Just Interpolate: Kernel "Ridgeless" Regression Can Generalize

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Abstract

In the absence of explicit regularization, Kernel "Ridgeless" Regression with nonlinear kernels has the potential to fit the training data perfectly. It has been observed empirically, however, that such interpolated solutions can still generalize well on test data. We isolate a phenomenon of implicit regularization for minimum-norm interpolated solutions which is due to a combination of high dimensionality of the input data, curvature of the kernel function, and favorable geometric properties of the data such as an eigenvalue decay of the empirical covariance and kernel matrices. In addition to deriving a data-dependent upper bound on the out-of-sample error, we present experimental evidence suggesting that the phenomenon occurs in the MNIST dataset.

1 Introduction

According to conventional wisdom, explicit regularization should be added to the least-squares objective when the Hilbert space $\mathcal{H}$ is high- or infinite-dimensional (Golub et al., 1979; Wahba, 1990; Smola and Schölkopf, 1998; Shawe-Taylor and Cristianini, 2004; Evgeniou et al., 2000; De Vito et al., 2005; Alvarez et al., 2012):

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} (f(x_i) - y_i)^2 + \lambda \|f\|_{\mathcal{H}}^2 . \tag{1.1}$$

The regularization term is introduced to avoid "overfitting" since kernels provide enough flexibility to fit training data exactly (i.e. interpolate it). From the theoretical point of view, the regularization parameter λ is a knob for balancing bias and variance, and should be chosen judiciously. Yet, as noted by a number of researchers in the last few years,[1] the best out-of-sample performance, empirically, is often attained by setting the regularization parameter to *zero* and finding the minimum-norm solution among those that interpolate the training data. The mechanism for good out-of-sample performance of this interpolation method has been largely unclear (Zhang et al., 2016; Belkin et al., 2018b).

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As a concrete motivating example, consider the prediction performance of Kernel Ridge Regression for various values[2] of the regularization parameter λ on subsets of the MNIST dataset. For virtually all pairs of digits, the best out-of-sample mean squared error is achieved at $\lambda = 0$. Contrary to the standard bias-variance-tradeoffs picture we have in mind, the test error is monotonically decreasing as we decrease λ (see Figure 1 and further details in Section 5).

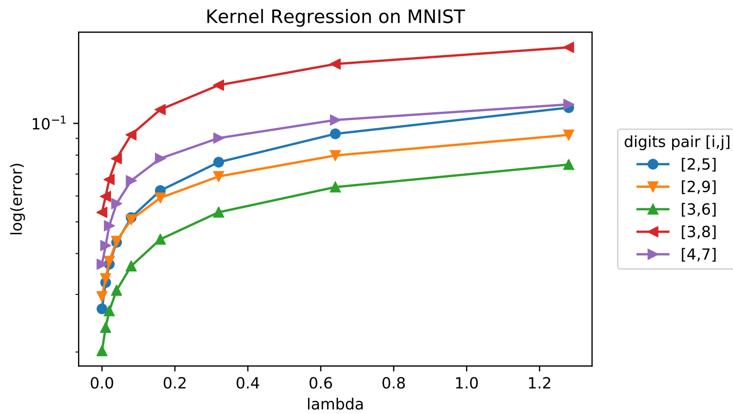

Figure 1: Test performance of Kernel Ridge Regression on pairs of MNIST digits for various values of regularization parameter λ, normalized by variance of y in the test set (for visualization purposes).

We isolate what appears to be a new phenomenon of *implicit regularization* for interpolated minimum-norm solutions in Kernel "Ridgeless" Regression. This regularization is due to the curvature of the kernel function and "kicks in" only for high-dimensional data and for "favorable" data geometry. We provide out-of-sample statistical guarantees in terms of spectral decay of the empirical kernel matrix and the empirical covariance matrix, under additional technical assumptions.

Our analysis rests on the recent work in random matrix theory. In particular, we use a suitable adaptation of the argument of (El Karoui, 2010) who showed that high-dimensional random kernel matrices can be approximated in spectral norm by linear kernel matrices plus a scaled identity. While the message of (El Karoui, 2010) is often taken as "kernels do not help in high dimensions," we show that such a random matrix analysis helps in explaining the good performance of interpolation in Kernel "Ridgeless" Regression.

1.1 Literature Review

Grace Wahba (Wahba, 1990) pioneered the study of nonparametric regression in reproducing kernel Hilbert spaces (RKHS) from the computational and statistical perspectives. One of the key aspects in that work is the role of the decay of eigenvalues of the kernel (at the population level) in rates of convergence. The analysis relies on explicit regularization (ridge parameter λ) for the bias-variance trade-off. The parameter is either chosen to reflect the knowledge of the spectral decay at the population level (De Vito et al., 2005) (typically unknown to statistician), or by the means of cross-validation (Golub et al., 1979). Interestingly, the explicit formula of Kernel Ridge Regression

[2] We take $\lambda \in \{0, 0.01, 0.02, 0.04, 0.08, 0.16, 0.32, 0.64, 1.28\}$.

has been introduced as "kriging" in the literature before, and was widely used in Bayesian statistics (Cressie, 1990; Wahba, 1990).

In the learning theory community, Kernel Ridge Regression is known as a special case of Support Vector Regression (Vapnik, 1998; Shawe-Taylor and Cristianini, 2004; Vovk, 2013). Notions like metric entropy (Cucker and Smale, 2002) or "effective dimension" (Caponnetto and De Vito, 2007) were employed to analyze the guarantees on the excess loss of Kernel Ridge Regression, even when the model is misspecified. We refer the readers to Györfi et al. (2006) for more details. Again, the analysis leans crucially on the explicit regularization, as given by a careful choice of λ, for the model complexity and approximation trade-offs, and mostly focusing on the fixed dimension and large sample size setting. However, to the best of our knowledge, the literature stays relatively quiet in terms of what happens to the minimum norm interpolation rules, i.e., $\lambda = 0$. As pointed out by (Belkin et al., 2018b,a), the existing bounds in nonparametric statistics and learning theory do not apply to interpolated solution either in the regression or the classification setting. In this paper, we aim to answer when and why interpolation in RKHS works, as a starting point for explaining the good empirical performance of interpolation using kernels in practice (Zhang et al., 2016; Belkin et al., 2018b).

2 Preliminaries

2.1 Problem Formulation

Suppose we observe n i.i.d. pairs (x_i, y_i), $1 \le i \le n$, where x_i are the covariates with values in a compact domain $\Omega \subset \mathbb{R}^d$ and $y_i \in \mathbb{R}$ are the responses (or, labels). Suppose the n pairs are drawn from an unknown probability distribution $\mu(x, y)$. We are interested in estimating the conditional expectation function $f_*(x) = \mathbf{E}(\mathbf{y}|\mathbf{x} = x)$, which is assumed to lie in a Reproducing Kernel Hilbert Space (RKHS) $\mathcal{H}$. Suppose the RKHS is endowed with the norm $\|\cdot\|_{\mathcal{H}}$ and corresponding positive definite kernel $K(\cdot,\cdot) : \Omega \times \Omega \to \mathbb{R}$. The interpolation estimator studied in this paper is defined as

$$\widehat{f} = \underset{f \in \mathcal{H}}{\arg\min} \|f\|_{\mathcal{H}}, \quad \text{s.t.} \quad f(x_i) = y_i, \ \forall i \ . \tag{2.1}$$

