mathcal{H}_K \) is a Kreın space if there exist two Hilbert spaces \( \mathcal{H}_+ \) and \( \mathcal{H}_- \) such that

1) All \( f \in \mathcal{H}_K \) can be decomposed into \( f = f_+ + f_- \), where \( f_+ \in \mathcal{H}_+ \) and \( f_- \in \mathcal{H}_- \), respectively.
2) \( \forall f, g \in \mathcal{H}_K, \langle f, g \rangle_{\mathcal{H}_K} = \langle f_+, g_+ \rangle_{\mathcal{H}_+} - \langle f_-, g_- \rangle_{\mathcal{H}_-} \).

For \( f \in \mathcal{H}_K \), if \( \langle f, g \rangle_{\mathcal{H}_K} = 0 \) for any \( g \in \mathcal{H}_K \) implies that \( f = 0 \). From the definition, the decomposition \( \mathcal{H}_K = \mathcal{H}_+ + \mathcal{H}_- \) is not necessarily unique. For a fixed decomposition, the inner product \( \langle f, g \rangle_{\mathcal{H}_K} \) is given accordingly [2], [19]. The key difference with Hilbert spaces is that the inner products might be negative for Kreın spaces, i.e., there exists \( f \in \mathcal{H}_K \) such that \( \langle f, f \rangle_{\mathcal{H}_K} < 0 \). If \( \mathcal{H}_+ \) and \( \mathcal{H}_- \) are two RKHSs, the Kreın space \( \mathcal{H}_K \) is a RKKS associated with a unique indefinite reproducing kernel \( k \) such that the reproducing property holds, i.e., \( \forall f \in \mathcal{H}_K, f(x) = \langle f, k(x, \cdot) \rangle_{\mathcal{H}_K} \).

**Proposition 1.** (positive decomposition [24]) An indefinite kernel \( k \) associated with a RKKS admits a positive decomposition \( k = k_+ - k_- \), with two positive definite kernels \( k_+ \) and \( k_- \).

Typical examples include a wide range of commonly used indefinite kernels, such as a linear combination of PD kernels [10], and conditionally PD kernels [25], [26].

**Definition 2. (Associated RKHS of RKKS [1])** Let \( \mathcal{H}_K \) be a RKKS with decomposition into two RKHSs \( \mathcal{H}_+ \) and \( \mathcal{H}_- \). Then \( \forall f, g \in \mathcal{H}_K \), the associated Hilbert space \( \mathcal{H}_K \) is defined as

\[ \mathcal{H}_K = \mathcal{H}_+ \oplus \mathcal{H}_- \text{, and } \langle f, g \rangle_{\mathcal{H}_K} = \langle f_+, g_+ \rangle_{\mathcal{H}_+} + \langle f_-, g_- \rangle_{\mathcal{H}_-}. \]

Note that \( \mathcal{H}_K \) is the smallest Hilbert space majorizing the RKKS \( \mathcal{H}_K \) with \( |\langle f, f \rangle_{\mathcal{H}_K}| \leq \|f\|_{\mathcal{H}_K}^2 = \|f_+\|_{\mathcal{H}_+}^2 + \|f_-\|_{\mathcal{H}_-}^2 \). Denote \( C(X) \) as the space of continuous functions on \( X \) with the norm \( \| \cdot \|_{\infty} \).
and suppose that \( \kappa := \sqrt{2} \sup_{x \in X} \sqrt{k_+(x, x) + k_-(x, x')} < \infty \). The reproducing property in RKKS indicates that \( \forall f \in \mathcal{H}_K \), we have
\[
\|f\|_\infty = \sup_{x \in X} |\langle f, k(x, \cdot) \rangle| \leq \kappa \|f\|_{\mathcal{H}_K}.
\]

**Definition 3.** (The empirical covariance operator in RKKS [23]) Let \( k \) be an indefinite kernel associated with a RKKS \( \mathcal{H}_K \), \( \psi : X \to \mathcal{H}_K \) be a mapping of the data in \( \mathcal{H}_K \) and \( \Psi = [\psi(x_1), \psi(x_2), \ldots, \psi(x_m)] \) be a sequence of images of the training data in \( \mathcal{H}_K \), then its empirical non-centered covariance operator \( T : \mathcal{H}_K \to \mathcal{H}_K \) is defined by
\[
T = \frac{1}{m} \Psi \Psi^*,
\]
which is not positive definite in the Hilbert sense, but it is in the Kreǐn sense satisfying \( \langle \zeta, T\zeta \rangle_{\mathcal{H}_K} \geq 0 \) for \( \zeta \neq 0 \).

The operator \( T \) actually depends on the sample set and it can be linked to an empirical kernel [27]. In our paper, we choose the mapping \( \psi(x) := k(x, \cdot) \) to obtain the empirical covariance operator \( T \). Since \( \langle f, Tf \rangle_{\mathcal{H}_K} \) is nonnegative, we use it as a regularizer to aid our proof.

### 3 Least Squares Regularized Regression Problem in RKKS

In this section, we aim to obtain a globally optimal solution to problem [2], and then provide another regularization scheme to aid our analysis.

#### 3.1 Eigenvalue Assumption of Indefinite Kernel Matrices

Let \( K = V \Sigma V^\top \) be the eigenvalue decomposition with the orthogonal matrix \( V \) and the diagonal matrix \( \Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_m) \). The spectrum of positive semi-definite (PSD) kernel matrix has been fully studied, but the eigenvalue assumption for indefinite \( K \) has not been investigated before. Actually, because of \( K = K_+ - K_- \) with two PSD matrices \( K_{\pm} \), we can easily make the assumption for \( K \) based on \( K_\pm \). Here we present the assumption for the spectrum of \( K \).

**Definition 4.** (Eigenvalue assumption) Assume that the indefinite kernel matrix \( K = V \Sigma V^\top \) has \( p \) positive eigenvalues, \( q \) negative eigenvalues, and \( m - p - q \) zero eigenvalues, i.e., \( \Sigma = \Sigma_+ + \Sigma_- \), where \( \Sigma_+ = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_p, 0, \ldots, 0) \), \( \Sigma_- = \text{diag}(0, \ldots, 0, \sigma_{m-q+1}, \ldots, \sigma_m) \) with the decreasing order \( \sigma_1 \geq \cdots \geq \sigma_p > 0 > \sigma_{m-q+1} \geq \cdots \geq \sigma_m \) and \( \sigma_{p+1} = \sigma_{p+2} = \cdots = \sigma_{m-q} = 0 \). Here we assume that its (positive) largest eigenvalue satisfies \( \sigma_1 \geq c_1 m^{\eta_1} \) with \( c_1 > 0 \), \( \eta_1 > 0 \) and its negative eigenvalue with the largest absolute value admits \( \sigma_m \leq c_m m^{\eta_2} \) with \( c_m < 0 \), \( \eta_2 > 0 \). And we denote \( \eta := \min\{\eta_1, \eta_2\} \).

Bach [28] considers three eigenvalue decays of a PSD kernel matrix, including i) the exponential decay \( \sigma_i \propto me^{-ci} \) with \( c > 0 \), ii) the polynomial decay \( \sigma_i \propto m^{-2t} \) with \( t \geq 1 \), and iii) the slowest decay with \( \sigma_i \propto m/i \). Hence, for an indefinite kernel matrix \( K \), we assume that its largest positive eigenvalue satisfies \( \sigma_1 \geq c_1 m^{\eta_1} \) with \( c_1 > 0 \), \( \eta_1 > 0 \). Besides, its negative eigenvalue with the largest absolute value \( \sigma_m \) also follows with this property, i.e., \( \sigma_m \leq c_m m^{\eta_2} \) with \( c_m < 0 \) and \( \eta_2 > 0 \). So our condition just considers the lower bound of \( \sigma_1 \) and the upper bound of \( \sigma_m \), which is a natural generalization of the above three decays. Note that the number of positive/negative eigenvalues depends on the training data, but our theoretical results will be independent of the unknown \( p \) and \( q \).

Here we take two kernels associated with RKKS as examples including the Delta-Gaussian kernel [19] and the log kernel [9] to validate our assumption. The Delta-Gaussian kernel is \( k(x, x') = \exp \left(-\|x - x'\|^2 / \tau_1 \right) - \exp \left(-\|x - x'\|^2 / \tau_2 \right) \) with two kernel widths \( \tau_1 \) and \( \tau_2 \). It is clear that \( \sigma_1 \) and \( \sigma_m \) follow with the exponential decay in the same rate, i.e., \( \eta_1 = \eta_2 \). For the log kernel
Theorem 1. Let $F$ be an optimal solution to problem (2), then $F$ admits the expansion $f_* = \sum_{i=1}^m \alpha_i k(x_i, \cdot)$ by the reproducing kernel $k$ with $\alpha_i \in \mathbb{R}$.

Proof. The proof is similar to Theorem 2 in [19]. For the sake of completeness, we present the proof in Appendix A.

By virtue of Theorem 1 problem (2) can be formulated as

$$\alpha_{z, \lambda} := \arg\min_{\alpha \in \mathbb{R}^m: \alpha^\top K^2 \alpha \leq m^2} \left\{ \frac{1}{m} \| K\alpha - y \|_2^2 + \lambda \alpha^\top K\alpha \right\},$$

(5)

where the output is $y = [y_1, y_2, \cdots, y_m]^\top$. We can see that the above regularized risk minimization problem is in essence non-convex due to the non-positive definiteness of $K$. But more exactly, problem (5) is non-convex when $\frac{1}{m} K^2 + \lambda K$ is indefinite. This condition always holds in practice due to $m \gg \lambda$. Following [19], we do not strictly distinguish between the two differences in this paper. This is because, approximation analysis considers the $m \rightarrow \infty$ case, so it always holds true when $m$ is large enough. If we consider a finite number $m$, suppose that the negative eigenvalue of $K$ satisfies exponential decay $\sigma_1 \propto -me^{-ct}$ with $c > \gamma/m \ln m$, the polynomial decay $\sigma_1 \propto -m^{-2t}$ with $t \geq 1$, or the slowest decay with $\sigma_1 \propto -m/i$, we can derive that $\frac{1}{m} K^2 + \lambda K$ is still indefinite. Even if $\frac{1}{m} K^2 + \lambda K$ is PSD, our analysis for problem (5) is still applicable and reduces to a special case (i.e., using a RKHS regularizer), of which the learning rates are demonstrated by Corollary 2.

