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An empirical feature-based learning algorithm producing sparse approximations ☆

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ABSTRACT

A learning algorithm for regression is studied. It is a modified kernel projection machine (Blanchard et al., 2004 [2]) in the form of a least square regularization scheme with ℓ^1-regularizer in a data dependent hypothesis space based on empirical features (constructed by a reproducing kernel and the learning data). The algorithm has three advantages. First, it does not involve any optimization process. Second, it produces sparse representations with respect to empirical features under a mild condition, without assuming sparsity in terms of any basis or system. Third, the output function converges to the regression function in the reproducing kernel Hilbert space at a satisfactory rate. Our error analysis does not require any sparsity assumption about the underlying regression function.

1. Introduction

We propose a *learning algorithm* for regression. It is a modification of the kernel projection machine (KPM) introduced by Blanchard et al. [2] and analyzed by Zwald [23]. The main advantage of this algorithm is its strong learning ability while producing *sparse approximations* in a very general setting in learning theory, without any hypothesis on sparse representations.

In the regression setting, an input space X is a compact metric space and the output space $Y = \mathbb{R}$. Let $Z = X \times Y$ and ρ be a Borel probability measure on Z with ρ_X the marginal measure on X, and $\rho(\cdot|x)$ the conditional measure at $x \in X$. The *regression function* f_ρ is defined as

$$f_\rho(x) = \int_Y y \, \mathrm{d}\rho(y|x), \quad x \in X.$$

Our learning algorithm produces approximations of f_ρ in a *reproducing kernel Hilbert space* (RKHS). A symmetric continuous function $K : X \times X \to \mathbb{R}$ is called a Mercer kernel if for any finite subset $\{x_i\}_{i=1}^l$ of X, the $l \times l$ matrix $(K(x_i, x_j))_{i,j=1}^l$ is positive semi-definite. For $x \in X$, we denote $K_x = K(\cdot, x)$. The RKHS associated with the Mercer kernel K is a Hilbert

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space $\mathcal{H}_K$ completed by the span of $\{K_x\colon x \in X\}$ under the norm $\|\cdot\|_K$ induced by the inner product $\langle\cdot,\cdot\rangle = \langle\cdot,\cdot\rangle_K$ satisfying $\langle K_x, K_u\rangle = K(x,u)$. We define an *integral operator* L_K on $\mathcal{H}_K$ by

$$L_K(f) = \int_X K_x f(x)\,\mathrm{d}\rho_X(x), \quad f \in \mathcal{H}_K.$$

In this paper, we take a general setting in learning theory satisfying

$$f_\rho = L_K^r(g_\rho) \quad \text{for some } r > 0 \text{ and } g_\rho \in \mathcal{H}_K. \tag{1}$$

Since L_K is a compact, self-adjoint positive operator, we can arrange its eigenvalues $\{\lambda_i\}$ (with multiplicity) as a nonincreasing sequence tending to 0 and take an associated sequence of eigenfunctions $\{\phi_i\}$ to be an orthonormal basis of $\mathcal{H}_K$. Then the power L_K^r of L_K can be written by $L_K^r(\sum_i c_i\phi_i) = \sum_i c_i\lambda_i^r\phi_i$ and assumption (1) is equivalent to $f_\rho = \sum_i d_i\lambda_i^r\phi_i$ where $\{d_i\} \in \ell^2$ represents g_ρ as $g_\rho = \sum_i d_i\phi_i$. The exponent r in (1) measures the decay of the coefficients $\{d_i\lambda_i^r\}$ of f_ρ with respect to the orthonormal basis $\{\phi_i\}$ of $\mathcal{H}_K$. It can be regarded as a measurement for the regularity of the regression function f_ρ.

The eigenfunctions $\{\phi_i\}$ can be used to understand feature maps in learning theory. They can be approximated by *empirical features* $\{\phi_i^{\mathbf{x}}\}$ which are eigenfunctions of an *empirical operator* $L_K^{\mathbf{x}}$ associated with a sample $\mathbf{x} \in X^m$. Throughout this paper we assume that $\mathbf{z} = \{(x_i, y_i)\}_{i=1}^m$ is a sample drawn independently from ρ. We use $\mathbf{x}$ to denote the unlabeled part of the data $\mathbf{x} = \{x_1, \ldots, x_m\}$. The empirical operator $L_K^{\mathbf{x}}$ on $\mathcal{H}_K$ is defined by

$$L_K^{\mathbf{x}}(f) = \frac{1}{m}\sum_{i=1}^m f(x_i)K_{x_i} = \frac{1}{m}\sum_{i=1}^m \langle f, K_{x_i}\rangle K_{x_i}, \quad f \in \mathcal{H}_K,$$

where we have used the reproducing property of the RKHS that asserts $\langle f, K_x\rangle = f(x)$ for any $f \in \mathcal{H}_K$ and $x \in X$. So $L_K^{\mathbf{x}}$ is a normalized sum of m rank-one operators and it is self-adjoint, positive with rank at most m. Therefore we can write the eigensystem of $L_K^{\mathbf{x}}$ as $\{(\lambda_i^{\mathbf{x}}, \phi_i^{\mathbf{x}})\}_i$, with eigenvalues $\lambda_i^{\mathbf{x}}$ arranged in nonincreasing order and $\lambda_i^{\mathbf{x}} = 0$ when $i > m$, and the corresponding eigenfunctions $\{\phi_i^{\mathbf{x}}\}_{i=1}^\infty$ to form an orthonormal basis of $\mathcal{H}_K$. The first m eigenfunctions $\{\phi_i^{\mathbf{x}}\}_{i=1}^m$ can be used as empirical features for learning by regularization schemes in a data dependent hypothesis space $\mathrm{span}\{\phi_i^{\mathbf{x}}\}_{i=1}^m$. The data dependence nature is reflected by the empirical features $\{\phi_i^{\mathbf{x}}\}_{i=1}^m$ obtained from the data $\mathbf{x}$. This idea was used in [2] to introduce the KPM outputting $\sum_{i=1}^m c_{\gamma,i}^{\mathbf{z}}\phi_i^{\mathbf{z}}$ where the coefficient vector $c_\gamma^{\mathbf{z}} = (c_{\gamma,1}^{\mathbf{z}}, \ldots, c_{\gamma,m}^{\mathbf{z}})$ is given with a regularization parameter $\gamma > 0$ by

$$c_\gamma^{\mathbf{z}} = \arg\min_{c\in\mathbb{R}^m}\left\{\frac{1}{m}\sum_{i=1}^m V\left(\sum_{j=1}^m c_j\phi_j^{\mathbf{x}}(x_i), y_i\right) + \gamma\|c\|_0\right\}.$$

Here $V:\mathbb{R}^2 \to \mathbb{R}_+$ is a loss function and $\|c\|_0$ is the number of nonzero entries of the vector $c = (c_1, \ldots, c_m) \in \mathbb{R}^m$. The KPM was analyzed in [23] for classification with $V(f,y) = \max\{1 - yf, 0\}$ and for regression with $V(f,y) = (f-y)^2$ in a Gaussian white noise model.

In this paper we modify the KPM in the least square regression setting by using the ℓ^1-regularizer $\|c\|_1 = \sum_{i=1}^m |c_i|$ instead of the ℓ^0-penalty. Our learning algorithm now takes the form

$$c_\gamma^{\mathbf{z}} = \arg\min_{c\in\mathbb{R}^m}\left\{\frac{1}{m}\sum_{i=1}^m \left(\left(\sum_{j=1}^m c_j\phi_j^{\mathbf{x}}\right)(x_i) - y_i\right)^2 + \gamma\|c\|_1\right\}, \tag{2}$$

and the output function is

$$f_\gamma^{\mathbf{z}} = \sum_{i=1}^m c_{\gamma,i}^{\mathbf{z}}\phi_i^{\mathbf{x}}. \tag{3}$$

We use $f_\gamma^{\mathbf{z}}$ to approximate the regression function f_ρ in $\mathcal{H}_K$.

The following Theorem 1, to be proved in Section 3, represents the solution to problem (2) explicitly, and thus shows computational efficiency of our algorithm.

Theorem 1. *For $i \in \mathbb{N}$, denote*

$$S_i^{\mathbf{z}} = \begin{cases} \frac{1}{m\lambda_i^{\mathbf{x}}}\sum_{j=1}^m y_j\phi_i^{\mathbf{x}}(x_j), & \text{if } \lambda_i^{\mathbf{x}} > 0, \\ 0, & \text{otherwise.}\end{cases}$$

Then the solution to problem (2) *is given with $i = 1, \ldots, m$ by*

$$c^{\mathbf{z}}_{\gamma,i} = \begin{cases} 0, & \text{if } 2\lambda^{\mathbf{x}}_i |S^{\mathbf{z}}_i| \leqslant \gamma, \\ S^{\mathbf{z}}_i - \frac{\gamma}{2\lambda^{\mathbf{x}}_i}, & \text{if } 2\lambda^{\mathbf{x}}_i |S^{\mathbf{z}}_i| > \gamma \text{ and } S^{\mathbf{z}}_i > \frac{\gamma}{2\lambda^{\mathbf{x}}_i}, \\ S^{\mathbf{z}}_i + \frac{\gamma}{2\lambda^{\mathbf{x}}_i}, & \text{if } 2\lambda^{\mathbf{x}}_i |S^{\mathbf{z}}_i| > \gamma \text{ and } S^{\mathbf{z}}_i < -\frac{\gamma}{2\lambda^{\mathbf{x}}_i}. \end{cases} \tag{4}$$

In particular, $c^{\mathbf{z}}_{\gamma,i} = 0$ *if* $\lambda^{\mathbf{x}}_i = 0$.