Let $X \in \mathbb{R}^{n \times d}$ be the matrix with rows $x_1, \ldots, x_n$ and let Y be the vector of values $y_1, \ldots, y_n$. Slightly abusing the notation, we let $K(X, X) = [K(x_i, x_j)]_{ij} \in \mathbb{R}^{n \times n}$ be the kernel matrix. Extending this definition, for $x \in \Omega$ we denote by $K(x, X) \in \mathbb{R}^{1 \times n}$ the matrix of values $[K(x, x_1), \ldots, K(x, x_n)]$. When $K(X, X)$ is invertible, solution to (2.1) can be written in the closed form:

$$\widehat{f}(x) = K(x, X)K(X, X)^{-1}Y. \tag{2.2}$$

In this paper we study the case when $K(X, X)$ is full rank, taking (2.2) as the starting point. For this interpolating estimator, we provide high-probability (with respect to a draw of X) upper bounds on the integrated squared risk of the form

$$\mathbf{E}(\widehat{f}(\mathbf{x}) - f_*(\mathbf{x}))^2 \le \phi_{n,d}(X, f^*). \tag{2.3}$$

Here the expectation is over $\mathbf{x} \sim \mu$ and $Y|X$, and $\phi_{n,d}$ is a data-dependent upper bound. We remark that upper bounds of the form (2.3) also imply prediction loss bounds for excess square loss with respect to the class $\mathcal{H}$, as $\mathbf{E}(\widehat{f}(\mathbf{x}) - f_*(\mathbf{x}))^2 = \mathbf{E}(\widehat{f}(\mathbf{x}) - \mathbf{y})^2 - \mathbf{E}(f_*(\mathbf{x}) - \mathbf{y})^2$.

2.2 Notation and Background on RKHS

For an operator A, its adjoint is denoted by A^*. For real matrices, the adjoint is the transpose. For any $x \in \Omega$, let $K_x : \mathbb{R} \to \mathcal{H}$ be such that

$$f(x) = \langle K_x, f \rangle_{\mathcal{H}} = K_x^* f. \tag{2.4}$$

It follows that for any $x, z \in \Omega$

$$K(x, z) = \langle K_x, K_z \rangle_{\mathcal{H}} = K_x^* K_z. \tag{2.5}$$

Let us introduce the integral operator $\mathcal{T}_\mu : L^2_\mu \to \mathcal{H}$ with respect to the marginal measure $\mu(x)$:

$$\mathcal{T}_\mu f(z) = \int K(z, x) f(x) d\mu(x), \tag{2.6}$$

and denote the set of eigenfunctions of this integral operator by $e(x) = \{e_1(x), e_2(x), \ldots, e_p(x)\}$, where p could be ∞. We have that

$$\mathcal{T}_\mu e_i = t_i e_i, \quad \text{and} \quad \int e_i(x) e_j(x) d\mu(x) = \delta_{ij} \ . \tag{2.7}$$

Denote $T = \mathrm{diag}(t_1, \ldots, t_p)$ as the collection of non-negative eigenvalues. Adopting the spectral notation,

$$K(x, z) = e(x)^* T e(z).$$

Via this spectral characterization, the interpolation estimator (2.1) takes the following form

$$\widehat{f}(x) = e(x)^* T e(X) \left[e(X)^* T e(X) \right]^{-1} Y \ . \tag{2.8}$$

Extending the definition of K_x, it is natural to define the operator $K_X : \mathbb{R}^n \to \mathcal{H}$. Denote the sample version of the kernel operator to be

$$\widehat{\mathcal{T}} := \frac{1}{n} K_X K_X^* \tag{2.9}$$

and the associated eigenvalues to be $\lambda_j(\widehat{\mathcal{T}})$, indexed by j. The eigenvalues are the same as those of $\frac{1}{n} K(X, X)$. It is sometimes convenient to express $\widehat{\mathcal{T}}$ as the linear operator under the basis of eigenfunctions, in the following matrix sense

$$\widehat{\mathcal{T}} = T^{1/2} \left(\frac{1}{n} e(X) e(X)^* \right) T^{1/2}.$$

We write $\mathbf{E}_\mu[\cdot]$ to denote the expectation with respect to the marginal $\mathbf{x} \sim \mu$. Furthermore, we denote by

$$\|g\|^2_{L^2_\mu} = \int g^2 d\mu(x) = \mathbf{E}_\mu g^2(\mathbf{x})$$

the squared L^2 norm with respect to the marginal distribution. The expectation $\mathbf{E}_{Y|X}[\cdot]$ denotes the expectation over $y_1, \ldots, y_n$ conditionally on $x_1, \ldots, x_n$.

3 Main Result

We impose the following assumptions:

(A.1) High dimensionality: there exists universal constants $c, C \in (0, \infty)$ such that $c \le d/n \le C$. Denote by $\Sigma_d = \mathbf{E}_\mu[x_i x_i^*]$ the covariance matrix, assume that $\|\Sigma_d\| \le C$ and $\mathrm{Tr}(\Sigma_d)/d \ge c$.

(A.2) $(8+m)$-moments: $z_i := \Sigma_d^{-1/2} x_i \in \mathbb{R}^d$, $i = 1, \ldots, n$, are i.i.d. random vectors. Furthermore, the entries $z_i(k), 1 \le k \le d$ are i.i.d. from a distribution with $\mathbf{E} z_i(k) = 0, \mathrm{Var}(z_i(k)) = 1$ and $|z_i(k)| \le C \cdot d^{\frac{2}{8+m}}$, for some $m > 0$.

(A.3) Noise condition: there exists a $\sigma > 0$ such that $\mathbf{E}[(f_*(\mathbf{x}) - \mathbf{y})^2 | \mathbf{x} = x] \le \sigma^2$ for all $x \in \Omega$.

(A.4) Non-linear kernel: for any $x \in \Omega$, $K(x,x) \le M$. Furthermore, we consider the inner-product kernels of the form

$$K(x, x') = h\left(\frac{1}{d}\langle x, x'\rangle\right) \tag{3.1}$$

for a non-linear smooth function $h(\cdot) : \mathbb{R} \to \mathbb{R}$ in a neighborhood of 0.

While we state the main theorem for inner product kernels, the results follow under suitable modifications[3] for Radial Basis Function (RBF) kernels of the form

$$K(x, x') = h\left(\frac{1}{d}\||x - x'\|^2\right). \tag{3.2}$$

We postpone the discussion of the assumptions until after the statement of the main theorem.

Let us first define the following quantities related to curvature of h:

$$\alpha := h(0) + h''(0)\frac{\mathrm{Tr}(\Sigma_d^2)}{d^2}, \quad \beta := h'(0),$$
$$\gamma := h\left(\frac{\mathrm{Tr}(\Sigma_d)}{d}\right) - h(0) - h'(0)\frac{\mathrm{Tr}(\Sigma_d)}{d}. \tag{3.3}$$

Theorem 1. *Define*

$$\phi_{n,d}(X, f_*) := \frac{8\sigma^2\|\Sigma_d\|}{d} \sum_j \frac{\lambda_j\left(\frac{XX^*}{d} + \frac{\alpha}{\beta}11^*\right)}{\left[\frac{\gamma}{\beta} + \lambda_j\left(\frac{XX^*}{d} + \frac{\alpha}{\beta}11^*\right)\right]^2}$$
$$+ \|f_*\|_{\mathcal{H}}^2 \inf_{0 \le k \le n}\left\{\frac{1}{n}\sum_{j>k}\lambda_j(K_X K_X^*) + 2M\sqrt{\frac{k}{n}}\right\}. \tag{3.4}$$

Under the assumptions (A.1)-(A.4) and for d large enough, with probability at least $1 - 2\delta - d^{-2}$ *(with respect to a draw of design matrix* X*), the interpolation estimator* (2.2) *satisfies*

$$\mathbf{E}_{Y|X}\|\widehat{f} - f_*\|_{L^2_\mu}^2 \le \phi_{n,d}(X, f_*) + \epsilon(n, d). \tag{3.5}$$

Here the remainder term $\epsilon(n,d) = O(d^{-\frac{m}{8+m}} \log^{4.1} d) + O(n^{-\frac{1}{2}} \log^{0.5}(n/\delta))$.