To obtain a global minimum of problem (5), we need the following proposition.

Proposition 2. Problem (5) is equivalent to

$$\alpha_{z, \lambda} := \arg\min_{\alpha \in \mathbb{R}^m: \alpha^\top K^2 \alpha = m^2} \left\{ \frac{1}{m} \| K\alpha - y \|_2^2 + \lambda \alpha^\top K\alpha \right\}.$$

(6)

Proof. Denote the objective function in problem (5) as $F(\alpha) = \frac{1}{m} \| K\alpha - y \|_2^2 + \lambda \alpha^\top K\alpha$, we aim to prove that the solution $\alpha^* := \arg\min_{\alpha} F(\alpha)$ of this unconstrained optimization problem would be unbounded. Due to the non-positive definiteness of $\frac{1}{m} K^2 + \lambda K$, there exists an initial solution $\alpha_0$ such that

$$\alpha_0^\top \left( \frac{1}{m} K^2 + \lambda K \right) \alpha_0 < 0.$$

By constructing a solving sequence $\{ \alpha_i \}_{i=0}^\infty$ admitting $\alpha_{i+1} := c \alpha_i$ with $c > 1$, we have

$$F(c \alpha_{i+1}) - c F(\alpha_i) = c(c-1) \alpha_i^\top \left( \frac{1}{m} K^2 + \lambda K \right) \alpha_i - \frac{c-1}{m} \| y \|_2^2 < 0,$$

which indicates that, after the $t$-th iteration, $F(\alpha_i) < c^t F(\alpha_0) < 0$ and $\| \alpha_i \|_2 = c^t \| \alpha_0 \|_2$ with $c > 1$. Therefore, the minimum $F(\alpha^*)$ is unbounded, and tends to negative infinity. In this case, $\| \alpha^* \|_2$
would also approach to infinity, i.e., a meaningless solution. Based on the above analyses, for problem \( \min_{\alpha} F(\alpha) \), by introducing the constraint \( \alpha^\top K \alpha \leq m r^2 \), its solution is obtained on the hyper-sphere, i.e., \( \alpha^\top K \alpha = m r^2 \), which concludes the proof.

As demonstrated by Proposition \( \boxed{2} \), the inequality constraint in problem (5) can be transformed into an equality constraint, which is also suitable to problem (2). It can be found that, problem (6) is hidden convex \( \boxed{29} \) and strong duality holds. As a generalized trust-region subproblem, it can also be solved by the S-lemma with equality to yield a globally optimal solution \( \boxed{30}, \boxed{29} \). Also, this non-convex problem (6) can be formulated as solving a constrained eigenvalue problem \( \boxed{31}, \boxed{19} \) with a closed-form solution. Its optimal solution \( \alpha_{z,\lambda} \) with a closed form can be similarly obtained with \( \boxed{19} \), i.e.

\[
\alpha_{z,\lambda} = \frac{1}{m}(\lambda I - \mu K)^+ y,
\]

where the notation \((\cdot)^+\) denotes the pseudo-inverse, \( I \) is the identity matrix, and \( \mu \) is the smallest real eigenvalue of the matrix

\[
G = \begin{bmatrix}
\lambda K^+ & -I \\
-y y^\top/m^2 r^2 & \lambda K^+
\end{bmatrix},
\]

where \( K^+ \) is the pseudo-inverse of \( K \), i.e. \( K^+ = V \text{diag} (\Sigma_1, 0_{m-p-q}, \Sigma_2) V^\top \) with two invertible diagonal matrices

\[
\Sigma_1 = \text{diag} \left( \frac{\lambda}{\sigma_1}, \ldots, \frac{\lambda}{\sigma_p} \right), \quad \Sigma_2 = \text{diag} \left( \frac{\lambda}{\sigma_{m-q+1}}, \ldots, \frac{\lambda}{\sigma_m} \right).
\]

It is clear that we cannot directly calculate \( \mu \). However, \( \mu \) is very important in our analysis and thus we attempt to estimate it based on matrix perturbation theory \( \boxed{32} \). We will detail this in Section \( \boxed{5} \).

Besides, to aid our analysis, we introduce another nonnegative regularization scheme in RKKS to problem (2)

\[
\widetilde{f}_{z,\lambda} := \arg\min_{f \in B(r)} \left\{ \frac{1}{m} \sum_{i=1}^{m} (f(x_i) - y_i)^2 + \lambda \langle f, Tf \rangle_{H_K} \right\},
\]

where the empirical covariance operator \( T \) is defined in RKKS but nonnegative, see Definition \( \boxed{3} \). Based on the above regularized risk minimization problem, following Theorem \( \boxed{1} \) we can easily prove the following representer theorem with omitting the proof here.

**Theorem 2.** Let \( \widetilde{f}_{z,\lambda} \) be an optimal solution to the regularized risk minimization problem (10), then it admits the expansion \( \widetilde{f}_{z,\lambda} = \sum_{i=1}^{m} \alpha_i k(x_i, \cdot) \) by the reproducing kernel \( k \) with \( \alpha_i \in \mathbb{R} \).

By virtue of Theorem \( \boxed{2} \) and Eq. (4), the regularizer can be represented as

\[
\langle f, Tf \rangle_{H_K} = \frac{1}{m} \sum_{i,i'=1}^{m} \alpha_i \alpha_{i'} \sum_{j=1}^{m} k(x_i, x_j) k(x_{i'}, x_j) = \frac{1}{m} \alpha^\top K^2 \alpha.
\]

Accordingly, problem (10) can be formulated as

\[
\widetilde{\alpha}_{z,\lambda} := \arg\min_{\alpha \in \mathbb{R}^m : \alpha^\top K^2 \alpha = m r^2} \left\{ \frac{1}{m} \| \alpha K - y \|_2^2 + \frac{\lambda}{m} \alpha^\top K^2 \alpha \right\},
\]

with \( \widetilde{\alpha}_{z,\lambda} = -\frac{1}{m \mu} K^+ y \), and \( \mu \) is the smallest real eigenvalue of the matrix

\[
\widetilde{G} = \begin{bmatrix}
0_m & -I \\
-y y^\top/m^3 r^2 & 0_m
\end{bmatrix}.
\]
By Sylvester’s determinant identity, the largest and smallest real eigenvalues of \( \mathcal{G} \) are \( \|y\|_{\infty}/m^{1/2} \) and \( -\|y\|_{\infty}/m^{1/2} \), respectively. So we have \( \tilde{\mu} = -\|y\|_{\infty}/m^{1/2} < 0 \). Note that the regularizer in problem (10) can be also chosen to be other RKHS regularizers, such as \( \langle f, T f \rangle_{\mathcal{H}_K} \) in Definition 2. But using the empirical kernel regularizer \( \langle f, T f \rangle_{\mathcal{H}_K} \), one obtains elegant and concise theoretical results, i.e., directly compute \( \tilde{\mu} \).

4 Main Results on Approximation Analysis

In this section, we state and discuss our main results. To illustrate our analysis, we need the following notations and assumptions.

In learning theory, we assume that the target function \( f_\rho \) exists throughout the paper. This is a standard assumption in approximation analysis [20], but existence of \( f_\rho \) is not ensured if we consider a potentially infinite dimensional RKKS \( \mathcal{H}_K \), possibly universal [21]. Instead, the infinite dimensional RKKS is substituted by a finite one, i.e., \( \mathcal{H}_K^r = \{ f \in \mathcal{H}_K : \| f \| \leq r \} \) with \( r \) fixed a priori, where the norm \( \| f \| \) is defined in some associated Hilbert spaces, e.g., \( \mathcal{H}_K \). In this case, a minimizer of risk \( \mathcal{E} \) always exists but \( r \) is fixed with a prior and \( \mathcal{H}_K^r \) cannot be universal. Hence, assuming the existence of \( f_\rho \) implies that \( f_\rho \) belongs to a ball of radius \( r_\rho, \mathcal{H}_K \). So this is the reason why the spherical constraint is indeed taken into account in approximation analysis.

For the target function \( f_\rho \), we additionally suppose that there exits a constant \( M^* \geq 1 \), such that
\[
\| f_\rho \| \leq M^* \quad \text{for almost all } x \in X \quad \text{with respect to } \mu_X.
\]

In the least squares regression problem, the expected risk is defined as \( \mathcal{E}(f) = \int_X (f(x) - y)^2 d\rho \). The empirical risk functional is defined on the sample \( z \), i.e., \( \mathcal{E}_z(f) = \frac{1}{m} \sum_{i=1}^m (f(x_i) - y_i)^2 \). One aims to find a good approximation of \( f_\rho \) by \( f_{x,\lambda} \) as illustrated in Eq. (2). For a tighter bound, we need the following projection operator.

**Definition 5.** (projection operator [33]) For \( B > 0 \), the projection operator \( \pi := \pi_B \) is defined on the space of measurable functions \( f : X \rightarrow \mathbb{R} \) as
\[
\pi_B(f)(x) = \begin{cases} B, & \text{if } f(x) > B; \\ -B, & \text{if } f(x) < -B; \\ f(x), & \text{if } -B \leq f(x) \leq B, \end{cases}
\]
and then the projection of \( f \) is denoted as \( \pi_B(f)(x) = \pi_B(f(x)) \).