Remark 1. Let us show how the eigenpairs $\{(\lambda^{\mathbf{x}}_i, \phi^{\mathbf{x}}_i)\}$ can be found explicitly. Let $d^{\mathbf{x}} \leqslant m$ be the rank of the Gramian matrix $\mathbb{K} := (K(x_i, x_j))^m_{i,j=1}$. Denote its eigenvalues as $\hat{\lambda}^{\mathbf{x}}_1 \geqslant \cdots \geqslant \hat{\lambda}^{\mathbf{x}}_{d^{\mathbf{x}}} > \hat{\lambda}^{\mathbf{x}}_{d^{\mathbf{x}}+1} = \cdots = \hat{\lambda}^{\mathbf{x}}_m = 0$, and associated eigenvectors $\{\hat{\mu}_i\}^m_{i=1}$ to form an orthonormal basis of $\mathbb{R}^m$. We have

$$\lambda^{\mathbf{x}}_i = \frac{\hat{\lambda}^{\mathbf{x}}_i}{m} \quad \text{and} \quad \phi^{\mathbf{x}}_i = \frac{1}{\sqrt{\hat{\lambda}^{\mathbf{x}}_i}} \sum_{j=1}^m (\hat{\mu}_i)_j K_{x_j}, \quad \text{for } i = 1, \ldots, d^{\mathbf{x}}, \tag{5}$$

$$\lambda^{\mathbf{x}}_i = 0, \quad \text{and} \quad \phi^{\mathbf{x}}_i|_{\mathbf{x}} = 0, \quad \text{for } i = d^{\mathbf{x}} + 1, \ldots, m.$$

In fact, for $i = 1, \ldots, d^{\mathbf{x}}$, we see that

$$L^{\mathbf{x}}_K\left(\sum_{j=1}^m (\hat{\mu}_i)_j K_{x_j}\right) = \frac{1}{m}\sum_{l=1}^m \sum_{j=1}^m (\hat{\mu}_i)_j K(x_l, x_j) K_{x_l} = \frac{\hat{\lambda}^{\mathbf{x}}_i}{m} \sum_{l=1}^m (\hat{\mu}_i)_l K_{x_l}$$

and $\|\sum_{j=1}^m (\hat{\mu}_i)_j K_{x_j}\|^2_K = \hat{\mu}_i^T \mathbb{K} \hat{\mu}_i = \hat{\lambda}^{\mathbf{x}}_i > 0$.

For $i = d^{\mathbf{x}} + 1, \ldots, m$, $\lambda^{\mathbf{x}}_i > 0$ would imply $\phi^{\mathbf{x}}_i = \frac{1}{\lambda^{\mathbf{x}}_i} L^{\mathbf{x}}_K(\phi^{\mathbf{x}}_i) = \frac{1}{m\lambda^{\mathbf{x}}_i} \sum_{j=1}^m \phi^{\mathbf{x}}_i(x_j) K_{x_j}$ and $\mathbb{K}(\phi^{\mathbf{x}}_i|_{\mathbf{x}}) = m\lambda^{\mathbf{x}}_i \phi^{\mathbf{x}}_i|_{\mathbf{x}}$ where $\phi^{\mathbf{x}}_i|_{\mathbf{x}} = (\phi^{\mathbf{x}}_i(x_j))^m_{j=1}$ is the vector obtained by restricting the function $\phi^{\mathbf{x}}_i$ onto the sampling points. It would then yield $\phi^{\mathbf{x}}_i|_{\mathbf{x}} = 0$ and $\phi^{\mathbf{x}}_i = 0$, a contradiction. So we must have $\lambda^{\mathbf{x}}_i = 0$. It follows that $\langle L^{\mathbf{x}}_K(\phi^{\mathbf{x}}_i), \phi^{\mathbf{x}}_i\rangle = 0$, which means $\frac{1}{m}\sum_{j=1}^m \phi^{\mathbf{x}}_i(x_j)\phi^{\mathbf{x}}_i(x_j) = 0$ and $\phi^{\mathbf{x}}_i|_{\mathbf{x}} = 0$. In this case, $\phi^{\mathbf{x}}_i$ is perpendicular to $\operatorname{span}\{K_{x_i}\}^m_{i=1}$.

Note that for $i = d^{\mathbf{x}} + 1, \ldots, m$, $\lambda^{\mathbf{x}}_i = 0$ implies $c^{\mathbf{z}}_{\gamma,i} = 0$. So $(\sum_{j=1}^m c_j \phi^{\mathbf{x}}_j)(x_i) = (\sum_{j=1}^{d^{\mathbf{x}}} c_j \phi^{\mathbf{x}}_j)(x_i)$ and optimization problem (2) is the same as $c^{\mathbf{x}}_{\gamma,i} = 0$ for $i = d^{\mathbf{x}} + 1, \ldots, m$, and

$$\left(c^{\mathbf{x}}_{\gamma,i}\right)^{d^{\mathbf{x}}}_{i=1} = \arg\min_{c \in \mathbb{R}^{d^{\mathbf{x}}}} \left\{\frac{1}{m}\sum_{i=1}^m \left(\left(\sum_{j=1}^{d^{\mathbf{x}}} c_j \phi^{\mathbf{x}}_j\right)(x_i) - y_i\right)^2 + \gamma\|c\|_1\right\}.$$

We shall conduct analysis for the error $f^{\mathbf{z}}_\gamma - f_\rho$ in the $\mathcal{H}_K$-metric (stronger than the $L^2_{\rho_X}$-metric, as shown in [14]) and derive learning rate for algorithm (2). Note that learning rates with the metric in $\mathcal{H}_K$ yield those with the metric in $C^s(X)$ when K is C^{2s} with $X \subset \mathbb{R}^n$. See [21].

Let us illustrate our analysis by the following examples when the eigenvalues $\{\lambda_i\}$ have some special asymptotic behaviors. Throughout the paper we assume that $|y| \leqslant M$ almost surely for some constant $M > 0$. Denote $\kappa = \sup_{x\in X}\sqrt{K(x,x)}$.

Theorem 2. *Assume* (1) *and for some* $\frac{1}{2r} < \alpha_2 \leqslant \alpha_1 < (1+r)\alpha_2 - \frac{1}{2}$ *and* $0 < D_1, D_2$, *the eigenvalues* $\{\lambda_i\}$ *decay polynomially as*

$$D_1 i^{-\alpha_1} \leqslant \lambda_i \leqslant D_2 i^{-\alpha_2}, \quad \forall i. \tag{6}$$

Let $0 < \delta < 1$. *If we choose*

$$\gamma = \left(2^{1+2r} D_2^{1+r}\|g_\rho\|_K + C_{K,\rho}\left(\log\frac{4}{\delta}\right)^{1+r}\right)\Big/\sqrt{m}, \tag{7}$$

then we have with confidence $1 - \delta$ *that*

$$c^{\mathbf{z}}_{\gamma,i} = 0, \quad \forall m^{\frac{1}{2\alpha_2(1+r)}} + 1 \leqslant i \leqslant m, \tag{8}$$

and

$$\|f^{\mathbf{z}}_\gamma - f_\rho\|_K \leqslant C_1\left(\log\frac{4}{\delta}\right)^{1+r} m^{-\frac{2\alpha_2 r - 1 - 2(\alpha_1 - \alpha_2)}{4\alpha_2(1+r)}}, \tag{9}$$

where $C_{K,\rho} = 8\kappa^2\|g_\rho\|_K(\lambda_1^r + 2^{4r}\kappa^{2r}) + 16M\kappa$ *and* C_1 *is a constant independent of* δ *or* m (*which will be specified in the proof*).

Remark 2. Asymptotic behavior (6) for the eigenvalues $\{\lambda_i\}$ of the integral operator is typical for Sobolev smooth kernels on domains in Euclidean spaces, and the power indices α_1 and α_2 depend on the smoothness of the kernel [12]. When the kernel is smooth enough, α_2 can be arbitrarily large and learning rate (9) takes the form $m^{\epsilon-\frac{r}{2(1+r)}}$ with an arbitrarily small $\epsilon > 0$. When r is large enough, it behaves like $m^{\epsilon-\frac{1}{2}}$ with an arbitrarily small $\epsilon > 0$.