[3]We refer the readers to El Karoui (2010) for explicit extensions to RBF kernels.

A few remarks are in order. First, the upper bound is *data-dependent* and can serve as a certificate (assuming that an upper bound on $\sigma^2, \|f_*\|^2_{\mathcal{H}}$ can be guessed) that interpolation will succeed. The bound also suggests the regimes when the interpolation method should work. The first term refers to the eigenvalues of the data covariance matrix. This term is small when the data are low rank or have a fast decay of the eigenvalues. Similarly, the second term is small when the eigenvalues of the kernel matrix decay fast or the kernel matrix is effectively low rank. Note that under the assumption (A.1), the quantities α, β, γ are constants.

The two terms in the estimate of Theorem 1 represent upper bounds on the variance and bias of the estimator, respectively. Unlike the regularization analysis (e.g. (Caponnetto and De Vito, 2007)), the two terms are not controlled by a tunable parameter λ. Rather, the choice of the kernel K itself leads to an implicit control of the two terms through curvature of the kernel function, favorable properties of the data, and high dimensionality. As an example, we remark that for the linear kernel ($h(a) = a$), we have $\gamma = 0$, and the bound on the variance term can become very large in the presence of small eigenvalues. In contrast, curvature of h introduces regularization through a non-zero value of γ. We also remark that the bound "kicks in" in the high-dimensional regime: the error term decays with both d and n, and the variance term decays with d (all other quantities being equal).

Discussion of the assumptions

- The assumption in (A.1) that $c \le d/n \le C$ emphasizes that we work in a high-dimensional regime where d scales on the order of n. This assumption is used in the proof of (El Karoui, 2010), and the particular dependence on c, C can be traced in that work if desired. Rather than doing so, we "folded" these constants into mild additional power of $\log d$. The same goes for the assumption on the scaling of the trace of the population covariance matrix.

- The assumption in (A.2) that $Z_i(k)$ are i.i.d. across $k = 1, \ldots, d$ is a strong assumption that is required to ensure the favorable high-dimensional effect. Relaxing this assumption is left for future work.

- The existence of $(8+m)$-moments for $|z_i(k)|$ is enough to ensure $|z_i(k)| \le C \cdot d^{\frac{2}{8+m}}$ for $1 \le i \le n, 1 \le k \le d$ almost surely (see, Lemma 2.2 in Yin et al. (1988)). Remark that the assumption of existence of $(8+m)$-moments in (A.2) is relatively weak. In particular, for bounded or subgaussian variables, $m = \infty$ and the error term $\epsilon(n,d)$ scales as $d^{-1} + n^{-1/2}$, up to log factors. See Lemma A.1 for an explicit calculation in the Gaussian case.

- Finally, as already mentioned, the main result is stated for the inner product kernel, but can be extended to the RBF kernel using an adaptation of the analysis in (El Karoui, 2010).

4 Proofs

To prove Theorem 1, we decompose the mean square error into the bias and variance terms (Lemma 4.1), and provide data-dependent bound for each (Sections 4.2 and 4.3).

4.1 Bias-Variance Decomposition

The following is a standard bias-variance decomposition for an estimator. We remark that it is an equality, and both terms have to be small to ensure the desired convergence.

Lemma 4.1. *The following decomposition for the interpolation estimator* (2.2) *holds*

$$\mathbf{E}_{Y|X}\|\widehat{f} - f_*\|^2_{L^2_\mu} = \mathbf{V} + \mathbf{B}, \tag{4.1}$$

where

$$\mathbf{V} := \int \mathbf{E}_{Y|X} \left| K_x^* K_X (K_X^* K_X)^{-1}(Y - \mathbf{E}[Y|X])\right|^2 d\mu(x), \tag{4.2}$$

$$\mathbf{B} := \int \left| K_x^* \left[K_X (K_X^* K_X)^{-1} K_X^* - I\right] f_* \right|^2 d\mu(x). \tag{4.3}$$

Proof of Lemma 4.1. Recall the closed form solution of the interpolation estimator:

$$\widehat{f}(x) = K_x^* K_X (K_X^* K_X)^{-1} Y = K(x, X) K(X, X)^{-1} Y.$$

Define $E = Y - \mathbf{E}[Y|X] = Y - f_*(X)$. Since $\mathbf{E}_{Y|X} E = 0$, we have

$$\widehat{f}(x) - f_*(x) = K_x^* K_X (K_X^* K_X)^{-1} E + K_x^* \left[K_X (K_X^* K_X)^{-1} K_X^* - I\right] f_*$$

$$\mathbf{E}_{Y|X}(\widehat{f}(x) - f_*(x))^2 = \mathbf{E}_{Y|X}\left(K_x^* K_X (K_X^* K_X)^{-1} E\right)^2 + \left| K_x^* \left[K_X (K_X^* K_X)^{-1} K_X^* - I\right] f_* \right|^2.$$

Using Fubini's Theorem,

$$\begin{aligned} \mathbf{E}_{Y|X}\|\widehat{f} - f_*\|^2_{L^2_\mu} &= \int \mathbf{E}_{Y|X}(\widehat{f}(x) - f_*(x))^2 d\mu(x) \\ &= \int \mathbf{E}_{Y|X}\left| K_x^* K_X (K_X^* K_X)^{-1} E\right|^2 d\mu(x) + \int \left| K_x^* \left[K_X (K_X^* K_X)^{-1} K_X^* - I\right] f_* \right|^2 d\mu(x). \end{aligned}$$

□

4.2 Variance

In this section, we provide upper estimates on the variance part $\mathbf{V}$ in (4.2).

Theorem 2 (Variance)**.** *Let $\delta \in (0, 1)$. Under the assumptions (A.1)-(A.4), with probability at least $1 - \delta - d^{-2}$ with respect to a draw of X,*

$$\mathbf{V} \le \frac{8\sigma^2 \|\Sigma_d\|}{d} \sum_j \frac{\lambda_j\left(\frac{XX^*}{d} + \frac{\alpha}{\beta} 11^*\right)}{\left[\frac{\gamma}{\beta} + \lambda_j\left(\frac{XX^*}{d} + \frac{\alpha}{\beta} 11^*\right)\right]^2} + \frac{8\sigma^2}{\gamma^2} d^{-(4\theta-1)} \log^{4.1} d, \tag{4.4}$$

for $\theta = \frac{1}{2} - \frac{2}{8+m}$ and for d large enough.

Remark 4.1. *Let us discuss the first term in Eq. (4.4) and its role in implicit regularization induced by the curvature of the kernel, eigenvalue decay, and high dimensionality. In practice, the data matrix X is typically centered, so $1^*X = 0$. Therefore the first term is effectively*

$$\sum_j f_c\left(\lambda_j\left(\frac{XX^*}{d}\right)\right), \text{ where } f_c(t) := \frac{t}{(c+t)^2} \le \frac{1}{4c}.$$

This formula explains the effect of implicit regularization, and captures the "effective rank" of the training data X. We would like to emphasize that this measure of complexity is distinct from the classical notion of effective rank for regularized kernel regression (Caponnetto and De Vito, 2007), where the "effective rank" takes the form $\sum_j g_c(t_j)$ with $g_c(t) = t/(c+t)$, with t_j is the eigenvalue of the population integral operator $\mathcal{T}$.