The projection operator is beneficial to the \( \| \cdot \|_\infty \)-bounds for sharp estimation. Besides, we consider the standard output assumption \( |y| \leq M \) (i.e. \( \|y\|_2 \leq \sqrt{m}M \)), and then we have \( \mathcal{E}_z(\pi_B(f_{x,\lambda})) \leq \mathcal{E}_z(f_{x,\lambda}) \). So it is more accurate to estimate \( f_\rho \) by \( \pi_{M^*}(f_{x,\lambda}) \) instead of \( f_{x,\lambda} \). Therefore, our approximation analysis attempts to bound the error \( \| \pi_{M^*}(f_{x,\lambda}) - f_\rho \|_{L^p_{\rho_X}}^2 \) in the space \( L^p_{\rho_X} \) with some \( p^* > 0 \), where \( L^p_{\rho_X} \) is a weighted \( L^p \)-space with the norm \( \| f \|_{L^p_{\rho_X}} = \left( \int_X |f(x)|^p d\rho_X(x) \right)^{1/p^*} \). Specifically, in our analysis, the excess error is exactly the distance in \( L^2_{\rho_X} \) due to the strong convexity of the squared loss.

To derive the learning rates, we need to consider the approximation ability of \( \mathcal{H}_K \) with respect to its capacity and \( f_\rho \) in \( L^2_{\rho_X} \), which can be characterised by the regularization error.

**Definition 6.** The regularization error of the triple \( (\mathcal{H}_K, f_\rho, \mu_X) \) is defined as
\[
D(\lambda) = \inf_{f \in \mathcal{H}_K} \left\{ \mathcal{E}(f) - \mathcal{E}(f_\rho) + \lambda \langle f, T f \rangle_{\mathcal{H}_K} \right\}.
\]

2. For unbounded outputs, the moment hypothesis [22] is suitable but the introduced hypothesis error in our analysis depends on the standard output assumption.
The target function $f_\rho$ can be approximated by $\mathcal{H}_K$ with exponent $0 < \beta \leq 1$ if there exists a constant $C_0$ such that

$$D(\lambda) \leq C_0\lambda^\beta, \quad \forall \lambda > 0. \quad (14)$$

Note that $\beta = 1$ is the best choice as we expect, which is equivalent to $f_\rho \in \mathcal{H}_K$ when $\mathcal{H}_K$ is dense. Furthermore, to quantitatively understand how the complexity of $\mathcal{H}_K$ affects the learning ability of algorithm $\text{(2)}$, we need the capacity (roughly speaking the “size”) of $\mathcal{H}_K$ measured by covering numbers.

**Definition 7.** (covering numbers $[18, 34]$) For a subset $Q$ of $C(X)$ and $\epsilon > 0$, the covering number $\mathcal{N}(Q, \epsilon)$ is the minimal integer $l \in \mathbb{N}$ such that there exist $l$ disks with radius $\epsilon$ covering $Q$.

In this paper, the covering numbers of balls are defined by

$$\mathcal{B}_R = \{ f \in \mathcal{H}_K : \sqrt{\langle f, Tf \rangle_{\mathcal{H}_K}} \leq R \}, \quad (15)$$

as subsets of $L^\infty(X)$. Our approximation analysis considers the above bounded hyper-sphere determined by $R$ instead of $r$ used in problem $\text{(2)}$. Following $[18, 22, 34]$, we assume that for some $s > 0$ and $C_s > 0$ such that

$$\log \mathcal{N}(\mathcal{B}_1, \epsilon) \leq C_s \left(\frac{1}{\epsilon}\right)^s, \quad \forall \epsilon > 0. \quad (16)$$

When $X$ is bounded in $\mathbb{R}^d$ and $k \in C^\gamma(X \times X)$, Eq. (16) holds true with $s = \frac{2d}{\gamma}$. In particular, if $k \in C^\infty(X \times X)$, Eq. (16) is still valid for an arbitrary small $s > 0$.

Formally, our main result about least squares regularized regression in RKKS is stated as follows.

**Theorem 3.** Suppose that $|f_\rho(x)| \leq M^*$ with $M^* \geq 1$, $\rho$ satisfies the condition in Eq. (14) with $0 < \beta \leq 1$, the indefinite kernel matrix $K$ satisfies the eigenvalue assumption in Definition $[2]$ with $\eta = \min\{\eta_1, \eta_2\} > 0$. Assume that for some $s > 0$, take $\tilde{\lambda} := m^{-\gamma}$ with $0 < \gamma \leq 1$. Let

$$0 < \epsilon < \frac{1}{s} - (\gamma + s\gamma - 1)(2 + s). \quad (17)$$

Then for $0 < \delta < 1$ with confidence $1 - \delta$, when $\gamma + \eta > 1$, we have

$$\|\pi_M(f_{x, \lambda}) - f_\rho\|_{L^2_{\mathbb{P}_X}}^2 \leq \tilde{C} \left(\log \frac{2}{\epsilon}\right)^2 \log \frac{2}{\delta} m^{-\Theta},$$

where $\tilde{C}$ is a constant independent of $m$ or $\delta$ and the power index $\Theta$ is

$$\Theta = \min \left\{ \gamma\beta, \gamma + \eta - 1, \frac{2 - s\gamma(1 - \beta)}{2(1 + s)}, \frac{2 - s(1 - \eta)}{2(1 + s)}, \frac{1 - s(\gamma + s\gamma - 1)(2 + s) - s\epsilon}{1 + s} \right\}, \quad (18)$$

where $\eta$ is further restricted by $\max\{0, 1 - 2/s\} < \eta < 1$ for a positive $\Theta$, i.e., a valid learning rate.

We hence directly have the following corollary that corresponds to learning rates in RKHS.

**Corollary 1.** (link to learning rates in RKHS) When $\eta \geq 1$, the power index $\Theta$ in Eq. (18) can be simplified as

$$\Theta = \min \left\{ \gamma\beta, \frac{2 - s\gamma(1 - \beta)}{2(1 + s)}, \frac{1 - (s\gamma(1 + s) - s)(2 + s) - s\epsilon}{1 + s} \right\}, \quad (19)$$

which is actually the learning rate for least squares regularized regression in RKHS, independent of $\eta$.

**Remark:** We provide learning rates in RKKS in Theorem 3 and also demonstrate the relation of the derived learning rates between RKKS and RKHS in Corollary 1. We make the following
In Theorem 3, our results choose $\lambda := m^{-\gamma}$ and the radius $R$ (or $r$) is implicit in Eq. (18). The estimation for $R$ depends on a bound for $\lambda(f_z, T f_z)_{H_K}$, see Lemma 4 for details. Note that $s$ can be arbitrarily small when the kernel $k$ is $C^\infty(X \times X)$. In this case, $\Theta$ in Eq. (18) can be arbitrarily close to $\min(\gamma \beta, \gamma + \eta - 1)$.

Corollary 1 derives the learning rates in RKHS, which recovers the result of [22] for least squares in RKHS. That is, when choosing $\beta = 1$ and $s$ is small enough, the derived learning rate in Corollary 1 can be arbitrarily close to 1, and hence is optimal [22].

Based on Theorem 3 and Corollary 1, we find that if $\eta = \min\{\eta_1, \eta_2\} \geq 1$, our analysis for RKKS is the same as that in RKHS. This is the best case. However, if $\eta = \min\{\eta_1, \eta_2\} \leq 1$, the derived learning rate in RKKS demonstrated by Eq. (18) is not faster than that in RKHS. It is reasonable since the spanning space of RKKS is larger than that of RKHS.

The proof of Theorem 3 is fairly technical and lengthy, and we briefly sketch some main ideas in the next section.

Furthermore, if problem (2) considers some nonnegative regularizers, such as $\langle f, T f \rangle_{H_K}$ in problem (10), or $\|f\|_{H_{\bar{K}}}$ in Definition 2, the analysis would be simplified due to the used nonnegative regularizer. To be specific, denote $f_z, \lambda := \arg \inf_{f \in B(r)} \{E_z(f) + \lambda \|f\|^2_{H_K}\}$ as demonstrated by [19], its learning rate could be given by the following corollary.

**Corollary 2.** Under the same assumption with Theorem 3 (without the eigenvalue assumption), by defining the regularization error as

$$D'(\lambda) = \inf_{f \in H_K} \left\{ E(f) - E(f_\rho) + \lambda \|f\|^2_{H_K} \right\},$$

satisfying $D'(\lambda) \leq C'_0 \lambda^{\beta'}$, with a constant $C'_0$ and $\beta' \in (0, 1]$, we have

$$\|\pi_{M^*}(f_{z, \lambda}) - f_\rho\|_{L^2_{\beta_X}}^2 \leq \tilde{C}' \left( \log \frac{2}{\delta} \right)^2 \log \frac{2}{\delta} m^{-\Theta'},$$

where $\tilde{C}'$ is a constant independent of $m$ or $\delta$ and the power index $\Theta'$ is defined as Eq. (19) with $\beta'$.

Note that the learning rates would be effected by different regularizers. In Table 1 we summarize the learning rates of problem (2) with different regularizers. Although the associated Hilbert space norms generated by different decompositions of the Krein space are topologically equivalent [35], the derived learning rates cannot be ensured to be the same due to their respective spanning/solving spaces.

**TABLE 1**

| learning problem in RKKS | learning rates |
|---------------------------|----------------|
| $f_{z, \lambda} := \arg \inf_{f \in B(r)} \{ E_z(f) + \lambda(f, f)_{H_K} \}$ | Eq. (18) |
| $\overline{f}_{z, \lambda} := \arg \inf_{f \in B(r)} \{ E_z(f) + \lambda(f, f)_{H_K} \}$ | Corollary 2 |
| $\tilde{f}_{z, \lambda} := \arg \inf_{f \in B(r)} \{ E_z(f) + \lambda(f, T f)_{H_K} \}$ | Corollary 2 ($\beta$ is different) |

5 **FRAMEWORK OF PROOFS**

In this section, we establish the framework of proofs for Theorem 3. By the modified error decomposition technique in section 5.1, the total error can be decomposed into the regularization
error, the sample error, and an additional hypothesis error. We detail the estimates for the hypothesis error in section 5.2. These two points are the main elements on novelty in the proof. We briefly introduce estimates for the sample error in section 5.3 and derive the learning rates in section 5.4.