Observe from (8) that the number of nonzero coefficients in the representation $f_\gamma^{\mathbf{z}} = \sum_{i=1}^m c_{\gamma,i}^{\mathbf{z}} \phi_i^{\mathbf{x}}$ is at most $m^{\frac{1}{2\alpha_2(1+r)}}$ which can be much smaller than the sample size m when α_2 and r are large.

Theorem 3. *Assume* (1) *and for some* $1 < \beta_2 \leqslant \beta_1 < \beta_2^{1+r}$ *and* $0 < D_1, D_2$, *the eigenvalues* $\{\lambda_i\}$ *decay exponentially as*

$$D_1 \beta_1^{-i} \leqslant \lambda_i \leqslant D_2 \beta_2^{-i}, \quad \forall i. \tag{10}$$

Let $0 < \delta < 1$ *and choose*

$$\gamma = \left(2^{1+2r} D_2^{1+r} \|g_\rho\|_K + C_{K,\rho}\left(\log\frac{4}{\delta}\right)^{1+r}\right) \Big/ \sqrt{m},$$

then we have with confidence $1-\delta$ *that*

$$c_{\gamma,i}^{\mathbf{z}} = 0, \quad \forall \frac{\log(m+1)}{2(1+r)\log\beta_2} + 1 \leqslant i \leqslant m, \tag{11}$$

and

$$\|f_\gamma^{\mathbf{z}} - f_\rho\|_K \leqslant C_2 \left(\log\frac{4}{\delta}\right)^{1+r} \sqrt{\log(m+1)}\, m^{-\frac{r-(\log\frac{\beta_1}{\beta_2}/\log\beta_2)}{2(1+r)}}, \tag{12}$$

where C_2 *is a constant independent of* δ *or* m (*which will be specified in the proof*).

Remark 3. Asymptotic behavior (10) for the eigenvalues $\{\lambda_i\}$ of the integral operator is typical for analytic kernels on domains in Euclidean spaces [13]. When r is large enough (meaning that f_ρ has high regularity), learning rate (12) behaves like $m^{\epsilon-\frac{1}{2}}$ with an arbitrarily small $\epsilon > 0$.

Again we observe from (11) that the number of nonzero coefficients in the representation $f_\gamma^{\mathbf{z}} = \sum_{i=1}^m c_{\gamma,i}^{\mathbf{z}} \phi_i^{\mathbf{x}}$ is at most $\frac{\log(m+1)}{2(1+r)\log\beta_2}$ which is much smaller than the sample size m.

Theorems 2 and 3 will be proved in Section 6.

2. General analysis

Our general analysis for algorithm (2) is the following theorem to be proved in Section 5.

Theorem 4. *Assume* (1). *Let* $p \in \{1, \ldots, m\}$ *and* $0 < \delta < 1$. *Choose* γ *to satisfy*

$$2^{1+2r} \|g_\rho\|_K \lambda_p^{1+r} + C_{K,\rho} \frac{(\log\frac{4}{\delta})^{1+r}}{\sqrt{m}} \leqslant \gamma, \tag{13}$$

then with confidence $1-\delta$ *we have*

$$\|f_\gamma^{\mathbf{z}} - f_\rho\|_K \leqslant \|g_\rho\|_K \lambda_p^r + \frac{\sqrt{2p}\gamma}{\lambda_p} + \frac{C_3 \log\frac{4}{\delta}}{\lambda_p\sqrt{m}} + C_4 \lambda_p^{\min\{r-1,0\}} \left(\sum_{i=p+1}^{\infty} \lambda_i^{\max\{2r,2\}}\right)^{1/2}, \tag{14}$$

where $C_3 = 16\sqrt{2}M\kappa + 2^{3+\max\{2r,1\}}\|g_\rho\|_K \lambda_1^r \kappa^2$ *and* $C_4 = 2^{\max\{r,1\}}\|g_\rho\|_K$.

Let us give a concrete example with $\mathcal{H}_K$ being the Sobolev space $H^s(X)$ of integer index $s > \frac{n}{2}$ and X being the unit ball $X = \{x \in \mathbb{R}^n\colon\ |x| \leqslant 1\}$ of $\mathbb{R}^n$. When ρ_X is the normalized Lebesgue measure on X, a classical result in the theory of function spaces (see e.g. [17]) asserts that condition (6) for the eigenvalues $\{\lambda_i\}$ holds with $\alpha_1 = \alpha_2 = \frac{2s}{n}$. Also, if $f_\rho \in H^{(2r+1)s}(X)$ for some $r > \frac{n}{4s}$, we know that condition (1) holds true. Then the following learning rate can be derived from Theorem 4, as in the proof of Theorem 2.

Example 1. Let $X = \{x \in \mathbb{R}^n\colon |x| \leqslant 1\}$ and ρ_X be the normalized Lebesgue measure on X. If K is the reproducing kernel of the Sobolev space $H^s(X)$ of integer index $s > \frac{n}{2}$ and $f_\rho \in H^{(2r+1)s}(X)$ for some $r > \frac{n}{4s}$, then by taking $\gamma = C_{s,f_\rho}(\log\frac{4}{\delta})^{1+r}/\sqrt{m}$, we have with confidence $1-\delta$,

$$\left\| f_\gamma^{\mathbf{z}} - f_\rho \right\|_K \leqslant C_1' \left(\log\frac{4}{\delta}\right)^{1+r} m^{-\frac{4sr-n}{8s(1+r)}},$$

where C_{s,f_ρ} and C_1' are constants independent of δ or m.

3. Explicit formula for the coefficients

In this section we prove the representer theorem for algorithm (2). The ℓ^1-regularizer is important in the process. The proof is an immediate consequence of the classical result on soft-thresholding in the context of orthogonal regressors [19], once the orthogonality of $\{\phi_i^{\mathbf{x}}\}$ on the data is derived (see (15) below). We give the proof here for completeness.

Proof of Theorem 1. Let $i \in \mathbb{N}$. Since $(\lambda_i^{\mathbf{x}}, \phi_i^{\mathbf{x}})$ is an eigenpair of $L_K^{\mathbf{x}}$, we have

$$\lambda_i^{\mathbf{x}} \phi_i^{\mathbf{x}} = L_K^{\mathbf{x}} \phi_i^{\mathbf{x}} = \frac{1}{m}\sum_{j=1}^m \phi_i^{\mathbf{x}}(x_j) K_{x_j}.$$

It follows from the reproducing property $\langle K_{x_j}, \phi_l^{\mathbf{x}}\rangle = \phi_l^{\mathbf{x}}(x_j)$ that

$$\delta_{i,l}\lambda_i^{\mathbf{x}} = \left\langle \lambda_i^{\mathbf{x}}\phi_i^{\mathbf{x}}, \phi_l^{\mathbf{x}}\right\rangle = \frac{1}{m}\sum_{j=1}^m \phi_i^{\mathbf{x}}(x_j)\phi_l^{\mathbf{x}}(x_j), \quad i, l \in \mathbb{N}, \tag{15}$$

where $\delta_{i,l} = 1$ if $i = l$ and $\delta_{i,l} = 0$ otherwise. In particular, when $\lambda_i^{\mathbf{x}} = 0$ (which is the case when $i > m$), we have $\phi_i^{\mathbf{x}}(x_j) = 0$ for each $j \in \{1,\dots,m\}$. Consider the minimization problem (2). Note from the definition of $S_i^{\mathbf{z}}$ that $\frac{1}{m}\sum_{j=1}^m y_j \phi_i^{\mathbf{x}}(x_j) = \lambda_i^{\mathbf{x}} S_i^{\mathbf{z}}$. Apply (15). The empirical error part takes the form

$$\begin{aligned}
\frac{1}{m}\sum_{i=1}^m \left(\left(\sum_{j=1}^m c_j\phi_j^{\mathbf{x}}\right)(x_i) - y_i\right)^2 &= \sum_{p,q=1}^m c_p c_q \frac{1}{m}\sum_{i=1}^m \phi_p^{\mathbf{x}}(x_i)\phi_q^{\mathbf{x}}(x_i) - \frac{2}{m}\sum_{i,j=1}^m y_i c_j \phi_j^{\mathbf{x}}(x_i) + \frac{1}{m}\sum_{i=1}^m y_i^2 \\
&= \sum_{p,q=1}^m c_p c_q \delta_{p,q}\lambda_p^{\mathbf{x}} - 2\sum_{i=1}^m \lambda_i^{\mathbf{x}} S_i^{\mathbf{z}} c_i + \frac{1}{m}\sum_{i=1}^m y_i^2 = \sum_{i=1}^m \lambda_i^{\mathbf{x}} c_i^2 - 2\sum_{i=1}^m \lambda_i^{\mathbf{x}} S_i^{\mathbf{z}} c_i + \frac{1}{m}\sum_{i=1}^m y_i^2.
\end{aligned}$$