Proof of Theorem 2. From the definition of $\mathbf{V}$ and $E[Y|X] = f_*(X)$,

$$\begin{aligned}\mathbf{V} &= \int \mathbf{E}_{Y|X}\mathrm{Tr}\left(K_x^*K_X(K_X^*K_X)^{-1}(Y-f_*(X))(Y-f_*(X))^*(K_X^*K_X)^{-1}K_X^*K_x\right)d\mu(x) \\ &\le \int \|(K_X^*K_X)^{-1}K_X^*K_x\|^2\|\mathbf{E}_{Y|X}\left[(Y-f_*(X))(Y-f_*(X))^*\right]\|d\mu(x).\end{aligned}$$

Due to the fact that $\mathbf{E}_{Y|X}\left[(Y_i - f_*(X_i))(Y_j - f_*(X_j))\right] = 0$ for $i \ne j$, and $\mathbf{E}_{Y|X}\left[(Y_i - f_*(X_i))^2\right] \le \sigma^2$, we have that $\|\mathbf{E}_{Y|X}\left[(Y - f_*(X))(Y - f_*(X))^*\right]\| \le \sigma^2$ and thus

$$\mathbf{V} \le \sigma^2 \int \|(K_X^*K_X)^{-1}K_X^*K_x\|^2 d\mu(x) = \sigma^2\mathbf{E}_\mu\|K(X,X)^{-1}K(X,\mathbf{x})\|^2.$$

Let us introduce two quantities for the ease of derivation. For α, β, γ defined in (3.3), let

$$K^{\mathrm{lin}}(X,X) := \gamma I + \alpha 11^T + \beta\frac{XX^*}{d} \in \mathbb{R}^{n\times n}, \tag{4.5}$$

$$K^{\mathrm{lin}}(X,x) := \beta\frac{Xx^*}{d} \in \mathbb{R}^{n\times 1}, \tag{4.6}$$

and $K^{\mathrm{lin}}(x,X)$ being the transpose of $K^{\mathrm{lin}}(X,x)$. By Proposition A.2, with probability at least $1-\delta-d^{-2}$, for $\theta = \frac{1}{2} - \frac{2}{8+m}$ the following holds

$$\left\|K(X,X) - K^{\mathrm{lin}}(X,X)\right\| \le d^{-\theta}(\delta^{-1/2} + \log^{0.51} d).$$

As a direct consequence, one can see that

$$\left\|K(X,X)^{-1}\right\| \le \frac{1}{\gamma - d^{-\theta}(\delta^{-1/2} + \log^{0.51} d)} \le \frac{2}{\gamma}, \tag{4.7}$$

$$\begin{aligned}\left\|K(X,X)^{-1}K^{\mathrm{lin}}(X,X)\right\| &\le 1 + \|K(X,X)^{-1}\|\cdot\|K(X,X) - K^{\mathrm{lin}}(X,X)\| \\ &\le \frac{\gamma}{\gamma - d^{-\epsilon'}(\delta^{-1/2} + \log^{0.51} d)} \le 2,\end{aligned} \tag{4.8}$$

provided d is large enough, in the sense that

$$d^{-\theta}(\delta^{-1/2} + \log^{0.51} d) \le \gamma/2.$$

By Lemma A.2 (for Gaussian case, Lemma A.1),

$$\mathbf{E}_\mu \left\| K(\mathbf{x}, X) - K^{\rm lin}(\mathbf{x}, X) \right\|^2 \le d^{-(4\theta-1)} \log^{4.1} d. \tag{4.9}$$

Let us proceed with the bound

$$\begin{aligned}
\mathbf{V} &\le \sigma^2 \mathbf{E}_\mu \|K(X,X)^{-1} K(X,\mathbf{x})\|^2 \\
&\le 2\sigma^2 \mathbf{E}_\mu \|K(X,X)^{-1} K^{\rm lin}(X,\mathbf{x})\|^2 + 2\sigma^2 \left\| K(X,X)^{-1} \right\|^2 \cdot \mathbf{E}_\mu \|K(X,\mathbf{x}) - K^{\rm lin}(X,\mathbf{x})\|^2 \\
&\le 2\sigma^2 \left\| K(X,X)^{-1} K^{\rm lin}(X,X) \right\|^2 \mathbf{E}_\mu \|K^{\rm lin}(X,X)^{-1} K^{\rm lin}(X,\mathbf{x})\|^2 + \frac{8\sigma^2}{\gamma^2} d^{-(4\theta-1)} \log^{4.1} d \\
&\le 8\sigma^2 \mathbf{E}_\mu \|K^{\rm lin}(X,X)^{-1} K^{\rm lin}(X,\mathbf{x})\|^2 + \frac{8\sigma^2}{\gamma^2} d^{-(4\theta-1)} \log^{4.1} d
\end{aligned}$$

where the the third inequality relies on (4.9) and (4.7), and the fourth inequality follows from (4.8). One can further show that

$$\begin{aligned}
&\mathbf{E}_\mu \|K^{\rm lin}(X,X)^{-1} K^{\rm lin}(X,\mathbf{x})\|^2 \\
&= \mathbf{E}_\mu \mathrm{Tr}\left(\left[\gamma I + \alpha 11^* + \beta \frac{XX^*}{d}\right]^{-1} \beta \frac{X\mathbf{x}}{d} \beta \frac{\mathbf{x}^* X^*}{d} \left[\gamma I + \alpha 11^* + \beta \frac{XX^*}{d}\right]^{-1} \right) \\
&= \mathrm{Tr}\left(\left[\gamma I + \alpha 11^* + \beta \frac{XX^*}{d}\right]^{-1} \beta^2 \frac{X\Sigma_d X^*}{d^2} \left[\gamma I + \alpha 11^* + \beta \frac{XX^*}{d}\right]^{-1} \right) \\
&\le \frac{1}{d} \|\Sigma_d\| \mathrm{Tr}\left(\left[\gamma I + \alpha 11^* + \beta \frac{X^*X}{d}\right]^{-1} \beta^2 \frac{X^*X}{d} \left[\gamma I + \alpha 11^* + \beta \frac{X^*X}{d}\right]^{-1} \right) \\
&\le \frac{1}{d} \|\Sigma_d\| \mathrm{Tr}\left(\left[\gamma I + \alpha 11^* + \beta \frac{X^*X}{d}\right]^{-1} \left[\beta^2 \frac{X^*X}{d} + \alpha\beta 11^*\right] \left[\gamma I + \alpha 11^* + \beta \frac{X^*X}{d}\right]^{-1} \right) \\
&= \frac{1}{d} \|\Sigma_d\| \sum_j \frac{\lambda_j \left(\frac{XX^*}{d} + \frac{\alpha}{\beta} 11^* \right)}{\left[\frac{\gamma}{\beta} + \lambda_j \left(\frac{XX^*}{d} + \frac{\alpha}{\beta} 11^* \right) \right]^2}.
\end{aligned}$$

We conclude that with probability at least $1 - \delta - d^{-2}$,

$$\mathbf{V} \le 8\sigma^2 \mathbf{E}_\mu \|K^{\rm lin}(X,X)^{-1} K^{\rm lin}(X,\mathbf{x})\|^2 + \frac{8\sigma^2}{\gamma^2} d^{-(4\theta-1)} \log^{4.1} d \tag{4.10}$$

$$\le \frac{8\sigma^2 \|\Sigma_d\|}{d} \sum_j \frac{\lambda_j \left(\frac{XX^*}{d} + \frac{\alpha}{\beta} 11^* \right)}{\left[\frac{\gamma}{\beta} + \lambda_j \left(\frac{XX^*}{d} + \frac{\alpha}{\beta} 11^* \right) \right]^2} + \frac{8\sigma^2}{\gamma^2} d^{-(4\theta-1)} \log^{4.1} d \tag{4.11}$$

for d large enough. □

4.3 Bias

Theorem 3 (Bias)**.** *Let $\delta \in (0,1)$. The bias, under the only assumptions that $K(x,x) \le M$ for $x \in \Omega$, and X_i's are i.i.d. random vectors, is upper bounded as*

$$\mathbf{B} \le \|f_*\|_{\mathcal{H}}^2 \cdot \inf_{0 \le k \le n} \left\{ \frac{1}{n} \sum_{j>k} \lambda_j(K(X,X)) + 2\sqrt{\frac{k}{n}} \sqrt{\frac{\sum_{i=1}^n K(x_i,x_i)^2}{n}} \right\} + 3M\sqrt{\frac{\log 2n/\delta}{2n}}, \tag{4.12}$$

with probability at least $1-\delta$.