5.1 Error Decomposition

In order to estimate error $\|\pi_M(f_{z,\lambda}) - f_p\|$ in the $L^2_{\mu_X}$ space, i.e., to bound $\|\pi_B(f_{z,\lambda}) - f_p\|$ for any $B \geq M^*$, we need to estimate the excess error $E(\pi_B(f_{z,\lambda})) - E(f_p)$ which can be conducted by an error decomposition technique [18]. However, since $\langle f_{z,\lambda}, f_{z,\lambda} \rangle_{H_K}$ might be negative, traditional techniques are invalid. Formally, our modified error decomposition technique is given by the following proposition by introducing an additional hypothesis error.

**Proposition 3.** Let $f_\lambda = \arg\min_{f \in H_K} \{ E(f) - E(f_\rho) + \lambda(f, T)f \}_{H_K}$, then $E(\pi_B(f_{z,\lambda})) - E(f_\rho)$ can be bounded by

$$E(\pi_B(f_{z,\lambda})) - E(f_\rho) \leq E(\pi_B(f_{z,\lambda})) - E(f_\rho) + \lambda(f_{z,\lambda}, T f_{z,\lambda})_{H_K} \leq D(\lambda) + S(z, \lambda) + P(z, \lambda),$$

where $D(\lambda)$ is the regularization error defined by Eq. (13). The sample error $S(z, \lambda)$ is given by

$$S(z, \lambda) = E(\pi_B(f_{z,\lambda})) - E_z(\pi_B(f_{z,\lambda})) + E_z(f_\lambda) - E(f_\lambda).$$

The introduced hypothesis error $P(z, \lambda)$ is defined by

$$P(z, \lambda) = E_z(f_{z,\lambda}) + \lambda(f_{z,\lambda}, T f_{z,\lambda})_{H_K} - E_z(f_{z,\lambda}) - \lambda(f_{z,\lambda}, T f_{z,\lambda})_{H_K},$$

where $f_{z,\lambda}$ and $\tilde{f}_{z,\lambda}$ are optimal solutions of problem (2) and problem (10), respectively.

**Proof.** We write $E(\pi_B(f_{z,\lambda})) - E(f_\rho) + \lambda(f_{z,\lambda}, T f_{z,\lambda})_{H_K}$ as

$$E(\pi_B(f_{z,\lambda})) - E(f_\rho) + \lambda(f_{z,\lambda}, T f_{z,\lambda})_{H_K} = \{ E(\pi_B(f_{z,\lambda})) - E_z(\pi_B(f_{z,\lambda})) \} + \{ E_z(\pi_B(f_{z,\lambda})) + \lambda(f_{z,\lambda}, T f_{z,\lambda})_{H_K} \} - \{ E_z(f_{\lambda}) + \lambda(f_{\lambda}, T f_{\lambda})_{H_K} \} + \{ E_z(f_{\lambda}) - E(f_{\lambda}) \} + \{ E(f_{\lambda}) - E(f_\rho) + \lambda(f_{\lambda}, T f_{\lambda})_{H_K} \} \leq D(\lambda) + P(z, \lambda) + S(z, \lambda),$$

where we use $E_z(\pi_B(f_{z,\lambda})) \leq E_z(f_{z,\lambda})$ in the first inequality, and the second inequality holds by the condition that $f_{z,\lambda}$ is a global minimizer of problem (10).

It can be found that the additional hypothesis error stems from the difference between $\langle f_{z,\lambda}, f_{z,\lambda} \rangle_{H_K}$-regularization and $\langle f_{z,\lambda}, T f_{z,\lambda} \rangle_{H_K}$-regularization in essence. Hence, we estimate the introduced hypothesis error in the following descriptions.

5.2 Bound Hypothesis Error

Since $\tilde{f}_{z,\lambda}$ is an optimal solution of problem (10), obviously, we have $P(z, \lambda) \geq 0$. To bound the hypothesis error, we need to estimate the objective function value difference of the two learning problems (2) and (11) by the following proposition.
Proposition 4. Suppose that the spectrum of the indefinite kernel matrix $K$ satisfies the assumption in Definition 4 denote the condition number of two invertible matrices $\Sigma_1$, $\Sigma_2$ in Eq. (9) as $C_1, C_2 < \infty$. When $\eta + \gamma > 1$ with $\eta = \min\{\eta_1, \eta_2\}$, the following expression holds with probability 1 such that

$$P(z, \lambda) \leq \tilde{C}_1 m^{-\theta_1},$$

where $\tilde{C}_1 := 2Mr + 2M^2\left(\frac{c_m}{c_2} + \frac{M^2}{r^2} + \frac{c_1}{c_1}\right)$ and the power index is $\theta_1 = \min\{1, \gamma + \eta - 1\}$.

Proof. The proof can be found in Appendix B. \hfill \square

Remark: We require that the condition number of invertible matrices is finite. This condition is mild as demonstrated by [36]. To prove this proposition, we firstly estimate $\mu$ and then derive the bound for $P(z, \lambda)$.

5.2.1 Estimate $\mu$

As aforementioned, $\mu$ is the smallest real eigenvalue of a non-Hermitian matrix $G$, but we cannot directly calculate it and thus attempt to estimate it based on matrix perturbation theory [32]. There are three classical and well-known perturbation bounds for matrix eigenvalues, including the Bauer-Fike theorem and the Hoffman-Wielandt theorem for diagonalizable matrices [37], and Weyl’s theorem for Hermitian matrices [32]. However, $G$ is neither Hermitian nor diagonalizable, and thus we need the following lemma.

Lemma 1. (Henrici theorem [38]) Let $A$ be an $m \times m$ matrix with Schur decomposition $Q^H A Q = D + U$, where $Q$ is unitary, $D$ is a diagonal matrix and $U$ is a strict upper triangular matrix, with $(\cdot)^H$ denoting the Hermitian transpose. For each eigenvalue $\tilde{\sigma}$ of $A + \Delta$, there exists an eigenvalue $\sigma(A)$ of $A$ such that

$$|\tilde{\sigma} - \sigma(A)| \leq \max(\varsigma, b\sqrt{\varsigma}), \text{ where } \varsigma := \|\Delta\|_2 \sum_{i=1}^{b-1} \|U\|_2^i,$$

where $b \leq m$ is the smallest integer satisfying $U^b = 0$, i.e., the nilpotent index of $U$.

Based on the above lemma, we can estimate $\mu$.

Proposition 5. Under the assumption of Proposition 4 $\mu$ can be represented as

$$\mu := c_a \tilde{\mu} + c_b \tilde{\mu}^2 + \left[\frac{C_2}{c_m} + \tilde{c}_d \left(\frac{C_1}{c_1} - \frac{C_2}{c_m}\right)\right] m^{-(\gamma + \eta)}.$$

with $c_a \in [-1, 0] \cup (0, 1], c_b \in [-1, 1]$, and $c_d \in [0, 1]$.

Proof. The matrix $G$ in Eq. (8) can be reformulated as

$$G = \begin{bmatrix} \lambda K^\dagger & -I \\ 0_{m \times m} & \lambda K^\dagger \end{bmatrix}_{\equiv G_1} + \begin{bmatrix} 0_{m \times m} & 0_{m \times m} \\ -yy^T/m^2r^2 & 0_{m \times m} \end{bmatrix}_{\equiv G_2}.$$

Here $G$ can be represented as a sum of a block upper triangular matrix $G_1$ with a non-Hermitian perturbation $G_2$. To estimate $G_1$, by Lemma 1 from the definition of Schur decomposition on $G_1$, it can be easily verified that $D$ and $U$ are

$$D = \text{diag}\left(\frac{\lambda}{\sigma_1}, \ldots, \frac{\lambda}{\sigma_p}, 0, \ldots, 0, \frac{\lambda}{\sigma_{m-q+1}}, \ldots, \frac{\lambda}{\sigma_m}, \frac{\lambda}{\sigma_1}, \ldots, \frac{\lambda}{\sigma_p}, 0, \ldots, 0, \frac{\lambda}{\sigma_{m-p+1}}, \ldots, \frac{\lambda}{\sigma_m}\right),$$

and $U = \begin{bmatrix} 0_m & -I \\ 0_m & 0_m \end{bmatrix}$. 


Accordingly, $U$ is a nilpotent matrix with $U^2 = 0$, and thus we have $b = 2$. According to Lemma 1, there exists an eigenvalue of $G_1$ denoting as $\sigma(G_1)$ such that

$$|\mu - \sigma(G_1)| \leq \max(\varsigma, \sqrt[3]{\varsigma}) \leq \varsigma + \sqrt[3]{\varsigma},$$

where $\varsigma$ is given by

$$\varsigma := \|G_2\|_2 \sum_{i=1}^{b-1} \|U\|_2^i = \|G_2\|_2 \|U\|_2 = \|G_2\|_2 = \frac{\|y\|^2}{m^3r^2}.$$

Then we consider the following three cases based on the sign of $\sigma(G_1)$.