Hence we have an equivalent form of (2) as

$$c_\gamma^{\mathbf{z}} = \arg\min_{c\in\mathbb{R}^m} \sum_{i=1}^m \left\{\lambda_i^{\mathbf{x}}\left(c_i - S_i^{\mathbf{z}}\right)^2 + \gamma|c_i|\right\}.$$

Thus for $i \in \{1,\dots,m\}$, when $\lambda_i^{\mathbf{x}} = 0$, we have $c_{\gamma,i}^{\mathbf{z}} = 0$. When $\lambda_i^{\mathbf{x}} > 0$, the component $c_{\gamma,i}^{\mathbf{z}}$ can be found by solving the following optimization problem

$$c_{\gamma,i}^{\mathbf{z}} = \arg\min_{c\in\mathbb{R}} \left\{\left(c - S_i^{\mathbf{z}}\right)^2 + \frac{\gamma}{\lambda_i^{\mathbf{x}}}|c|\right\}$$

which has the solution given by (4). This proves the theorem. □

Remark 4. The algorithm can be divided into two parts: computing eigenpairs $\{(\lambda_i^{\mathbf{x}}, \phi_i^{\mathbf{x}})\}$ and solving the minimization problem (2). So the algorithm can be extended to a semi-supervised learning setting: if other than the labeled data $\{(x_i, y_i)\}_{i=1}^m$, we have some extra unlabeled data $\{x_i\}_{i=m+1}^{m'}$, then we can enhance the learning of the eigenfunctions in the first step by making full use of all the data $\{x_i\}_{i=1}^{m'}$.

4. Preliminary analysis for sparsity

Theorem 1 tells us that $c_{\gamma,i}^{\mathbf{z}} = 0$ whenever $2\lambda_i^{\mathbf{x}}|S_i^{\mathbf{z}}| \leqslant \gamma$. We shall choose suitable $p = p(m)$ with $\frac{p(m)}{m} \to 0$ and γ depending on δ such that with confidence $1-\delta$,

$$2\lambda_i^{\mathbf{x}}\left|S_i^{\mathbf{z}}\right| \leqslant \gamma, \quad i = p+1,\dots,m, \tag{16}$$

which would yield the desired sparsity: $c^{\mathbf{z}}_{\gamma,i} = 0$ for $i = p+1, \ldots, m$. The preliminary analysis for sparsity is an important tool for our error analysis.

To achieve the required condition (16), we need to estimate $\lambda^{\mathbf{x}}_i$ and $S^{\mathbf{z}}_i$. The eigenvalue $\lambda^{\mathbf{x}}_i$ is easier to deal with, by the following Hoffman–Wielandt inequality (see [7] for the original inequality for matrices, [8] for the generalization to self-adjoint operators on Hilbert spaces, [9] for an application to approximation of integral operators, and [1] for more general discussion).

Lemma 1. *We have*

$$\sum_{i=1}^{\infty} \big(\lambda_i - \lambda^{\mathbf{x}}_i\big)^2 \leqslant \big\|L_K - L^{\mathbf{x}}_K\big\|^2_{\mathrm{HS}},$$

where $\|\cdot\|_{\mathrm{HS}}$ is the Hilbert–Schmidt norm of $\mathrm{HS}(\mathcal{H}_K)$, the Hilbert space of all Hilbert–Schmidt operators on $\mathcal{H}_K$.

Recall that $\langle A_1, A_2\rangle_{\mathrm{HS}} = \sum_j \langle A_1 e_j, A_2 e_j\rangle_K$ for $A_1, A_2 \in \mathrm{HS}(\mathcal{H}_K)$, where $\{e_j\}$ is an orthonormal basis of $\mathcal{H}_K$. The space $\mathrm{HS}(\mathcal{H}_K)$ is a subspace of the space of bounded linear operators on $\mathcal{H}_K$ with norms satisfying $\|A\|_{\mathcal{H}_K \to \mathcal{H}_K} \leqslant \|A\|_{\mathrm{HS}}$.

The quantity $\|L_K - L^{\mathbf{x}}_K\|_{\mathrm{HS}}$ has been bounded in the literature [4,9,20,14,22].

Lemma 2. *For $0 < \delta < 1$, we have with confidence $1-\delta$,*

$$\big\|L_K - L^{\mathbf{x}}_K\big\|_{\mathrm{HS}} \leqslant \frac{4\kappa^2 \log\frac{2}{\delta}}{\sqrt{m}}. \tag{17}$$

Bounding the coefficients $\{S^{\mathbf{z}}_i\}$ towards (16) is more involved. We first show that $\lambda^{\mathbf{x}}_i S^{\mathbf{z}}_i$ is close to $\lambda^{\mathbf{x}}_i \langle f_\rho, \phi^{\mathbf{x}}_i\rangle$, by means of the following probability inequality in [15] derived from [11,14].

Lemma 3. *Let $\{\xi_i\}_{i=1}^m$ be a set of independent random variables with values in a Hilbert space. If $\|\xi_i\| \leqslant \widetilde{M} < \infty$ almost surely for each $i = 1, \ldots, m$, then for $0 < \delta < 1$, with confidence $1-\delta$ we have*

$$\left\|\frac{1}{m}\sum_{i=1}^m (\xi_i - \mathbb{E}\xi_i)\right\| \leqslant \frac{4\widetilde{M}\log\frac{2}{\delta}}{\sqrt{m}}.$$

Lemma 4. *For $0 < \delta < 1$, with confidence $1-\delta$ we have*

$$\left(\sum_{j\in\mathbb{N}} \big(\lambda^{\mathbf{x}}_j\big(S^{\mathbf{z}}_j - \langle f_\rho, \phi^{\mathbf{x}}_j\rangle\big)\big)^2\right)^{1/2} \leqslant \frac{8M\kappa \log\frac{2}{\delta}}{\sqrt{m}}. \tag{18}$$

Proof. Consider the set of independent random variables $\{\xi_i = (y_i - f_\rho(x_i))K_{x_i}\}_{i=1}^m$ with values in the Hilbert space $\mathcal{H}_K$. They satisfy $\|\xi_i\| = |y_i - f_\rho(x_i)|\sqrt{K(x_i,x_i)} \leqslant 2M\kappa$ and $\mathbb{E}\xi_i = 0$. So by Lemma 3, we know that for any $0 < \delta < 1$, with confidence $1-\delta$ we have $\|\frac{1}{m}\sum_{i=1}^m (y_i - f_\rho(x_i))K_{x_i}\|_K \leqslant \frac{8M\kappa\log\frac{2}{\delta}}{\sqrt{m}}$.

By the definition of $S^{\mathbf{z}}_j$ and the relation $\lambda^{\mathbf{x}}_j \phi^{\mathbf{x}}_j = L^{\mathbf{x}}_K(\phi^{\mathbf{x}}_j) = \frac{1}{m}\sum_{i=1}^m \phi^{\mathbf{x}}_j(x_i)K_{x_i}$, for each $j \in \mathbb{N}$ we have

$$\lambda^{\mathbf{x}}_j\big(S^{\mathbf{z}}_j - \langle f_\rho, \phi^{\mathbf{x}}_j\rangle\big) = \frac{1}{m}\sum_{i=1}^m \big(y_i - f_\rho(x_i)\big)\phi^{\mathbf{x}}_j(x_i) = \left\langle \frac{1}{m}\sum_{i=1}^m \big(y_i - f_\rho(x_i)\big)K_{x_i}, \phi^{\mathbf{x}}_j\right\rangle.$$

But $\{\phi^{\mathbf{x}}_j\}_{j\in\mathbb{N}}$ is an orthonormal basis of $\mathcal{H}_K$, so we have

$$\sum_{j\in\mathbb{N}} \big(\lambda^{\mathbf{x}}_j\big(S^{\mathbf{z}}_j - \langle f_\rho, \phi^{\mathbf{x}}_j\rangle\big)\big)^2 = \left\|\frac{1}{m}\sum_{i=1}^m \big(y_i - f_\rho(x_i)\big)K_{x_i}\right\|^2,$$

and our conclusion follows. □

Next we need to estimate $\lambda^{\mathbf{x}}_i\langle f_\rho, \phi^{\mathbf{x}}_i\rangle$. Since $\{\phi_j\}$ and $\{\phi^{\mathbf{x}}_i\}$ are orthonormal bases of $\mathcal{H}_K$, we observe that

$$\big(L_K - L^{\mathbf{x}}_K\big)\phi^{\mathbf{x}}_i = \sum_{j=1}^{\infty}\langle \phi^{\mathbf{x}}_i, \phi_j\rangle L_K\phi_j - \lambda^{\mathbf{x}}_i\sum_{j=1}^{\infty}\langle\phi^{\mathbf{x}}_i, \phi_j\rangle\phi_j = \sum_{j=1}^{\infty}\langle\phi^{\mathbf{x}}_i, \phi_j\rangle\big(\lambda_j - \lambda^{\mathbf{x}}_i\big)\phi_j.$$

Then the definition of the Hilbert–Schmidt norm tells us that

$$\left\|L_K - L_K^{\mathbf{x}}\right\|_{\mathrm{HS}}^2 = \sum_{i=1}^{\infty} \left\|\left(L_K - L_K^{\mathbf{x}}\right)\phi_i^{\mathbf{x}}\right\|_K^2 = \sum_{i,j=1}^{\infty} \left(\lambda_j - \lambda_i^{\mathbf{x}}\right)^2 \left(\langle \phi_i^{\mathbf{x}}, \phi_j\rangle\right)^2. \tag{19}$$

We shall use expression (19) a few times in our analysis for both sparsity and error bounds.