Proof of Theorem 3. For the bias, it is easier to work in the frequency domain using the spectral decomposition. Recalling the spectral characterization in the preliminary section,

$$\begin{aligned}
\mathbf{B} &= \int \left| e^*(x)T^{1/2}\left[T^{1/2}e(X)(e(X)^*Te(X))^{-1}e(X)^*T^{1/2} - I\right]T^{-1/2}f_* \right|^2 d\mu(x) \\
&\le \int \left\| \left[T^{1/2}e(X)(e(X)^*Te(X))^{-1}e(X)^*T^{1/2} - I\right]T^{1/2}e(x) \right\|^2 d\mu(x) \cdot \|T^{-1/2}f_*\|^2 \\
&= \|f_*\|_{\mathcal{H}}^2 \int \left\| \left[T^{1/2}e(X)(e(X)^*Te(X))^{-1}e(X)^*T^{1/2} - I\right]T^{1/2}e(x) \right\|^2 d\mu(x).
\end{aligned}$$

Next, recall the empirical Kernel operator with its spectral decomposition $\widehat{T} = \widehat{U}\widehat{\Lambda}\widehat{U}^*$, with $\widehat{\Lambda}_{jj} = \frac{1}{n}\lambda_j\left(K(X,X)\right)$. Denote the top k columns of $\widehat{U}$ to be $\widehat{U}_k$, and $P_{\widehat{U}_k}^{\perp}$ to be projection to the eigenspace orthogonal to $\widehat{U}_k$. By observing that $T^{1/2}e(X)(e(X)^*Te(X))^{-1}e(X)^*T^{1/2}$ is a projection matrix, it is clear that for all $k \le n$,

$$\mathbf{B} \le \|f_*\|_{\mathcal{H}}^2 \int \left\| P_{\widehat{U}}^{\perp}\left(T^{1/2}e(x)\right) \right\|^2 d\mu(x) \le \|f_*\|_{\mathcal{H}}^2 \int \left\| P_{\widehat{U}_k}^{\perp}\left(T^{1/2}e(x)\right) \right\|^2 d\mu(x). \tag{4.13}$$

We continue the study of the last quantity using techniques from Shawe-Taylor and Cristianini (2004). Denote the function g indexed by rank-k projection U_k as

$$g_{U_k}(x) := \left\| P_{U_k}\left(T^{1/2}e(x)\right) \right\|^2 = \mathrm{Tr}\left(e^*(x)T^{1/2}U_kU_k^T T^{1/2}e(x)\right). \tag{4.14}$$

Clearly, $\|U_kU_k^T\|_F = \sqrt{k}$. Define the function class

$$\mathcal{G}_k := \{g_{U_k}(x) : U_k^T U_k = I_k\}.$$

It is clear that $g_{\widehat{U}_k} \in \mathcal{G}_k$. Observe that $g_{\widehat{U}_k}$ is a random function that depends on the data X, and we will bound the bias term using empirical process theory. It is straightforward to verify that

$$\begin{aligned}
\mathbf{E}_\mu \left\| P_{\widehat{U}_k}^{\perp}\left(T^{1/2}e(\mathbf{x})\right) \right\|^2 &= \int \left\| P_{\widehat{U}}^{\perp}\left(T^{1/2}e(x)\right) \right\|^2 d\mu(x), \\
\widehat{\mathbf{E}}_n \left\| P_{\widehat{U}_k}^{\perp}\left(T^{1/2}e(\mathbf{x})\right) \right\|^2 &= \frac{1}{n}\sum_{i=1}^n \left\| P_{\widehat{U}_k}^{\perp}\left(T^{1/2}e(x_i)\right) \right\|^2 \\
&= \mathrm{Tr}\left(P_{\widehat{U}_k}^{\perp}\widehat{T}P_{\widehat{U}_k}^{\perp}\right) = \sum_{j>k}\widehat{\Lambda}_{jj} = \frac{1}{n}\sum_{j>k}\lambda_j(K(X,X)).
\end{aligned}$$

Using symmetrization Lemma A.3 with $M = \sup_{x\in\Omega} K(x,x)$, with probability at least $1-2\delta$,

$$
\begin{aligned}
&\int \left\| P^{\perp}_{\widehat{U}_k}\left(T^{1/2}e(x)\right)\right\|^2 d\mu(x) - \frac{1}{n}\sum_{j>k}\lambda_j(K(X,X)) \\
=&\mathbf{E}_\mu \left\| P^{\perp}_{\widehat{U}_k}\left(T^{1/2}e(\mathbf{x})\right)\right\|^2 - \widehat{\mathbf{E}}_n \left\| P^{\perp}_{\widehat{U}_k}\left(T^{1/2}e(\mathbf{x})\right)\right\|^2 \\
\leq& \sup_{U_k: U_k^T U_k = I_k} \left(\mathbf{E} - \widehat{\mathbf{E}}_n\right) \left\| P^{\perp}_{\widehat{U}_k}\left(T^{1/2}e(\mathbf{x})\right)\right\|^2 \\
\leq& 2\mathbf{E}_\epsilon \sup_{U_k: U_k^T U_k = I_k} \frac{1}{n}\sum_{i=1}^n \epsilon_i \left(\left\|T^{1/2}e(x_i)\right\|^2 - \left\|P_{U_k}\left(T^{1/2}e(x_i)\right)\right\|^2\right) + 3M\sqrt{\frac{\log 1/\delta}{2n}}
\end{aligned}
$$

by the Pythagorean theorem. Since ϵ_i's are symmetric and zero-mean and $\left\|T^{1/2}e(x_i)\right\|^2$ does not depend on U_k, the last expression is equal to

$$
2\mathbf{E}_\epsilon \sup_{g\in\mathcal{G}_k} \frac{1}{n}\sum_{i=1}^n \epsilon_i g(x_i) + 3M\sqrt{\frac{\log 1/\delta}{2n}}.
$$