**Case 1.** $\sigma(G_1) = 0$

The inequality in Eq. (21) can be formulated as

$$- \frac{\|y\|^2}{m^{\sqrt{mr}}} - \frac{\|y\|^2}{m^3r^2} \leq \mu \leq \frac{\|y\|^2}{m^{\sqrt{mr}}} + \frac{\|y\|^2}{m^3r^2}.$$  

(22)

**Case 2.** $\sigma(G_1) > 0$

Without loss of generality, we assume that $\sigma(G_1)$ is $\lambda/\sigma_l$ with $l \in \{1, 2, \cdots, p\}$. According to the definition of condition number $C_1$, we have

$$0 < \frac{1}{\sigma_l} \leq 1 \leq \frac{C_1}{c_1} m^{-\eta} \leq \frac{C_1}{c_1} m^{-\eta}, \quad \eta = \min\{\eta_1, \eta_2\}.$$

Then, the inequality in Eq. (21) can be formulated as

$$- \frac{\|y\|^2}{m^{\sqrt{mr}}} - \frac{\|y\|^2}{m^3r^2} \leq \frac{C_1}{c_1} m^{-(\gamma + \eta)} + \frac{\|y\|^2}{m^{\sqrt{mr}}} + \frac{\|y\|^2}{m^3r^2}.$$  

(23)

**Case 3.** $\sigma(G_1) < 0$

Likewise, we assume that $\sigma(G_1)$ is $\lambda/\sigma_l$ with $l \in \{m - q + 1, m - q + 2, \cdots, m\}$. According to the definition of condition number $C_2$, we have

$$0 > \frac{1}{\sigma_m} \geq 1 \geq \frac{C_2}{c_m} m^{-\eta_2} \geq \frac{C_2}{c_m} m^{-\eta}, \quad \eta = \min\{\eta_1, \eta_2\}.$$

Then, the inequality in Eq. (21) can be formulated as

$$\frac{C_2}{c_m} m^{-(\gamma + \eta)} - \frac{\|y\|^2}{m^{\sqrt{mr}}} - \frac{\|y\|^2}{m^3r^2} \leq \frac{\|y\|^2}{m^{\sqrt{mr}}} + \frac{\|y\|^2}{m^3r^2}.$$  

(24)

Combining Eq. (22), Eq. (23) and Eq. (24), we have

$$\begin{cases} 
\mu \geq \frac{C_2}{c_m} m^{-(\gamma + \eta)} - \frac{\|y\|^2}{m^{\sqrt{mr}}} - \frac{\|y\|^2}{m^3r^2} \\
\mu \leq \frac{C_1}{c_1} m^{-(\gamma + \eta)} + \frac{\|y\|^2}{m^{\sqrt{mr}}} + \frac{\|y\|^2}{m^3r^2}, 
\end{cases}$$

which can be further written as

$$\frac{C_2}{c_m} m^{-(\gamma + \eta)} + \tilde{\mu}^2 \leq \mu \leq \frac{C_1}{c_1} m^{-(\gamma + \eta)} - \tilde{\mu} + \tilde{\mu}^2.$$

Therefore, we have $\lim_{m \to \infty} \mu = 0$, and its convergence rate is $O(\frac{1}{m})$ due to $\gamma + \eta > 1$. Finally, $\mu$ can be represented in Eq. (20) with $\tilde{c}_a \neq 0$, which concludes the proof.
5.2.2 Derive the convergence rate of the hypothesis error

After giving the expression for \( \mu \) with the convergence rate \( \mathcal{O}(\frac{1}{m}) \) in Proposition 5, we are ready to present the estimates for \( P(z, \lambda) \). We firstly prove the consistency, i.e., \( \lim_{m \to \infty} P(z, \lambda) = 0 \), and then derive its convergence rate as demonstrated by Proposition 4.

**Lemma 2.** Under the assumption of Proposition 4, the coefficient \( \tilde{c}_a \in [-1, 0] \bigcup (0, 1] \) in Eq. (20) can be further improved to \( \tilde{c}_a = 1 \). The estimates for \( P(z, \lambda) \) are consistent if for any given \( \varepsilon > 0 \)

\[
\lim_{m \to \infty} P(z, \lambda) = 0.
\]

**Proof.** The hypothesis error \( P(z, \lambda) \) is defined as

\[
P(z, \lambda) = \varepsilon_z(f_{z, \lambda}) + \lambda f_{z, \lambda}^H_{H_K} - \varepsilon_z(f_{z, \lambda}) - \lambda f_{z, \lambda}^H_{H_K},
\]

where \( f_{z, \lambda} \) and \( \tilde{f}_{z, \lambda} \) are optimal solutions of problem (2) and problem (10), respectively. Hence, they are both obtained on the hyper-sphere and thus the regularizer is \( \alpha_{z, \lambda}^T K^2 \alpha_{z, \lambda} = m \sigma^2 \) can be canceled out in \( P(z, \lambda) \). Based on this, \( P(z, \lambda) \) can be represented as

\[
P(z, \lambda) = \frac{1}{m} \sum_{i=1}^{m} (f_{z, \lambda}(x_i) - y_i)^2 + \lambda f_{z, \lambda}^H_{H_K} - \frac{1}{m} \sum_{i=1}^{m} (f_{z, \lambda}(x_i) - y_i)^2 - \lambda f_{z, \lambda}^H_{H_K}
\]

\[
= \frac{1}{m} \| K \alpha_{z, \lambda} - y \|_2^2 - \frac{1}{m} \| K \tilde{f}_{z, \lambda} - y \|_2^2
\]

\[
= \frac{2}{m} y^T K \alpha_{z, \lambda} - \frac{2}{m} y^T K \tilde{f}_{z, \lambda},
\]

Due to \( P(z, \lambda) \geq 0 \) for any \( m \in \mathbb{N} \), we can conclude that \( \lim_{m \to \infty} (P_1(z, \lambda) + P_2(z, \lambda)) \geq 0 \) if the limits \( \lim_{m \to \infty} P_1(z, \lambda) \) and \( \lim_{m \to \infty} P_2(z, \lambda) \) exist. Hence, we analyse \( P_1(z, \lambda) \) and \( P_2(z, \lambda) \), respectively. Here \( P_1(z, \lambda) \) is given by

\[
P_1(z, \lambda) = \frac{2}{m} y^T K \alpha_{z, \lambda} = -\frac{2}{m^2 \mu} y^T K K^T y
\]

\[
= -\frac{2}{m^2 \mu} y^T \left( \sum_{i=1}^{p} v_i v_i^T + \sum_{i=m-q+1}^{m} v_i v_i^T \right) y
\]

\[
\leq \frac{2 \| y \|_2^2}{\sqrt{m}},
\]

where \( v_i \) is the \( i \)-th column of the orthogonal matrix \( V \) from the eigenvalue decomposition \( K = V \Sigma V^T \). The inequality in the above equation holds by \( y^T \Sigma y = y^T (I - \sum_{i=p+1}^{m-q} v_i v_i^T) y \leq y^T y \). Besides, \( P_2(z, \lambda) = -\frac{2}{m} y^T K \alpha_{z, \lambda} \) can be rewritten as

\[
P_2(z, \lambda) = -\frac{2}{m^2} y^T K (\lambda I - \mu K)^T y
\]

\[
= \frac{2}{m^2} y^T \left( \sum_{i=1}^{p} \frac{v_i v_i^T}{\lambda - \mu} + \sum_{i=m-q+1}^{m} \frac{v_i v_i^T}{\lambda - \mu} \right) y.
\]

Since the function \( h(\sigma_i) = \frac{1}{\sigma_i - \mu} \) is an increasing function of \( \sigma_i \), \( P_2(z, \lambda) \) can be bounded by

\[
-\frac{2}{m^2} \cdot \frac{1}{\lambda - \mu} y^T \Xi y \leq P_2(z, \lambda) \leq -\frac{2}{m^2} \cdot \frac{1}{\lambda - \mu} y^T \Xi y.
\]
By Proposition \[5\] plugging Eq. (20) into the above inequality, when \(\eta + \gamma > 1\), we have
\[
\lim_{m \to \infty} - \frac{2}{m^2} \cdot \frac{1}{\sigma_{m-q+1}} \cdot \mathbf{y}^\top \Xi = \lim_{m \to \infty} - \frac{2}{m^2} \cdot \frac{1}{\sigma_{m-q+1}} \cdot \mathbf{y}^\top \Xi = \lim_{m \to \infty} \frac{2}{\sqrt{m}} \cdot \frac{r}{\sqrt{m}} \leq \lim_{m \to \infty} \frac{2}{\sqrt{m}} \cdot \frac{r}{\sqrt{m}} < \infty,
\]
which holds by \(\|\mathbf{y}\|_2 = O(\sqrt{m})\) and \(\tilde{c}_a \neq 0\). According to the squeeze theorem, we conclude that the limit \(\lim_{m \to \infty} P_2(z, \lambda)\) exists. Because of \(P(z, \lambda) \geq 0\), we have
\[
0 \leq \lim_{m \to \infty} \left( P_1(z, \lambda) + P_2(z, \lambda) \right) \leq \lim_{m \to \infty} \left[ \frac{2}{\sqrt{m}} \cdot \left( 1 - \frac{1}{\tilde{c}_a} \right) \right],
\]
which indicates that \(1 - \frac{1}{\tilde{c}_a} \geq 0\), i.e., \(\tilde{c}_a \geq 1\). Due to \(\tilde{c}_a \in [-1, 0) \cup (0, 1]\), we have \(\tilde{c}_a = 1\). Then we conclude that \(\lim_{m \to \infty} \left( P_1(z, \lambda) + P_2(z, \lambda) \right) = 0\), which concludes the consistency for \(P(z, \lambda)\). \(\square\)

Accordingly, based on Lemma \[2\] we derive the convergence rate for \(P(z, \lambda)\) as demonstrated by Proposition \[4\]. The proof can be found in Appendix \[B\]

### 5.3 Estimate Sample Error

The sample error can be decomposed into \(S(z, \lambda) = S_1(z, \lambda) + S_2(z, \lambda)\) with
\[
S_1(z, \lambda) = \mathcal{E}\left( \pi_B(f_{z,\lambda}) \right) - \mathcal{E}(f_\rho) - \mathcal{E}_z\left( \pi_B(f_{z,\lambda}) \right) + \mathcal{E}_z(f_\rho),
\]
\[
S_2(z, \lambda) = \left\{ \mathcal{E}_z(f_\lambda) - \mathcal{E}_z(f_\rho) \right\} - \left\{ \mathcal{E}(f_\lambda) - \mathcal{E}(f_\rho) \right\}.
\]

Note that \(S_1(z, \lambda)\) involves the samples \(z\). Thus a uniform concentration inequality for a family of functions containing \(f_{z,\lambda}\) is needed to estimate \(S_1(z, \lambda)\). Since we have \(f_{z,\lambda} \in \mathcal{B}_R\) defined by Eq. (15), we shall bound \(S_1\) by the following proposition with a properly chosen \(R\). Considering that the estimates for \(S_1(z, \lambda)\) and \(S_2(z, \lambda)\) have been extensively investigated in \[16\], \[18\], \[39\], we directly present the corresponding results in Appendix \[C\]