Lemma 5. *Let $I \subseteq \mathbb{N}$. If $f_\rho = L_K^r(g_\rho)$ for some $r > 0$ and $g_\rho \in \mathcal{H}_K$, then*

$$\left(\sum_{i\in I}\left|\lambda_i^{\mathbf{x}}\langle f_\rho, \phi_i^{\mathbf{x}}\rangle\right|^2\right)^{1/2} \leqslant \lambda_1^r \|g_\rho\|_K \left\|L_K - L_K^{\mathbf{x}}\right\|_{\mathrm{HS}} + 2^r \|g_\rho\|_K \left(\sum_{i\in I}\left(\lambda_i^{\mathbf{x}}\right)^{2(1+r)}\right)^{1/2}.$$

Proof. Write $g_\rho = \sum_{j=1}^{\infty} d_j \phi_j$ with $\{d_j\} \in \ell^2$ and $\|\{d_j\}\|_{\ell^2} = \|g_\rho\|_K$. Then $f_\rho = \sum_{j=1}^{\infty} \lambda_j^r d_j \phi_j$, and for $i \in I$,

$$\lambda_i^{\mathbf{x}}\langle f_\rho, \phi_i^{\mathbf{x}}\rangle = \lambda_i^{\mathbf{x}} \sum_{j=1}^{\infty} \lambda_j^r d_j \langle \phi_j, \phi_i^{\mathbf{x}}\rangle = \lambda_i^{\mathbf{x}} \sum_{j:\ \lambda_j > 2\lambda_i^{\mathbf{x}}} \lambda_j^r d_j \langle \phi_j, \phi_i^{\mathbf{x}}\rangle + \lambda_i^{\mathbf{x}} \sum_{j:\ \lambda_j \leqslant 2\lambda_i^{\mathbf{x}}} \lambda_j^r d_j \langle \phi_j, \phi_i^{\mathbf{x}}\rangle.$$

When $\lambda_j > 2\lambda_i^{\mathbf{x}}$, we have $\lambda_i^{\mathbf{x}} \leqslant \lambda_j - \lambda_i^{\mathbf{x}}$. Hence by the Schwarz inequality,

$$\left|\lambda_i^{\mathbf{x}} \sum_{j:\ \lambda_j > 2\lambda_i^{\mathbf{x}}} \lambda_j^r d_j \langle \phi_j, \phi_i^{\mathbf{x}}\rangle\right| \leqslant \lambda_1^r \left\|\{d_l\}\right\|_{\ell^2} \left(\sum_{j:\ \lambda_j > 2\lambda_i^{\mathbf{x}}} \left(\lambda_j - \lambda_i^{\mathbf{x}}\right)^2 \left(\langle \phi_j, \phi_i^{\mathbf{x}}\rangle\right)^2\right)^{1/2}.$$

It follows from (19) that

$$\left(\sum_{i\in I}\left|\lambda_i^{\mathbf{x}}\langle f_\rho, \phi_i^{\mathbf{x}}\rangle\right|^2\right)^{1/2} \leqslant \lambda_1^r \left\|\{d_j\}\right\|_{\ell^2} \left\|L_K - L_K^{\mathbf{x}}\right\|_{\mathrm{HS}} + 2^r \left\|\{d_j\}\right\|_{\ell^2} \left(\sum_{i\in I}\left(\lambda_i^{\mathbf{x}}\right)^{2(1+r)}\right)^{1/2}.$$

The proof is completed. □

Now we can present our preliminary analysis for sparsity of algorithm (2). The ℓ^1*-regularizer* plays a key role to produce sparse approximations. The phenomenon that the ℓ^1-regularizer can be used to reproduce sparsity has been observed in LASSO [19] and compressed sensing [3,6], usually under the assumption that the approximated function has a sparse representation with respect to some basis or redundant system. Here we show that sparsity of $f_\gamma^{\mathbf{z}}$ in representation (3) can be *produced* under assumption (1) which does not impose any sparse representation and is a common mild condition in learning theory (e.g. [4,14,10]). The choice of the empirical features $\{\phi_i^{\mathbf{x}}\}_{i=1}^m$ is important to ensure the sparsity and convergence rates for the algorithm.

Theorem 5. *Under the same condition as in Theorem* 4*, with confidence* $1 - \delta$ *we have*

$$c_{\gamma,i}^{\mathbf{z}} = 0, \quad \forall i = p+1, \ldots, m.$$

Proof. By Lemmas 2 and 4, we know that for any $0 < \delta < \frac{1}{2}$ there exists a subset Z_δ of Z^m of measure at least $1 - 2\delta$ such that both (17) and (18) hold for each $\mathbf{z} \in Z_\delta$.

Let $i \in \{1, \ldots, m\}$ and $\mathbf{z} \in Z_\delta$. Then from (18), we see that

$$2\lambda_i^{\mathbf{x}}\left|S_i^{\mathbf{z}}\right| \leqslant 2\lambda_i^{\mathbf{x}}\left|\langle f_\rho, \phi_i^{\mathbf{x}}\rangle\right| + 2\lambda_i^{\mathbf{x}}\left|S_i^{\mathbf{z}} - \langle f_\rho, \phi_i^{\mathbf{x}}\rangle\right| \leqslant 2\lambda_i^{\mathbf{x}}\left|\langle f_\rho, \phi_i^{\mathbf{x}}\rangle\right| + \frac{16M\kappa \log\frac{2}{\delta}}{\sqrt{m}}.$$

Applying Lemma 5 to $I = \{i\}$, we have

$$2\lambda_i^{\mathbf{x}}\left|S_i^{\mathbf{z}}\right| \leqslant \lambda_1^r \|g_\rho\|_K \frac{8\kappa^2 \log\frac{2}{\delta}}{\sqrt{m}} + 2^{1+r}\|g_\rho\|_K \left(\lambda_i^{\mathbf{x}}\right)^{1+r} + \frac{16M\kappa \log\frac{2}{\delta}}{\sqrt{m}}. \tag{20}$$

By Lemma 1, $|\lambda_i^{\mathbf{x}} - \lambda_i| \leqslant \|L_K - L_K^{\mathbf{x}}\|_{\mathrm{HS}}$, so $(\lambda_i^{\mathbf{x}})^{1+r} \leqslant (\lambda_i + \|L_K - L_K^{\mathbf{x}}\|_{\mathrm{HS}})^{1+r} \leqslant 2^r(\lambda_i^{1+r} + \|L_K - L_K^{\mathbf{x}}\|_{\mathrm{HS}}^{1+r})$. It follows that for $i = 1, \ldots, m$, the right-hand side of (20) has an upper bound

$$2^{1+2r}\|g_\rho\|_K \lambda_i^{1+r} + C_{K,\rho}\frac{(\log\frac{2}{\delta})^{1+r}}{\sqrt{m}}.$$

Therefore, when

$$2^{1+2r}\|g_\rho\|_K \lambda_p^{1+r} + C_{K,\rho}\frac{(\log\frac{2}{\delta})^{1+r}}{\sqrt{m}} \leqslant \gamma, \tag{21}$$

we know that

$$2\lambda_i^{\mathbf{x}}\left|S_i^{\mathbf{z}}\right| \leqslant \gamma, \quad \forall i = p+1, \ldots, m,$$

which by Theorem 1 yields $c_{\gamma,i}^{\mathbf{z}} = 0$ for $i = p+1, \ldots, m$. Then the conclusion of Theorem 5 follows by scaling 2δ to δ, for which (21) corresponds to (13). □

From Theorem 5 we see immediately that when the eigenvalues $\{\lambda_i\}$ decay polynomially, the sparsity can be explicitly derived by taking p to be $\lceil m^{\frac{1}{2\alpha(1+r)}}\rceil$, the smallest integer greater than or equal to $m^{\frac{1}{2\alpha(1+r)}}$.

Corollary 1. *Assume* (1). *If for some $D_2 > 0$ and $\alpha > 0$, $\lambda_i \leqslant D_2 i^{-\alpha}$ holds for each i, then when $\gamma \geqslant (2^{1+2r} D_2^{1+r}\|g_\rho\|_K + C_{K,\rho}(\log\frac{4}{\delta})^{1+r})/\sqrt{m}$, we have with confidence $1-\delta$,*

$$c_{\gamma,i}^{\mathbf{z}} = 0, \quad \forall m^{\frac{1}{2\alpha(1+r)}} + 1 \leqslant i \leqslant m.$$

5. Error analysis

In this section, we prove our error bounds stated in Theorem 4.