We further bound the Rademacher complexity of the set $\mathcal{G}_k$

$$
\begin{aligned}
&\mathbf{E}_\epsilon \sup_{g\in\mathcal{G}_k} \frac{1}{n}\sum_{i=1}^n \epsilon_i g(x_i) = \mathbf{E}_\epsilon \sup_{U_k} \frac{1}{n}\sum_{i=1}^n \epsilon_i g_{U_k}(x_i) \\
&= \mathbf{E}_\epsilon \frac{1}{n} \sup_{U_k} \left\langle U_k U_k^T, \sum_{i=1}^n \epsilon_i T^{1/2} e(x_i) e^*(x_i) T^{1/2} \right\rangle \\
&\leq \frac{\sqrt{k}}{n}\mathbf{E}_\epsilon \left\| \sum_{i=1}^n \epsilon_i T^{1/2} e(x_i) e^*(x_i) T^{1/2} \right\|_F
\end{aligned}
$$

by the Cauchy-Schwarz inequality and the fact that $\|U_k U_k^T\|_F \leq \sqrt{k}$. The last expression is can be further evaluated by the independence of ϵ_i's

$$
\begin{aligned}
\frac{\sqrt{k}}{n}\left\{\mathbf{E}_\epsilon \left\| \sum_{i=1}^n \epsilon_i T^{1/2} e(x_i) e^*(x_i) T^{1/2} \right\|_F^2 \right\}^{1/2} &= \frac{\sqrt{k}}{n}\left\{\sum_{i=1}^n \left\| T^{1/2} e(x_i) e^*(x_i) T^{1/2} \right\|_F^2 \right\} \\
&= \sqrt{\frac{k}{n}}\sqrt{\frac{\sum_{i=1}^n K(x_i,x_i)^2}{n}}.
\end{aligned}
$$

Therefore, for all $k \leq n$, with probability at least $1-2n\delta$,

$$
\mathbf{B} \leq \|f_*\|_{\mathcal{H}}^2 \cdot \inf_{0\leq k\leq n} \left\{ \frac{1}{n}\sum_{j>k}\lambda_j(K(X,X)) + 2\sqrt{\frac{k}{n}}\sqrt{\frac{\sum_{i=1}^n K(x_i,x_i)^2}{n}} + 3M\sqrt{\frac{\log 1/\delta}{2n}} \right\}.
$$

□

Remark 4.2. *Let us compare the bounds obtained in this paper to those one can obtain for classification with a margin.*[4] *For classification, Thm. 21 in Bartlett and Mendelson (2002) shows that the misclassification error is upper bounded with probability at least $1-\delta$ as*

$$\mathbf{E}\mathbf{1}(\mathbf{y}\widehat{f}(\mathbf{x}) < 0) \le \mathbf{E}\phi_\gamma(\mathbf{y}\widehat{f}(\mathbf{x})) \le \widehat{\mathbf{E}}_n\phi_\gamma(\mathbf{y}\widehat{f}(\mathbf{x})) + \frac{C_\delta}{\gamma\sqrt{n}}\sqrt{\frac{\sum_{i=1}^n K(x_i,x_i)}{n}}$$

where $\phi_\gamma(t) := \max(0, 1-t/\gamma)\wedge 1$ is the margin loss surrogate for the indicator loss $\mathbf{1}(t<0)$. By tuning the margin γ, one obtains a family of upper bounds.

Now consider the noiseless regression scenario (i.e. $\sigma = 0$ in (A.1)). In this case, the variance contribution to the risk is zero, and

$$\begin{aligned}\mathbf{E}_{Y|X}\|\widehat{f}-\mathbf{y}\|^2_{L^2_\mu} = \mathbf{E}_{Y|X}\|\widehat{f}-f_*\|^2_{L^2_\mu} &= \mathbf{E}[P_n^\perp f_*]^2 \le \mathbf{E}[P_k^\perp f_*]^2 \\ &\le \widehat{\mathbf{E}}_n[P_k^\perp f_*]^2 + C'_\delta\sqrt{\frac{k}{n}}\sqrt{\frac{\sum_{i=1}^n K(x_i,x_i)^2}{n}}\end{aligned}$$

where P_k is the best-rank k projection (based on X) and $P_k^\perp$ denotes its orthogonal projection. By tuning the parameter k (similar as the $1/\gamma$ in classification), one can balance the RHS to obtain the optimal trade-offs.

However, classification is easier than regression in the following sense: $\widehat{f}$ can present a non-vanishing bias in estimating f_*, but as long as the bias is below the empirical margin level, it plays no effect in the margin loss $\phi_\gamma(\cdot)$. In fact, for classification, under certain conditions, one can prove exponential convergence for the generalization error (Koltchinskii and Beznosova, 2005).

5 Experiments: MNIST

In this section we provide full details of the experiments on MNIST (LeCun et al., 2010). Our first experiment considers the following problem: for each pair of distinct digits (i,j), $i,j \in \{0,1,\dots,9\}$, label one digit as 1 and the other as -1, then fit the Kernel Ridge Regression with Gaussian kernel $k(x,x') = \exp(-\|x-x'\|^2/d)$, where d is the dimension as analyzed in our theory (also the default choice in Scikit-learn package (Pedregosa et al., 2011)). For each of the $\binom{10}{2} = 45$ pairs of experiments, we chose $\lambda = 0$ (no regularization, interpolation estimator), $\lambda = 0.1$ and $\lambda = 1$. We evaluated the performance on the *out-of-sample* test dataset, with the error metric

$$\frac{\sum_i(\widehat{f}(x_i)-y_i)^2}{\sum_i(\bar{y}-y_i)^2}. \tag{5.1}$$

Remarkably, among all 45 experiments, no-regularization performs the best. We refer to the table in Section B for a complete list of numerical results.

The second experiment is to perform the similar task on a finer grid of regularization parameter $\lambda \in \{0, 0.01, 0.02, 0.04, 0.08, 0.16, 0.32, 0.64, 1.28\}$. Again, in all but one pair, the interpolation estimator performs the best in out-of-sample prediction. We refer to Figure 2 for details.

To conclude the experiments, we plot the eigenvalue decay of the empirical kernel matrix and the sample covariance matrix for the 5 experiments shown in the introduction. The two plots are shown

[4] We thank B. Recht for discussions on this point.

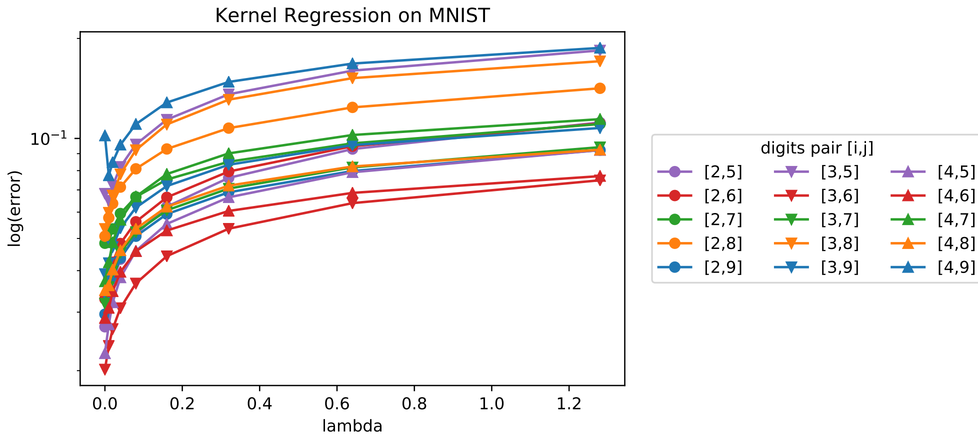

Figure 2: Test error, normalized as in (5.1). The y-axis is on the log scale.