### 5.4 Derive Learning Rates

Combining the bounds in Proposition \[3\] and estimates for the sample error, the excess error \(\mathcal{E}\left( \pi_B(f_{z,\lambda}) \right) - \mathcal{E}(f_\rho)\) can be estimated. Specifically, as aforementioned, algorithmically, the radius \(r\) or \(R\) in Eq. (15) is determined by cross validation in our experiments. Theoretically, in our analysis, it is estimated by giving a bound for \(\lambda(f_{z,\lambda}, T f_{z,\lambda})_{H_K}\). This is conducted by the iteration technique \[16\] to improve learning rates. The proof for learning rates in Theorem \[3\] can be found in the supplemental materials, see Appendix \[D\]

### 6 Numerical Experiments

In this section, we validate our theoretical results by numerical experiments in the following three aspects.
6.1 Eigenvalue assumption

Here we verify the justification of our eigenvalue assumption in Definition 4 on four indefinite kernels, including

- the spherical polynomial (SP) kernel \[ k_p(x, x') = (1 + \langle x, x' \rangle)^p \] with \( p = 10 \) on the unit sphere is shift-invariant but indefinite.
- the TL1 kernel \[ k_{\tau'}(x, x') = \max\{\tau' - \|x - x'|_1, 0\} \] with \( \tau' = 0.7d \) as suggested.
- the Delta-Gauss kernel \[ k(x, x') = \exp\left(-\|x - x'|^2 / \tau_1\right) - \exp\left(-\|x - x'|^2 / \tau_2\right) \] with \( \tau_1 = 1 \) and \( \tau_2 = 0.1 \).
- the log kernel \[ k(x, x') = -\log(1 + \|x - x'|) \].

Figure 1 shows eigenvalue distributions of the above four indefinite kernels on the monks3 dataset. It can be found that our eigenvalue assumption: \( \sigma_1 \geq c_1m^{\eta_1} \) (\( c_1 > 0, \eta_1 > 0 \)) and \( \sigma_m \leq c_mm^{\eta_2} \) (\( c_m < 0, \eta_2 > 0 \)) in Definition 4 is reasonable. Specifically, our experiments on the log kernel verify that it has only one negative eigenvalue admitting \( \sigma_m = -\sum_{i=1}^{m-1} \sigma_i \). Note that the SP and TL1 kernels have not been proved as reproducing kernels in RKKS. It is still an open problem to verify that a kernel admits the decomposition. However, our eigenvalue assumption still covers them, which demonstrates the feasibility of our assumption.

6.2 Empirical validations of derived learning rates

Here we verify the derived convergence rates on the monks3 dataset effected by different indefinite kernels. In our experiment, we choose \( \lambda = 1/m \) and two indefinite kernels including the Delta-Gauss kernel and the log kernel on monks3 to study in what degree they would effect the learning.

Fig. 2. The log-log plot of the theoretical and observed risk convergence rates averaged on 100 trials.
rates. Since the selected two kernels are \(C^\infty(X \times X)\), \(s\) can be arbitrarily small. In this case, by Theorem 3 and Corollary 2, the learning rate of problem \((2)\) with the RKKS regularizer \(\langle f, f \rangle_{\mathcal{H}_K}\) or the RKHS regularizer \(\|f\|_{\mathcal{H}_K}^2\) is close to \(\min\{\beta, \eta\}\). Here the two parameters \(\beta\) and \(\eta\) indicate the approximation ability for \(f\) and the size of RKKS by different indefinite kernels, and thus they will influence the expected risk rate. Figure 2(a) shows the observed learning rate associated with the Delta-Gauss kernel is \(O(1/\sqrt{m})\), while the excess risk associated with the \(\log\) kernel converges at \(O(m^{-1/3})\) in Figure 2(b). Hence, Figure 2 demonstrates this difference that the excess risk of problem \((2)\) with the Delta-Gauss kernel converges faster than that with the \(\log\) kernel. This is reasonable and demonstrated by Theorem 3 i.e., different \(\mathcal{H}_K\) spanned by various indefinite kernels lead to different convergence rates due to their different approximation ability for \(f\).

The above experiments validate the rationality of our eigenvalue assumption and the consistency with theoretical results.

7 Conclusion

In this paper, we provide approximation analysis of the least squares problem associated with the \(\langle f, f \rangle_{\mathcal{H}_K}\) regularization scheme in RKKS. For this non-convex problem with the bounded hyper-sphere constraint, we can get an attainable optimal solution, which makes it possible to conduct approximation analysis in RKKS. Accordingly, we start the analysis from the learning problem that has an analytical solution, and thus obtain the first-step to understand the learning behavior in RKKS. Our analysis and experimental validation bridge the gap between the regularized risk minimization problem in RKHS and RKKS.

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APPENDIX A
PROOF OF THEOREM 1

Proof. According to Definition 1, all \( f \in \mathcal{H}_K \) can be decomposed into \( f = f_+ + f_- \), where \( f_+ \in \mathcal{H}_+ \) and \( f_- \in \mathcal{H}_- \). Further, we decompose \( f_\pm \) Denote two empirical Hilbert spaces \( \mathcal{H}_\pm(X) = \text{span}\{k_\pm(x, \cdot) \in \mathcal{H}_\pm | x \in X\} \), which are spanned by evaluation functionals on the data \( X := \{x_i\}_{i=1}^m \). Further, \( f_\pm \) can be represented as
\[
    f_\pm = u_\pm + v_\pm,
\]
where \( u_\pm \in \mathcal{H}_\pm(X) \) and \( v_\pm \bot \mathcal{H}_\pm(X) \). Then, for any \( x \in X \), we have
\[
    \langle v_\pm, k_\pm(x, \cdot) \rangle_{\mathcal{H}_\pm} = 0.
\]
Accordingly, by the reproducing property in RKKS, the hypothesis \( f \) evaluated at \( x \) admits
\[
    f(x) = \langle f, k(x, \cdot) \rangle_{\mathcal{H}_K} = \langle f_+ + f_-, k(x, \cdot) \rangle_{\mathcal{H}_K} = \langle u_+ + v_+, k_+(x, \cdot) \rangle_{\mathcal{H}_+} - \langle u_- + v_, k_-(x, \cdot) \rangle_{\mathcal{H}_-} = u_+(x) - u_-(x),
\]
which indicates that \( f(x) \) is independent of \( v_\pm \). Besides, \( \langle f, f \rangle_{\mathcal{H}_K} \) can be decomposed as
\[
    \langle f, f \rangle_{\mathcal{H}_K} = \|f_+\|^2_{\mathcal{H}_+} - \|f_-\|^2_{\mathcal{H}_-} = \|u_+\|^2_{\mathcal{H}_+} + \|v_+\|^2_{\mathcal{H}_+} - \|u_-\|^2_{\mathcal{H}_+} - \|v_-\|^2_{\mathcal{H}_-}.
\]
Based on the above equations, problem (2) can be expressed as
\[
    \begin{align*}
    \min_{f \in \mathcal{H}_K} & \quad \frac{1}{m} \sum_{i=1}^m (u_+(x_i) - u_-(x_i) - y_i)^2 + \lambda \left( \|u_+\|^2_{\mathcal{H}_+} + \|v_+\|^2_{\mathcal{H}_+} - \|u_-\|^2_{\mathcal{H}_+} - \|v_-\|^2_{\mathcal{H}_-} \right) \\
    \text{s.t.} & \quad \frac{1}{m} \sum_{i=1}^m (u_+(x_i) - u_-(x_i))^2 \leq r^2 \quad \text{with} \quad f = u_+ + v_+ + u_- + v_-
    \end{align*}
\]
(25)
Since the constraint is independent of \( v_\pm \), the above optimization problem obtains the optimal solution \( f^* \) at \( v_\pm = 0 \). Therefore, \( f^* \) only involves with \( u_+ \in \mathcal{H}_+(X) \) and \( u_- \in \mathcal{H}_-(X) \), and thus can be expressed as
\[
    f^* = \sum_{i=1}^m \alpha_i k(x_i, \cdot), \quad \text{with} \quad \alpha_i \in \mathbb{R},
\]
which concludes the proof. \(\square\)

APPENDIX B
PROOF FOR PROPOSITION 4

Proof. For notational simplicity, we denote \( \tilde{c}_e := \left[ \frac{C_2}{c_m} + \tilde{c}_d \left( \frac{c_1}{c_m} - \frac{C_1}{C_2} \right) \right] \). Then, by Lemma 2, we have
\[
    P = P_1(z, \lambda) + P_2(z, \lambda)
\]
\[
    \leq \frac{2\|y\|^2_{2r}}{\sqrt{m}} + \frac{2\|y\|^2_2}{m^2} \cdot \frac{1}{\sigma_{m-q+1}^2} - \mu
\]
\[
    \leq \frac{2\|y\|^2_{2r}}{\sqrt{m}} + \frac{2\|y\|^2_2}{m} \left( \frac{1}{\sigma_{m-q+1}^2} - \frac{1}{m^1\gamma - \|y\|^2_{2r}} \right) - \frac{\tilde{c}_e \|y\|^2_{2r}}{m^1\gamma - \|y\|^2_{2r}} - \tilde{c}_e m^{-\gamma}
\]
\[
    \leq \frac{2\|y\|^2_{2r}}{\sqrt{m}} + \frac{2\|y\|^2_2}{m} \left( \frac{\sqrt{mr} - C_m}{C_2} \cdot m^{-\gamma - \eta} + \frac{\|y\|^2_{2M} m^{-1} + |\tilde{c}_e|m^{-(\gamma + \eta)}}{C_1} \right) m^{-\Theta_1}
\]
\[
    \leq \left( 2Mr + 2M^2 \left( \frac{C_m}{C_2} + \frac{M^2}{C_1} \right) \right) m^{-\Theta_1}
\]
\[
    \triangleq \tilde{C}_1 m^{-\Theta_1},
\]
we conclude the proof for Proposition 4.