Proof of Theorem 4. We follow the proof of Theorem 5 and know that for any $0 < \delta < \frac{1}{2}$ there exists a subset Z_δ of Z^m of measure at least $1 - 2\delta$ such that both (17) and (18) hold for each $\mathbf{z} \in Z_\delta$. Moreover, when (21) is satisfied and $\mathbf{z} \in Z_\delta$, we have $c_{\gamma,i}^{\mathbf{z}} = 0$ for every $i \in \{p+1, \ldots, m\}$ and those $i \in \{1, \ldots, p\}$ with $\lambda_i^{\mathbf{x}} \leqslant \frac{\lambda_p}{2}$, which follows directly from (20). Hence

$$f_\gamma^{\mathbf{z}} = \sum_{i \in \mathcal{S}} c_{\gamma,i}^{\mathbf{z}} \phi_i^{\mathbf{x}},$$

where $\mathcal{S}$ is defined by $\mathcal{S} = \{i \in \{1, \ldots, p\}\colon \lambda_i^{\mathbf{x}} > \frac{\lambda_p}{2}\}$. It follows from the orthogonal expansion in terms of the orthonormal basis $\{\phi_i^{\mathbf{x}}\}$ that

$$\left\|f_\gamma^{\mathbf{z}} - f_\rho\right\|_K^2 = \sum_{i \in \mathbb{N}\setminus\mathcal{S}} \left(\left\langle f_\rho, \phi_i^{\mathbf{x}}\right\rangle\right)^2 + \sum_{i \in \mathcal{S}} \left(\left\langle f_\rho, \phi_i^{\mathbf{x}}\right\rangle - c_{\gamma,i}^{\mathbf{z}}\right)^2 =: \Delta_1 + \Delta_2. \tag{22}$$

Let $\mathbf{z} \in Z_\delta$ in the following proof.

We bound the first term Δ_1 on the right-hand side of (22) by decomposing it further into two parts with $f_\rho = \sum_{j=1}^\infty \lambda_j^r d_j \phi_j = \sum_{j=p+1}^\infty \lambda_j^r d_j \phi_j + \sum_{j=1}^p \lambda_j^r d_j \phi_j$. Here we have written $g_\rho = \sum_{j=1}^\infty d_j \phi_j$ with $\{d_j\} \in \ell^2$ and $\|\{d_j\}\|_{\ell^2} = \|g_\rho\|_K$.

The part with $\sum_{j=p+1}^\infty$ is easy to deal with: since $\{\phi_i^{\mathbf{x}}\}$ is an orthonormal basis, we have

$$\left(\sum_{i=1}^\infty \left\langle \sum_{j=p+1}^\infty \lambda_j^r d_j \phi_j, \phi_i^{\mathbf{x}}\right\rangle^2\right)^{1/2} = \left\|\sum_{j=p+1}^\infty \lambda_j^r d_j \phi_j\right\|_K \leqslant \|g_\rho\|_K \lambda_{p+1}^r. \tag{23}$$

The part with $\sum_{j=1}^p$ can be estimated by the Schwarz inequality as

$$\left(\sum_{i \in \mathbb{N}\setminus\mathcal{S}} \left\langle \sum_{j=1}^p \lambda_j^r d_j \phi_j, \phi_i^{\mathbf{x}}\right\rangle^2\right)^{1/2} \leqslant \left(\sum_{i \in \mathbb{N}\setminus\mathcal{S}} \left\|\{d_l\}\right\|_{\ell^2}^2 \sum_{j=1}^p \lambda_j^{2r} \left\langle \phi_j, \phi_i^{\mathbf{x}}\right\rangle^2\right)^{1/2}.$$

We continue to bound $\sum_{i \in \mathbb{N}\setminus\mathcal{S}} \sum_{j=1}^p \lambda_j^{2r} \langle \phi_j, \phi_i^{\mathbf{x}}\rangle^2$ in two cases.

Case 1: $r \geqslant 1$. For $i \geqslant p+1$, we observe that $\lambda_j^{2r} \leqslant 2^{2r-1}(\lambda_i^{2r} + (\lambda_j - \lambda_i)^{2r})$ and

$$(\lambda_j - \lambda_i)^{2r} \leqslant \lambda_1^{2r-2}(\lambda_j - \lambda_i)^2 \leqslant 2\lambda_1^{2r-2}\left(\left|\lambda_j - \lambda_i^{\mathbf{x}}\right|^2 + \left|\lambda_i - \lambda_i^{\mathbf{x}}\right|^2\right).$$

It follows that

$$\sum_{j=1}^p \lambda_j^{2r}\left\langle \phi_j, \phi_i^{\mathbf{x}}\right\rangle^2 \leqslant 2^{2r-1} \sum_{j=1}^p \left(\lambda_i^{2r} + 2\lambda_1^{2r-2}\left|\lambda_i - \lambda_i^{\mathbf{x}}\right|^2 + 2\lambda_1^{2r-2}\left|\lambda_j - \lambda_i^{\mathbf{x}}\right|^2\right)\left\langle \phi_j, \phi_i^{\mathbf{x}}\right\rangle^2,$$

which in connection with Lemma 1 and (19) yields

$$\sum_{i=p+1}^{\infty}\sum_{j=1}^{p}\lambda_j^{2r}\langle\phi_j,\phi_i^{\mathbf{x}}\rangle^2 \leqslant 2^{2r-1}\sum_{i=p+1}^{\infty}\lambda_i^{2r}+2^{2r}\lambda_1^{2r-2}\left(\sum_{i=1}^{\infty}\left|\lambda_i-\lambda_i^{\mathbf{x}}\right|^2+\sum_{i,j=1}^{\infty}\left|\lambda_j-\lambda_i^{\mathbf{x}}\right|^2\langle\phi_j,\phi_i^{\mathbf{x}}\rangle^2\right)$$
$$\leqslant 2^{2r-1}\sum_{i=p+1}^{\infty}\lambda_i^{2r}+2^{1+2r}\lambda_1^{2r-2}\left\|L_K-L_K^{\mathbf{x}}\right\|_{\mathrm{HS}}^2.$$

For $i\in\{1,\dots,p\}\setminus\mathcal{S}$ and $j\leqslant p$, we have $|\lambda_j-\lambda_i^{\mathbf{x}}|\geqslant\frac{\lambda_j}{2}$ and hence $\lambda_j^{2r}\leqslant 4\lambda_1^{2r-2}|\lambda_j-\lambda_i^{\mathbf{x}}|^2$. So by (19),

$$\sum_{i\in\{1,\dots,p\}\setminus\mathcal{S}}\sum_{j=1}^{p}\lambda_j^{2r}\langle\phi_j,\phi_i^{\mathbf{x}}\rangle^2\leqslant 4\lambda_1^{2r-2}\sum_{i,j=1}^{\infty}\left|\lambda_j-\lambda_i^{\mathbf{x}}\right|^2\langle\phi_j,\phi_i^{\mathbf{x}}\rangle^2\leqslant 4\lambda_1^{2r-2}\left\|L_K-L_K^{\mathbf{x}}\right\|_{\mathrm{HS}}^2.$$

Thus in the first case we have

$$\sum_{i\in\mathbb{N}\setminus\mathcal{S}}\sum_{j=1}^{p}\lambda_j^{2r}\langle\phi_j,\phi_i^{\mathbf{x}}\rangle^2\leqslant 2^{2r-1}\sum_{i=p+1}^{\infty}\lambda_i^{2r}+4\lambda_1^{2r-2}\left(2^{2r-1}+1\right)\left\|L_K-L_K^{\mathbf{x}}\right\|_{\mathrm{HS}}^2.$$

Case 2: $r<1$. we notice that $\lambda_j^{2r}\leqslant\lambda_p^{2r-2}\lambda_j^2$ and obtain from the above estimate

$$\sum_{i\in\mathbb{N}\setminus\mathcal{S}}\sum_{j=1}^{p}\lambda_j^{2r}\langle\phi_j,\phi_i^{\mathbf{x}}\rangle^2\leqslant 2\lambda_p^{2r-2}\sum_{i=p+1}^{\infty}\lambda_i^{2}+12\lambda_p^{2r-2}\left\|L_K-L_K^{\mathbf{x}}\right\|_{\mathrm{HS}}^2.$$

The bounds for the two cases together with (23) give a bound for Δ_1 as

$$\sqrt{\Delta_1}\leqslant\begin{cases}\|g_\rho\|_K\lambda_{p+1}^r+2^r\left\|\{d_j\}\right\|_{\ell^2}\left(\left(\sum_{i=p+1}^{\infty}\lambda_i^{2r}\right)^{1/2}+2^{1+r}\lambda_1^{r-1}\left\|L_K-L_K^{\mathbf{x}}\right\|_{\mathrm{HS}}\right), & \text{if } r\geqslant 1,\\ \|g_\rho\|_K\lambda_{p+1}^r+2\left\|\{d_j\}\right\|_{\ell^2}\lambda_p^{r-1}\left(\left(\sum_{i=p+1}^{\infty}\lambda_i^{2}\right)^{1/2}+2\left\|L_K-L_K^{\mathbf{x}}\right\|_{\mathrm{HS}}\right), & \text{if } r<1.\end{cases}$$