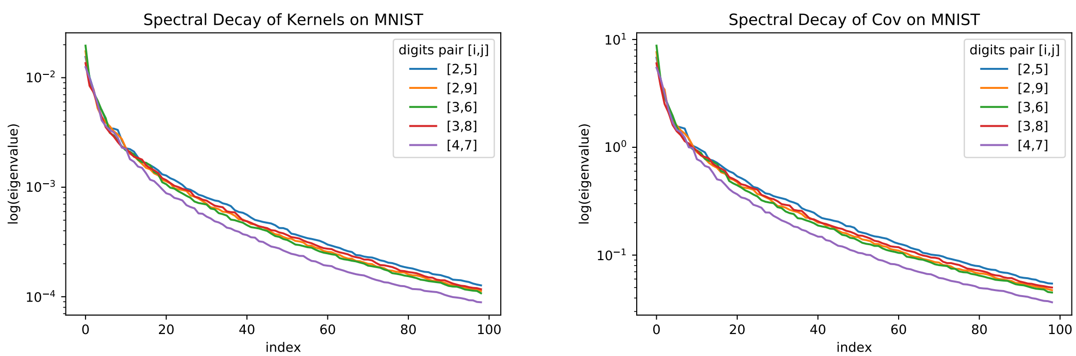

Figure 3: Spectral decay. The y-axis is on the log scale.

in Figure 3. Both plots exhibit a fast decay of eigenvalues, supporting the theoretical finding that interpolation performs well on a test set in such situations.

On the other hand, it is easy to construct examples where the eigenvalues do not decay and interpolation performs poorly. This is the case, for instance, if X_i are i.i.d. from spherical Gaussian. One can show that in the high-dimensional regime, the variance term itself (and not just the upper bound on it) is large. Since the bias-variance decomposition is an equality, it is not possible to establish good L^2_μ convergence.

6 Discussion

This paper is motivated by the work of Belkin et al. (2018b) and Zhang et al. (2016), who, among others, observed the good out-of-sample performance of interpolating rules. This paper continues the line of work in (Belkin et al., 2018a,c; Belkin, 2018) on understanding theoretical mechanisms for the good out-of-sample performance of interpolation.

From an algorithmic point of view, the minimum-norm interpolating solution can be found either by inverting the kernel matrix, or by performing gradient descent on the least-squares objective (starting from 0). Our analysis can then be viewed in the light of recent work on implicit regularization of optimization procedures (Yao et al., 2007; Neyshabur et al., 2014; Gunasekar et al., 2017; Li et al., 2017).

The paper also highlights a novel type of implicit regularization. If one explicitly parametrizes the choice of the kernel by, say, the bandwidth, we are likely to see the familiar picture of the bias-variance trade-off, despite the fact that the estimator is always interpolating. Whether one can achieve optimal rates of estimation (under appropriate assumptions) for the right choice of the bandwidth appears to be an interesting and difficult statistical question. Another open question is whether one can characterize situations when the interpolating minimum-norm solution is dominating the regularized solution in terms of expected performance.

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A Appendix

A.1 Propositions

We first borrow a technical result for concentration of quadratic forms under a mild moment condition.

Proposition A.1 (Adapted from Lemma A.3 in (El Karoui, 2010))**.** *Let $\{Z_i\}_{i=1}^n$ be i.i.d. random vectors in $\mathbb{R}^d$, whose entries are i.i.d., mean 0, variance 1 and $|Z_i(k)| \le C \cdot d^{\frac{2}{8+m}}$. Under the assumption (A.1), for $\theta = \frac{1}{2} - \frac{2}{8+m}$, we have with probability at least $1 - d^{-2}$,*

$$\max_{i,j} \left| \frac{Z_i^* \Sigma Z_j}{d} - \delta_{ij} \frac{\mathrm{Tr}(\Sigma)}{d} \right| \le d^{-\theta} \log^{0.51} d, \tag{A.1}$$

for d large enough.

Proof. The proof follows almost exactly as in Lemma A.3 (El Karoui, 2010). The only point of clarification is that one can assert

$$P\left(\max_{i,j} \left| \frac{Z_i^* \Sigma Z_j}{d} - \delta_{ij} \frac{\mathrm{Tr}(\Sigma)}{d} \right| > 3d^{-\theta} (\log d)^{0.51} \right) \le 2n^2 \exp(-c(\log d)^{1.02}), \tag{A.2}$$

and thus for d large enough, say $c(\log d)^{1.02} \ge 4\log d + \log 2/c^2$, we have that $2n^2 \exp(-c(\log d)^{1.02}) \le d^{-2}$. □

The following proposition is a non-asymptotic adaptation of Theorem 2.1 in (El Karoui, 2010). Our contribution here is only to carefully spell out the terms and emphasize that the error rate can be very slow (this is why (El Karoui, 2010) only provides a convergence in probability result).

Proposition A.2. *Under the assumptions (A.1), (A.2), and (A.4), for $\theta = \frac{1}{2} - \frac{2}{8+m}$, with probability at least $1 - \delta - d^{-2}$,*

$$\left\| K(X,X) - K^{\mathrm{lin}}(X,X) \right\| \le d^{-\theta}(\delta^{-1/2} + \log^{0.51} d), \tag{A.3}$$

for d large enough and δ small enough.

Proof. In (El Karoui, 2010), the approximation error can be decomposed into first-order term E_1 (diagonal approximation), second-order off-diagonal term E_2, and third-order off-diagonal approximation E_3,

$$K(X,X) - K^{\mathrm{lin}}(X,X) := E_1 + E_2 + E_3 \tag{A.4}$$

where $\|E_1\| \le \frac{1}{2} d^{-\theta} \log^{0.51} d$, $\|E_3\| \le \frac{1}{2} d^{-\theta} \log^{0.51} d$ with probability at least $1 - d^{-2}$. However, for E_2 only convergence in probability is obtained. On Page 19 in (El Karoui, 2010), the last line reads

$$\mathbf{E}\mathrm{Tr}(E_2^4) \le C d^{-4\theta}, \tag{A.5}$$

therefore by Chebyshev bound, we have

$$P\left(\|E_2\| \ge d^{-\theta} \delta^{-1/2} \right) \le P(\mathrm{Tr}(E_2^4) \ge d^{-4\theta}\delta^{-2}) \le \frac{\mathbf{E}\mathrm{Tr}(E_2^4)}{d^{-4\theta}\delta^{-2}} \le C\delta^2 \le \delta. \tag{A.6}$$

□

A.2 Lemmas

Lemma A.1 (Gaussian case)**.** *Under the assumptions (A.1), (A.4), and that* $x_i \sim \mathcal{N}(0, \Sigma_d)$ *i.i.d. Then with probability at least* $1 - d^{-2}$ *with respect to a draw of* X*,*

$$\mathbf{E}_\mu \|K(\mathbf{x}, X) - K^{\mathrm{lin}}(\mathbf{x}, X)\|^2 \le d^{-1} \log^{4.1} d, \tag{A.7}$$

with d *large enough.*

Proof. Start with entry-wise Taylor expansion,

$$K(\mathbf{x}, x_j) - K^{\mathrm{lin}}(\mathbf{x}, x_j) = \frac{h''(\xi_j)}{2} \left(\frac{\mathbf{x}^* x_j}{d} \right)^2 .$$

Conditionally on $x_j, 1 \le j \le n$, with probability at least $1 - 2\exp(-t^2/2)$ on $\mathbf{x}$ drawn from $\mathcal{N}(0, \Sigma)$,

$$\left| \frac{\mathbf{x}^* x_j}{d} \right| = \left| \frac{\langle \Sigma^{1/2} x_j, \Sigma^{-1/2} \mathbf{x} \rangle}{d} \right| \le \|\Sigma\| \frac{\|\Sigma^{-1/2} x_j\|}{\sqrt{d}} \frac{t}{\sqrt{d}}, \ \forall j.$$