APPENDIX C
PROOF FOR THE SAMPLE ERROR

The asymptotical behaviors of $S_1(z, \lambda)$ and $S_2(z, \lambda)$ are usually illustrated by the convergence of the empirical mean $\frac{1}{m}\sum_{i=1}^{m}\xi_i$ to its expectation $E\xi$, where $\{\xi_i\}_{i=1}^{m}$ are independent random variables on $(Z, \rho)$ defined as

$$\xi(x, y) := (y - f_\lambda(x))^2 - (y - f_\rho(x))^2.$$ 

For $R \geq 1$, denote

$$\mathcal{W}(R) = \left\{ z \in Z^m : \sqrt{\langle f_z, T_f_z \rangle_{\mathcal{H}_\lambda}} \leq R \right\}.$$

Lemma 3. If $\xi$ is a symmetric real-valued function on $X \times Y$ with mean $E\xi$. Assume that $E\xi \geq 0$, $|\xi - E\xi| \leq T$ almost surely and $E\xi^2 \leq c_1'(E\xi)^\theta$ for some $0 \leq \theta \leq 1$ and $c_1' \geq 0$, $T \geq 0$. Then for every $\epsilon > 0$ there holds

$$\text{Prob}\left\{ \frac{1}{m}\sum_{i=1}^{m}\xi(z_i) - E\xi \geq \epsilon^{1-\theta} \right\} \leq \exp\left\{ -m\epsilon^{2-\theta} \right\}.$$

Now we can bound $S_2(z, \lambda)$ by the following proposition.

Proposition 6. Suppose that $|f_\rho(x)| \leq M^*$ with $M^* \geq 1$, for any $0 < \delta < 1$, there exists a subset of $Z_1$ of $Z^m$ with confidence at least $1 - \delta/2$, such that for any $\forall z \in Z_1$

$$S_2(z, \lambda) \leq \frac{1}{2}D(\lambda) + \frac{1}{m}\left( \kappa\sqrt{\frac{D(\lambda)}{\lambda}} + M^* + 12 \right) \log \frac{2}{\delta}.$$ 

Proof. From the definition of $f_\lambda$ in Proposition 3 combining Eq. (3) and Eq. (13), we have

$$\|f_\lambda\|_\infty \leq \kappa\sqrt{\langle f_\lambda, T f_\lambda \rangle_{\mathcal{H}_\lambda}} \leq \kappa\sqrt{\frac{D(\lambda)}{\lambda}} \leq \kappa\sqrt{C_0\lambda^{\frac{\theta+1}{2}}},$$

which leads to $\|f_\lambda\|_\infty \leq \kappa\sqrt{\frac{D(\lambda)}{\lambda}}$. The first equality holds because the reproducing kernel $k_+ + k_-$ associated with $\mathcal{H}_\lambda$ is the square root of the limiting kernel in [27] associated with the empirical covariance operator $T$. Due to $f_\rho(x)$ contained in $[-M^*, M^*]$, we can get

$$|\xi - E\xi| \leq \kappa\sqrt{\frac{D(\lambda)}{\lambda}} + M^*.$$ 

For least squared loss, $E(\xi^2) \leq 4E(\xi)$ indicates $c_1' = 4$ and $\theta = 1$. Applying Lemma 3 there exists a subset $Z_1$ of $Z^m$ with confidence $1 - \delta/2$, we have

$$\frac{1}{m}\sum_{i=1}^{m}\xi(z_i) - E\xi \leq \sqrt{(E(\xi)^\theta + \epsilon^\theta / 2)^{1-\frac{\theta}{2}}} \leq \frac{1}{2}E\xi + \frac{3}{2}\epsilon,$$

Then, we obtain

$$\frac{1}{m}\sum_{i=1}^{m}\xi(z_i) - E\xi \leq \frac{\theta}{2}(E(f_\lambda) - E(f_\rho)) + \frac{T + 3c_1'}{m}\log \frac{2}{\delta} \leq \frac{1}{2}D(\lambda) + \frac{\kappa\sqrt{D(\lambda) + M^* + 12}}{m}\log \frac{2}{\delta},$$
We can easily see that each function \( g \) where we use \( M \), which concludes the proof.

In the next, we attempt to bound \( S_1(z, \lambda) \) with respect to the samples \( z \). Thus a uniform concentration inequality for a family of functions containing \( f_{z,\lambda} \) is needed to estimate \( S_1 \). Since we have \( f_{z,\lambda} \in \mathcal{B}_R \), which is defined by Eq. (15), we shall bound \( S_1 \) by the following proposition with a properly chosen \( R \).

**Proposition 7.** Suppose that \( |f_\rho(x)| \leq M^* \) with \( M^* \geq 1 \), and Eq. (16), for any \( 0 < \delta < 1 \), \( R \geq 1 \), \( B > 0 \), there exists a subset \( Z_2 \) of \( Z^m \) with confidence at least \( 1 - \delta/2 \), such that for any \( z \in \mathcal{W}(R) \cap Z_2 \),

\[
S_1(z, \lambda) \leq \frac{136(M^* + B)}{m} \log \frac{2}{\delta} + \frac{1}{2} \left\{ \mathcal{E}(\pi_B(f_{z,\lambda})) - \mathcal{E}(f_\rho) \right\} + 144C_s(M^* + B)m^{-\frac{1}{1+\frac{\epsilon}{R}}} R^{\frac{\epsilon}{R}}.
\]

**Proof.** Consider the function set \( \mathcal{F}_R \) with \( R > 0 \) by

\[
\mathcal{F}_R := \left\{ (y - \pi_B(f)(x))^2 - (y - f_\rho(x))^2 : f \in \mathcal{B}_R \right\}.
\]

We can easily see that each function \( g \in \mathcal{F}_R \) satisfies \( \|g\|_{\infty} \leq B + M^* \), and thus we have \( |g - \mathbb{E}g| \leq B + M^* \). So using \( \mathcal{N}(\mathcal{F}_R, \epsilon) \leq \mathcal{N}(\mathcal{B}_1, \epsilon) \) and applying Lemma 3 to the function set \( \mathcal{F}_R \) with the covering number condition in Eq. (16), we have

\[
\text{Prob}_{z \in Z^m} \left\{ \sup_{f \in \mathcal{F}_R} \frac{\mathbb{E}g - \frac{1}{m} \sum_{i=1}^{m} g(x_i, y_i)}{\sqrt{(\mathbb{E}g)^\theta + \epsilon^\theta}} \geq 4\epsilon^{1-\frac{\theta}{2}} \right\} \leq \exp \left\{ C_s \left( \frac{R}{\epsilon} \right)^s - \frac{m \epsilon^{2-\theta}}{2c'_1 + \frac{2}{3}(B + M^*)\epsilon^{1-\theta}} \right\},
\]

with \( \mathbb{E}g = \mathcal{E}(\pi_B(f)) - \mathcal{E}(f_\rho) \). Hence there holds a subset \( Z_2 \) of \( Z^m \) with confidence at least \( 1 - \delta/2 \) such that \( \forall z \in Z_2 \cap \mathcal{W}(R) \)

\[
\sup_{f \in \mathcal{F}_R} \frac{\mathbb{E}g - \frac{1}{m} \sum_{i=1}^{m} g(x_i, y_i)}{\sqrt{(\mathbb{E}g)^\theta + \left( \epsilon^s(m, R, \frac{\delta}{2}) \right)^\theta}} \leq 4\left( \epsilon^s(m, R, \frac{\delta}{2}) \right)^{1-\frac{\theta}{2}},
\]

where \( \epsilon^s(m, R, \frac{\delta}{2}) \) is the smallest positive number \( \epsilon \) satisfying

\[
C_s \left( \frac{R}{\epsilon} \right)^s - \frac{m \epsilon^{2-\theta}}{2c'_1 + \frac{2}{3}(B + M^*)\epsilon^{1-\theta}} = \log \frac{\delta}{2},
\]

using Lemma 7.2 in [18], we have

\[
\epsilon^s \leq \max \left\{ \frac{48 + 2(M^* + B)}{3m} \log \frac{2}{\delta}, \left( \frac{48 + 4(B + M^*)}{3m} C_s R^s \right)^{\frac{1}{1+\frac{\epsilon}{R}}} \right\} \leq \frac{17(M^* + B)}{m} \log \frac{2}{\delta} + 18C_s(M^* + B)m^{-\frac{1}{1+\frac{\epsilon}{R}}} R^{\frac{\epsilon}{R}},
\]

where we use \( M^* \geq 1 \). For \( z \in \mathcal{B}(R) \cap Z_2 \), we have

\[
S_1(z, \lambda) \leq 8\epsilon^s(m, R, \frac{\delta}{2}) + \frac{1}{2} \left\{ \mathcal{E}(\pi_B(f_{z,\lambda})) - \mathcal{E}(f_\rho) \right\}.
\]

\[\square\]
**APPENDIX D**

**PROOF FOR LEARNING RATES**

Combining the bounds in Proposition 3, 4, 6, 7, and Eq. (26), let Eq. (16) with \( s > 0 \), Eq. (14) with \( 0 < \beta \leq 1 \), take \( \lambda = m^{-\gamma} \) with \( 0 < \gamma < 1 \), the excess error \( \mathcal{E}(\pi_B(f_{z,\lambda})) - \mathcal{E}(f_\rho) \) can be bounded by

\[
\mathcal{E}(\pi_B(f_{z,\lambda})) - \mathcal{E}(f_\rho) + \lambda(f_{z,\lambda}, T_{f_{z,\lambda}})_{\mathcal{H}_K} \leq 3C_0m^{-\gamma \beta} + \widetilde{C}_1m^{-\Theta_1} + \widetilde{C}_2 \log \frac{2}{\delta} m^{-1} + \widetilde{C}_3m^{-\frac{1}{\gamma(1 + \beta) + 1}} \log \frac{2}{\delta} + 2K\sqrt{C_0}m^{-(\frac{\gamma(\beta - 1)}{2} + 1)} \log \frac{2}{\delta},
\]

where \( \widetilde{C}_1 \) is given in Proposition 4. Two constants \( \widetilde{C}_2 \) and \( \widetilde{C}_3 \) are given by

\[
\widetilde{C}_2 = 274M^* + 272B + 24, \quad \widetilde{C}_3 = 288(M^* + B)C_s.
\]

In the next, we attempt to find a \( R > 0 \) by giving a bound for \( \lambda(f_{z,\lambda}, T_{f_{z,\lambda}})_{\mathcal{H}_K} \).