Now we turn to the second term Δ_2 on the right-hand side of (22). Observe that the case $c_{\gamma,i}^{\mathbf{z}}=0$ corresponds to $|S_i^{\mathbf{z}}|\leqslant\frac{\gamma}{2\lambda_i^{\mathbf{x}}}$. So for either $c_{\gamma,i}^{\mathbf{z}}=0$ or $c_{\gamma,i}^{\mathbf{z}}=S_i^{\mathbf{z}}\pm\frac{\gamma}{2\lambda_i^{\mathbf{x}}}$, we always have

$$\left|\langle f_\rho,\phi_i^{\mathbf{x}}\rangle-c_{\gamma,i}^{\mathbf{z}}\right|\leqslant\frac{\gamma}{2\lambda_i^{\mathbf{x}}}+\left|S_i^{\mathbf{z}}-\langle f_\rho,\phi_i^{\mathbf{x}}\rangle\right|\leqslant\frac{1}{2\lambda_i^{\mathbf{x}}}\left(\gamma+2\lambda_i^{\mathbf{x}}\left|\langle f_\rho,\phi_i^{\mathbf{x}}\rangle-S_i^{\mathbf{z}}\right|\right).$$

But for each $i\in\mathcal{S}$, there holds $2\lambda_i^{\mathbf{x}}\geqslant\lambda_p$. Hence

$$\sqrt{\Delta_2}=\left(\sum_{i\in\mathcal{S}}\left(\langle f_\rho,\phi_i^{\mathbf{x}}\rangle-c_{\gamma,i}^{\mathbf{z}}\right)^2\right)^{1/2}\leqslant\frac{\sqrt{2p}\gamma}{\lambda_p}+\frac{2\sqrt{2}}{\lambda_p}\left(\sum_{i\in\mathcal{S}}\left(\lambda_i^{\mathbf{x}}\left(S_i^{\mathbf{z}}-\langle f_\rho,\phi_i^{\mathbf{x}}\rangle\right)\right)^2\right)^{1/2}.$$

By Lemma 4, this implies

$$\sqrt{\Delta_2}\leqslant\frac{\sqrt{2p}\gamma}{\lambda_p}+\frac{16\sqrt{2}M\kappa\log\frac{2}{\delta}}{\lambda_p\sqrt{m}}.$$

Putting the bounds for Δ_1 and Δ_2 into (22), we know that for $\mathbf{z}\in Z_\delta$, $\|f_\gamma^{\mathbf{z}}-f_\rho\|_K$ is bounded by

$$\|g_\rho\|_K\lambda_p^r+\frac{\sqrt{2p}\gamma}{\lambda_p}+\frac{16\sqrt{2}M\kappa\log\frac{2}{\delta}}{\lambda_p\sqrt{m}}+\begin{cases}2^r\|g_\rho\|_K\left(\left(\sum_{i=p+1}^{\infty}\lambda_i^{2r}\right)^{1/2}+\frac{2^{3+r}\lambda_1^{r-1}\kappa^2\log\frac{2}{\delta}}{\sqrt{m}}\right), & \text{if } r\geqslant 1,\\ 2\|g_\rho\|_K\lambda_p^{r-1}\left(\left(\sum_{i=p+1}^{\infty}\lambda_i^{2}\right)^{1/2}+\frac{8\kappa^2\log\frac{2}{\delta}}{\sqrt{m}}\right), & \text{if } r<1.\end{cases}$$

Then the conclusion of Theorem 4 follows by scaling 2δ to δ. □

6. Achieving both sparsity and learning rates

We are in a position to derive both sparsity and learning rates in two special situations, based on our general analysis.

Proof of Theorem 2. We take $p=\lceil m^{1/(2\alpha_2(1+r))}\rceil$ to give $m^{1/(2\alpha_2(1+r))}\leqslant p\leqslant 2m^{1/(2\alpha_2(1+r))}$, so $\lambda_p^{1+r}\leqslant D_2^{1+r}/\sqrt{m}$. Thus the choice of γ in (7) implies condition (13) of Theorem 5. This verifies (8) as well as the condition of Theorem 4. We bound the first three terms of the right-hand side of (14) in Theorem 4 as follows. First,

$$\|g_\rho\|_K\lambda_p^r+\frac{\sqrt{2p}\gamma}{\lambda_p}+\frac{C_3}{\lambda_p\sqrt{m}}\log\frac{4}{\delta}\leqslant\|g_\rho\|_K D_2^r m^{-\frac{\alpha_2 r}{2\alpha_2(1+r)}}+2D_1^{-1}2^{\alpha_1}\gamma m^{(\frac{1}{2}+\alpha_1)\frac{1}{2\alpha_2(1+r)}}$$
$$+C_3D_1^{-1}2^{\alpha_1}\left(\log\frac{4}{\delta}\right)m^{-\frac{1}{2}+\frac{\alpha_1}{2\alpha_2(1+r)}}\leqslant\widetilde{C}_1\left(\log\frac{4}{\delta}\right)^{1+r}m^{-\frac{2\alpha_2 r-1-(\alpha_1-\alpha_2)}{4\alpha_2(1+r)}},$$

where $\widetilde{C}_1=\|g_\rho\|_K D_2^r+2^{1+\alpha_1}D_1^{-1}(2^{1+r}\|g_\rho\|_K D_2^{1+r}+C_{K,\rho})+C_3D_1^{-1}2^{\alpha_1}$.

When $r\geqslant 1$, since $2r\alpha_2>1$,

$$\sum_{i=p+1}^{\infty}\lambda_i^{\max\{2r,2\}}\leqslant D_2^{2r}\int_p^{\infty}x^{-2r\alpha_2}\,dx=\frac{D_2^{2r}p^{1-2r\alpha_2}}{2r\alpha_2-1}.$$

So the last term of the right-hand side of (14) can be bounded as

$$C_4\lambda_p^{\min\{r-1,0\}}\left(\sum_{i=p+1}^{\infty}\lambda_i^{\max\{2r,2\}}\right)^{1/2}\leqslant\frac{C_4D_2^r}{\sqrt{2r\alpha_2-1}}m^{\frac{1-2r\alpha_2}{4\alpha_2(1+r)}}.$$

Similarly, when $0<r<1$, since $\alpha_2>\frac{1}{2}+(1-r)\alpha_1$, we have

$$C_4\lambda_p^{\min\{r-1,0\}}\left(\sum_{i=p+1}^{\infty}\lambda_i^{\max\{2r,2\}}\right)^{1/2}\leqslant\frac{C_4D_1^{r-1}p^{-\alpha_1(r-1)}D_2p^{(1-2\alpha_2)/2}}{\sqrt{2\alpha_2-1}}\leqslant\frac{C_4D_1^{r-1}D_2}{\sqrt{2\alpha_2-1}}m^{\frac{1+2(1-r)\alpha_1-2\alpha_2}{4\alpha_2(1+r)}}.$$

Now we use Theorem 4 to obtain

$$\left\|f_\rho-f_\gamma^{\mathbf{z}}\right\|_K\leqslant C_1\left(\log\frac{4}{\delta}\right)^{1+r}m^{-\frac{2\alpha_2 r-1-2(\alpha_1-\alpha_2)}{4\alpha_2(1+r)}}$$

with confidence $1-\delta$, where

$$C_1=\widetilde{C}_1+\begin{cases}\frac{C_4D_2^r}{\sqrt{2r\alpha_2-1}}, & \text{when } r\geqslant 1,\\ \frac{C_4D_1^{r-1}D_2}{\sqrt{2\alpha_2-1}}, & \text{when } 0<r<1.\end{cases}$$

The proof of Theorem 2 is complete. □

Proof of Theorem 3. Choosing $p=\lceil\frac{\log(m+1)}{2(1+r)\log\beta_2}\rceil$, we have

$$\frac{\log(m+1)}{2(1+r)\log\beta_2}\leqslant p\leqslant 1+\frac{\log(m+1)}{2(1+r)\log\beta_2}.$$

It follows that

$$m^{\frac{1}{2(1+r)}}\leqslant\beta_2^p\leqslant\beta_1^p\leqslant\beta_1(2m)^{\frac{\log\beta_1}{2(1+r)\log\beta_2}}.$$

The assumption $\lambda_p\leqslant D_2\beta_2^{-p}$ in (10) tells us that

$$\lambda_p^{1+r}\leqslant\frac{D_2^{1+r}}{\sqrt{m}}.$$

Then

$$2^{1+2r}\|g_\rho\|_K\lambda_p^{1+r}+C_{K,\rho}\frac{(\log\frac{4}{\delta})^{1+r}}{\sqrt{m}}\leqslant 2^{1+2r}\|g_\rho\|_K\frac{D_2^{1+r}}{\sqrt{m}}+C_{K,\rho}\frac{(\log\frac{4}{\delta})^{1+r}}{\sqrt{m}}=\gamma.$$

So condition (13) in Theorem 5 holds, and thus we know that with confidence $1-\delta$, $c_{\gamma,i}^{\mathbf{z}}=0$ for $p+1\leqslant i\leqslant m$. This verifies the desired conclusion (11) for sparsity.

Now we turn to the error analysis. By Theorem 4, bound (14) holds with confidence $1-\delta$. We estimate the first three terms of the right-hand side of (14) as

$$\|g_\rho\|_K\lambda_p^r+\frac{\sqrt{2p}\gamma}{\lambda_p}+C_3\frac{\log\frac{4}{\delta}}{\lambda_p\sqrt{m}}\leqslant\|g_\rho\|_K D_2^r m^{-\frac{r}{2(1+r)}}+\widetilde{C}_2\left(\log\frac{4}{\delta}\right)^{1+r}\sqrt{\log(m+1)}m^{-\frac{r-(\log\frac{\beta_1}{\beta_2}/\log\beta_2)}{2(1+r)}}$$
$$+C_3D_1^{-1}\left(\log\frac{4}{\delta}\right)\beta_1 2^{\frac{\log\beta_1}{2(1+r)\log\beta_2}}m^{-\frac{r-(\log\frac{\beta_1}{\beta_2}/\log\beta_2)}{2(1+r)}},\tag{24}$$

Table 1
Parameters.

i	Coefficient A_i	Variation v_i^2	Center P_i
1	2.0	0.62^2	(0.3, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0)
2	−3.5	0.64^2	(0.6, 0.6, 0.6, 0.6, 0.6, 0.6, 0.6, 0.6, 0.6, 0.6)
3	0.7	0.65^2	$\frac{1}{9}$(0.9, 1.7, 2.5, 3.3, 4.1, 4.9, 5.7, 6.5, 7.3, 8.1)

where $\widetilde{C}_2 = (\frac{2}{\log 2} + \frac{1}{(1+r)\log\beta_2})^{1/2}(2^{1+2r}\|g_\rho\|_K D_2^{1+r} + C_{K,\rho})D_1^{-1}\beta_1 2^{\frac{\log\beta_1}{2(1+r)\log\beta_2}}$.

When $r \geqslant 1$, the last term on the right-hand side of (14) can be bounded as

$$C_4\left(\sum_{i=p+1}^{\infty}\lambda_i^{2r}\right)^{1/2} \leqslant C_4 D_2^r\left(\sum_{i=p+1}^{\infty}\beta_2^{-2ri}\right)^{1/2} = \frac{C_4 D_2^r \beta_2^{-pr}}{\sqrt{\beta_2^{2r}-1}} \leqslant \frac{C_4 D_2^r}{\sqrt{\beta_2^{2r}-1}} m^{-\frac{r}{2(1+r)}}. \tag{25}$$

Similarly, when $0 < r < 1$, we have

$$C_4\lambda_p^{r-1}\left(\sum_{i=p+1}^{\infty}\lambda_i^2\right)^{1/2} \leqslant C_4 D_1^{r-1}\beta_1^{1-r}(2m)^{\frac{(1-r)\log\beta_1}{2(1+r)\log\beta_2}}\frac{D_2 m^{-\frac{1}{2(1+r)}}}{\sqrt{\beta_2^2-1}}.$$

Putting this estimate in the case $0 < r < 1$ and (25) in the case $r \geqslant 1$ and (24) into bound (14) tells us that with confidence $1-\delta$, the desired bound (12) for the error holds true with the constant C_2 given by

$$C_2 = \frac{1}{\sqrt{\log 2}}\left(\|g_\rho\|_K D_2^r + C_3 D_1^{-1}\beta_1 2^{\frac{\log\beta_1}{2(1+r)\log\beta_2}}\right) + \widetilde{C}_2 + \frac{1}{\sqrt{\log 2}}\begin{cases} \frac{C_4 D_2^r}{\sqrt{\beta_2^{2r}-1}}, & \text{when } r \geqslant 1, \\ \frac{C_4 D_1^{r-1}\beta_1^{1-r}D_2}{\sqrt{\beta_2^2-1}}2^{\frac{(1-r)\log\beta_1}{2(1+r)\log\beta_2}}, & \text{when } 0 < r < 1. \end{cases}$$

The proof of Theorem 3 is complete. □

7. Further remarks and discussion

We have proposed a modified KPM (2) for regression with ℓ^1-regularizer. Analysis for the error in the $\mathcal{H}_K$-metric has been conducted by means of a priori condition (1) concerning the regularity of the regression with respect to the kernel K and the marginal distribution ρ_X. Our learning rates have been given in terms of special choices of the regularization parameter $\gamma > 0$ which depends on a priori condition (1). Condition (1) is a standard assumption for least square regularized regression with an infinitely dimensional $\mathcal{H}_K$ in the literature of learning theory [4,14,16,18] and almost all theoretical error bounds are based on similar a priori conditions. To the best of our knowledge, the only theoretical error analysis for a learning algorithm with a regularization parameter determined directly by the data was given recently in [5], where a cross-validation approach was rigorously proved.

It is a common practice to choose the regularization parameter by a cross-validation method, which often leads to satisfactory simulation. Here we present an example to show how to choose the regularization parameter γ for algorithm (2). Rigorous theoretical analysis for such a process will be considered in our further study.

Example 2. We generate the regression function f_ρ on $\mathbb{R}^{10}$ as

$$f_\rho(x) = \sum_{i=1}^{3} A_i \exp\left(-\frac{|x-P_i|^2}{2v_i^2}\right), \tag{26}$$

where the parameters are prescribed in Table 1. The data set $\{(x_i, y_i)\}_i^m$ is drawn independently with x_i's uniformly distributed on $[0,1]^{10}$, $y_i = f_\rho(x_i) + \epsilon_i$, and ϵ_i's being Gaussian noise with $\mu = 0$, $\sigma^2 = 0.5^2$ and truncated onto $[-1.5, 1.5]$. The Mercer kernel K is the Gaussian with variance 0.60^2. Table 2 shows the result of the simulation. For comparison, in the last three columns we list the error performance of the least squares regularized regression (LSR) algorithm

$$f_{\mathrm{LSR},\gamma_1}^{\mathbf{z}} = \arg\min_{f\in\mathcal{H}_K}\left\{\frac{1}{m}\sum_{i=1}^{m}\bigl(f(x_i)-y_i\bigr)^2 + \gamma_1\|f\|_K^2\right\}.$$

The notations γ^* and γ_1^* in the second and sixth columns denote the optimal γ and γ_1 respectively, which are selected from a geometric sequence $\{10^{-4}, \ldots, 10^{-2}\}$ of length 60 by 5-fold cross-validation. The learning error is estimated empirically by independently drawing another unlabeled sample set $\{\xi_j\}$ uniformly on $[0,1]^{10}$ of size 12,000 and with $f^{\mathbf{z}} = f_{\gamma^*}^{\mathbf{z}}$ or $f_{\mathrm{LSR},\gamma_1^*}^{\mathbf{z}}$ computing

Table 2
Learning error.

m	γ^*	$\|c^{\mathbf{z}}_{\gamma^*}\|_0$	Error 1	Error 2	γ_1^*	LSR Error 1	LSR Error 2
300	6.261e−3	16	9.708e−2	1.244e−1	6.769e−3	0.3936	0.4951
600	6.769e−3	13	8.472e−2	1.077e−1	5.790e−3	0.3986	0.5042
1200	3.625e−3	16	6.569e−2	9.000e−2	4.582e−3	0.5229	0.6534
1800	2.270e−3	25	5.054e−2	6.467e−2	3.101e−3	0.5500	0.6945
2400	2.099e−3	20	4.289e−2	6.249e−2	2.653e−3	0.5246	0.6764

$$\text{Error 1} = \frac{1}{12{,}000}\sum_{j=1}^{12{,}000} \left| f_\rho(\xi_j) - f^{\mathbf{z}}(\xi_j)\right|,$$

$$\text{Error 2} = \left(\frac{1}{12{,}000}\sum_{j=1}^{12{,}000} \left(f_\rho(\xi_j) - f^{\mathbf{z}}(\xi_j)\right)^2\right)^{1/2}.$$

We have observed sparsity for the coefficients in the representation (3) of the output function in our algorithm. This sparsity is different from that for the representation in terms of $\{K_{x_i}\}_{i=1}^m$. It would be interesting to extend our study to a semi-supervised learning setting as indicated in Remark 4. Another extension is to take empirical features in different ways by means of efficient numerical methods for the Gramian matrix $\mathbb{K}$. Exploring sparsity in such extended settings would be of much value for applications.

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