**Lemma 4.** Suppose that \( \rho \) satisfies the condition in Eq. (14) with \( 0 < \beta \leq 1 \). Assume that for some \( s > 0 \), take \( \lambda = m^{-\gamma} \) with \( 0 < \gamma \leq 1 \). Then for \( 0 < \epsilon < 1 \) and \( 0 < \delta < 1 \), we have

\[
\sqrt{\langle f_{z,\lambda}, T_{f_{z,\lambda}} \rangle_{\mathcal{H}_K}} \leq 4\widetilde{C}_3\widetilde{C}_X \left( \log \frac{2}{\epsilon} \right)^2 \sqrt{\log \frac{2}{\delta} m^{\theta_1}},
\]

where \( \widetilde{C}_X \) is given by

\[
\widetilde{C}_X = \left( 1 + \sqrt{\widetilde{C}_2} + \sqrt{2K\sqrt{\widetilde{C}_0} + \sqrt{3\widetilde{C}_0} + \sqrt{\widetilde{C}_1}} \right),
\]

and \( \theta_1 \) is

\[
\theta_1 = \max \left\{ \frac{\gamma(1 - \beta)}{2}, \frac{1 - \eta}{2}, \frac{\gamma - 1}{2}, \frac{\gamma(\beta - 1) + 2}{4}, \frac{1 - \eta}{2} \right\}.
\]

**Proof.** From Eq. (27), we know that for any \( R \geq 1 \) there exists a subset \( V_R \) of \( Z_m \) with measure at most \( \delta \) such that

\[
\sqrt{\langle f_{z,\lambda}, T_{f_{z,\lambda}} \rangle_{\mathcal{H}_K}} \leq a_mR^{\frac{\gamma}{1 + \beta}} + b_m, \quad \forall z \in \mathcal{W}(R) \setminus V_R,
\]

where \( a_m = \sqrt{\widetilde{C}_3m^{\frac{\gamma}{1 + \beta} - 2(1 + s)}} \), and \( b_m \) is defined as

\[
b_m = \left( \sqrt{\widetilde{C}_2 \log \frac{2}{\delta} + \sqrt{2K\sqrt{\widetilde{C}_0} \log \frac{2}{\delta} + \sqrt{3\widetilde{C}_0} + \sqrt{\widetilde{C}_1}} \right) m^{\zeta},
\]

where the power index \( \zeta \) is

\[
\zeta = \max \left\{ \frac{\gamma(1 - \beta)}{2}, \frac{\gamma - 1}{2}, \frac{\gamma(\beta - 1) + 2}{4}, \frac{1 - \eta}{2} \right\},
\]

\[
= \max \left\{ \frac{\gamma(1 - \beta)}{2}, \frac{1 - \eta}{2} \right\}.
\]

It tells us that \( \mathcal{W}(R) \subseteq \mathcal{W} \left( a_mR^{\frac{\gamma}{1 + \beta}} + b_m \right) \cup V_R \). Define a sequence \( \{R^{(j)}\}_{j=0}^{J} \) with \( R^{(j)} = a_m(R^{(j-1)})^{s/(2+2s)} + b_m \) with \( J \in \mathbb{N} \), we have \( Z_m = \mathcal{W}(R^{(0)}) \) satisfying

\[
\mathcal{W}(R^{(0)}) \subseteq \mathcal{W}(R^{(1)}) \cup V_{R^{(0)}} \subseteq \cdots \subseteq \mathcal{W}(R^{(J)}) \cup \bigcup_{j=0}^{J-1} V_{R^{(j)}}.
\]

Since each set \( V_{R^{(j)}} \) is at most \( \delta \), the set \( \mathcal{W}(R^{(J)}) \) has measure at least \( 1 - J\delta \).
Denote $\Delta = s/(2 + 2s) < 1/2$, the definition of the sequence $\{R^{(j)}\}_{j=0}^{\infty}$ indicates that

$$R^{(j)} = 0_m^{1+\Delta+\cdots+\Delta^{J-1}}(R^{(0)})^{\Delta_j} + \sum_{j=1}^{J-1}a_m^{1+\Delta+\cdots+\Delta^{j-1}}b_m^{\Delta_j} + b_m.$$  

The first term $R_1^{(J)}$ can be bounded by

$$R_1^{(J)} \leq \tilde{C}_3 m^{(\gamma(1+s)-1)(2+s)} m^{\frac{1}{\eta+2}} 2^{-J},$$  

where $J$ is chosen to be the smallest integer satisfying $J \geq \frac{\log(1/\epsilon)}{\log 2}$. Besides, $R_2^{(J)}$ can be bounded by

$$R_2^{(J)} \leq m^{(\gamma(1+s)-1)(2+s)} \tilde{C}_3 b_1 \sum_{j=0}^{J-1} m^{\left(\gamma - (\gamma(1+s)-1)(2+s)\right) \frac{s^j}{2(2+2s)^j}},$$

with $b_1 := \sqrt{C_2 \log \frac{2}{\epsilon}} + \sqrt{2\kappa \sqrt{C_0} \log \frac{2}{\epsilon}} + \sqrt{3C_0} + \sqrt{C_1}$. When $\zeta \leq (\gamma(1+s)-1)(2+s)$, $R_2^{(J)}$ can be bounded by $\tilde{C}_3 b_1 J m^{(\gamma(1+s)-1)(2+s)}$. When $\zeta > (\gamma(1+s)-1)(2+s)$, $R_2^{(J)}$ can be bounded by $\tilde{C}_3 b_1 J m^\zeta$. Based on the above discussion, we have

$$R^{(J)} \leq (\tilde{C}_3 + \tilde{C}_3 b_1 J)m^{\theta_\epsilon},$$

with $\theta_\epsilon = \max\{\zeta, (\gamma(1+s)-1)(2+s)+\epsilon\}$. So with confidence $1 - J\delta$, there holds

$$\sqrt{\langle f_{z,\lambda}, Tf_{z,\lambda}\rangle_{H_K}} \leq R^{(J)} \leq \tilde{C}_3 \tilde{C}_X J \sqrt{\log \frac{2}{\delta} m^\theta},$$

which follows by replacing $\delta$ by $\delta/J$ and noting $J \leq 2\log(2/\epsilon)$. Finally, we conclude the proof.  

Now, by Lemma 4 and Eq. (27), we are able to prove our main result in Theorem 3.

**Proof.** Take $R$ to be the right hand side of Eq. (28) by Lemma 4, there exists a subset $V'_R$ of $Z_m$ with measure at most $\delta$ such that $Z_m/V'_R \subseteq \mathcal{W}(R)$. Therefore, there exists another subset $V_R$ of $Z_m$ with measure at most $\delta$ such that for any $z \in \mathcal{W}(R)/V_R$, Eq. (27) can be formulated as

$$\mathcal{E}(\pi_B(f_{z,\lambda})) - \mathcal{E}(f_\rho) \leq 3C_0 m^{-\gamma\beta} + \tilde{C}_1 m^{-\theta_1} + \tilde{C}_2 \log \frac{2}{\delta} m^{-1} + 2\kappa \sqrt{C_0} m^{-(\frac{\zeta}{4} + 1)} \log \frac{2}{\delta}$$

$$\tilde{C}_4 \left(\log \frac{2}{\epsilon}\right) \sqrt{\log \frac{2}{\delta} m^{\theta_1}},$$

where $\tilde{C}_4 = \tilde{C}_X (4\tilde{C}_3)^{\frac{1}{\eta+2}}$. Accordingly, by setting the constant $\tilde{C}$ with

$$\tilde{C} = 3C_0 + \tilde{C}_1 + \tilde{C}_2 + 2\kappa \sqrt{C_0} + \tilde{C}_4,$$

we have the following error bound

$$\|\pi_{M^*}(f_{z,\lambda}) - f_\rho\|_{L_{p_x}}^2 \leq \tilde{C} \left(\log \frac{2}{\epsilon}\right)^2 \log \frac{2}{\delta} m^{-\theta},$$

with confidence $1 - \delta$ and the power index $\Theta$ is

$$\Theta = \min \left\{\gamma\beta, \gamma + \eta - 1, \frac{1 - s\theta_\epsilon}{1 + s}\right\},$$

(30)
provided that $\theta_c < 1/s$. Combining Eq. (29) and Eq. (30), when $0 < \eta < 1$, we have

$$\Theta = \min \left\{ \gamma \beta, \gamma + \eta - 1, \frac{2 - s \gamma (1 - \beta)}{2(1 + s)}, \frac{2 - s (1 - \eta)}{2(1 + s)}, \frac{1 - s (\gamma (1 + s) - 1)(2 + s) - s \epsilon}{1 + s} \right\},$$

where $\epsilon$ is given by Eq. (17) and $\eta$ needs to be further restricted by $\max\{0, 1 - 2/s\} < \eta < 1$. These two restrictions ensure that $\Theta$ is positive for a valid learning rate. Specifically, when $\eta \geq 1$, the power index $\Theta$ can be simplified as

$$\Theta = \min \left\{ \gamma \beta, \frac{2 - s \gamma (1 - \beta)}{2(1 + s)}, \frac{1 - s (\gamma (1 + s) - 1)(2 + s) - s \epsilon}{1 + s} \right\},$$

which concludes the proof. \qed