Using standard χ^2 concentration bound, we know that with probability at least $1 - d^{-2}$ on X

$$\max_j \frac{\|\Sigma^{-1/2} x_j\|^2}{d} \le 1 + \frac{\log^{0.51} d}{\sqrt{d}}. \tag{A.8}$$

Therefore with probability at least $1 - 2\exp(-t^2/2)$ on $\mathbf{x} \sim \mu$, conditionally on $x_j, 1 \le j \le n$

$$\begin{aligned}
\|K(\mathbf{x}, X) - K^{\mathrm{lin}}(\mathbf{x}, X)\| &\le C_1 \sqrt{d} \max_j \left(\frac{\mathbf{x}^* x_j}{d} \right)^2 \\
&\le C\sqrt{d} \cdot \max_j \frac{\|\Sigma^{-1/2} x_j\|^2}{d} \cdot d^{-1} t^2 \\
&\le C \max_j \frac{\|\Sigma^{-1/2} x_j\|^2}{d} \cdot d^{-1/2} t^2
\end{aligned}$$

and due to $E|X|^4 = \int_0^\infty 4t^3 P(|X| > t) dt$, one knows

$$\begin{aligned}
\mathbf{E}_\mu \|K(\mathbf{x}, X) - K^{\mathrm{lin}}(\mathbf{x}, X)\|^2 &\le \left(\max_j \frac{\|\Sigma^{-1/2} x_j\|^2}{d} \right)^2 \left(C d^{-1} \int_0^\infty 8t^3 \exp(-t^2/2) dt \right) \\
&\le d^{-1} \log^{4.1} d
\end{aligned}$$

with probability at least $1 - d^{-2}$ on X, for d large enough. ∎

Lemma A.2 (Weak moment case)**.** *Under the assumptions (A.1), (A.2), and (A.4), for* $\theta = \frac{1}{2} - \frac{2}{8+m}$*, we have with probability at least* $1 - d^{-2}$ *with respect to the draw of* X*, for* d *large enough,*

$$\mathbf{E}_\mu \|K(\mathbf{x}, X) - K^{\mathrm{lin}}(\mathbf{x}, X)\|^2 \le d^{-(4\theta - 1)} \log^{4.1} d. \tag{A.9}$$

Proof. Start with entry-wise Taylor expansion,

$$K(x, x_j) - K^{\mathrm{lin}}(x, x_j) = \frac{h''(\xi_j)}{2} \left(\frac{x^* x_j}{d} \right)^2 .$$

Conditionally on $X_j, 1 \le j \le n$, by Bernstein's inequality, with probability at least $1 - d^{-2}$ on $\mathbf{x}$, for all j

$$\begin{aligned}
\left| \frac{\mathbf{x}^* x_j}{d} \right| &= \left| \frac{\langle \Sigma^{1/2} x_j, \Sigma^{-1/2}\mathbf{x} \rangle}{d} \right| \\
&\le \sqrt{\frac{2\|\Sigma^{1/2} x_j\|^2}{d}} \frac{\log^{0.51} d}{\sqrt{d}} + \frac{1}{3} \frac{\|\Sigma^{1/2} x_j\|_\infty d^{\frac{2}{8+m}} \log^{1.02} d}{d}, \\
&\le \sqrt{\frac{2\|\Sigma^{1/2} x_j\|^2}{d}} \frac{\log^{0.51} d}{\sqrt{d}} + \frac{1}{3} \frac{\|\Sigma^{1/2} x_j\| d^{\frac{2}{8+m}} \log^{1.02} d}{d} \\
&= \sqrt{\frac{2\|\Sigma^{1/2} x_j\|^2}{d}} \frac{\log^{0.51} d}{\sqrt{d}} + \frac{1}{3} \frac{\|\Sigma^{1/2} x_j\|}{\sqrt{d}} d^{\frac{2}{8+m} - \frac{1}{2}} \log^{1.02} d \\
&= \sqrt{\frac{2\|\Sigma^{1/2} x_j\|^2}{d}} \frac{\log^{0.51} d}{\sqrt{d}} + \frac{1}{3} \frac{\|\Sigma^{1/2} x_j\|}{\sqrt{d}} d^{-\theta} \log^{1.02} d
\end{aligned}$$

Apply Proposition A.1, for all j, with probability at least $1 - d^{-2}$ on X

$$\max_j \frac{\|\Sigma^{1/2} x_j\|^2}{d} \le \|\Sigma\| \max_j \frac{\|\Sigma^{-1/2} x_j\|^2}{d} \le C(1 + d^{-\theta} \log^{0.51} d).$$

Therefore with probability at least $1 - d^{-2}$ on $\mathbf{x} \sim \mu$, conditionally on $x_j, 1 \le j \le n$

$$\begin{aligned}
\|K(\mathbf{x}, X) - K^{\mathrm{lin}}(\mathbf{x}, X)\| &\le C_1 \sqrt{d} \max_j \left(\frac{\mathbf{x}^* x_j}{d} \right)^2 \\
&\le C\sqrt{d} \max_j \frac{\|\Sigma^{1/2} x_j\|^2}{d} \left(d^{-1} \log^{1.02} d + d^{-2\theta} \log^{2.04} d \right) \\
&\le C\sqrt{d} \max_j \frac{\|\Sigma^{1/2} x_j\|^2}{d} \left(d^{-1/2} \log^{1.02} d + d^{-2\theta + 1/2} \log^{2.04} d \right).
\end{aligned}$$

Hence, we know the expectation satisfies

$$\begin{aligned}
\mathbf{E}_\mu \|K(\mathbf{x}, X) - K^{\mathrm{lin}}(\mathbf{x}, X)\|^2 \le & \left(\max_j \frac{\|\Sigma^{1/2} x_j\|^2}{d} \right)^2 \left(Cd^{-1} \log^{2.04} d + Cd^{-4\theta+1} \log^{4.08} d \right) \\
& + (M + Cd^{\frac{4}{8+m}})^2 d^{-2} \\
\le & \, d^{-4\theta+1} \log^{4.1} d
\end{aligned}$$

with probability at least $1 - d^{-2}$ on X, for d large enough.

□

Lemma A.3. *Let $g(x) \in \mathbb{R}$ that satisfies $\forall g \in \mathcal{G}$, $|g(x)| \le M$ for all x. Then with probability at least $1 - 2\delta$, we have for i.i.d. $x_i \sim \mu$*

$$\sup_{g\in\mathcal{G}} \left| \mathbf{E} g(\mathbf{x}) - \widehat{\mathbf{E}}_n g(\mathbf{x}) \right| \le \mathbf{E} \sup_{g\in\mathcal{G}} \left| \mathbf{E} g(\mathbf{x}) - \widehat{\mathbf{E}}_n g(\mathbf{x}) \right| + M\sqrt{\frac{\log 1/\delta}{2n}} \tag{A.10}$$

$$\le 2\mathbf{E} \sup_{g\in\mathcal{G}} \frac{1}{n} \sum_i \epsilon_i g(x_i) + M\sqrt{\frac{\log 1/\delta}{2n}} \tag{A.11}$$

$$\le 2\mathbf{E}_\epsilon \sup_{g\in\mathcal{G}} \frac{1}{n} \sum_i \epsilon_i g(x_i) + 3M\sqrt{\frac{\log 1/\delta}{2n}} \tag{A.12}$$

where $\mathbf{E}_\epsilon$ denotes the conditional expectation with respect to i.i.d. Rademacher random variables $\epsilon_1, \ldots, \epsilon_n$.

Proof. The proof is a standard exercise using McDiarmid's inequality and symmetrization. □

B MNIST Result

Here the error is in percentage, so 2.921 corresponds to an error 2.921%.

```
Digits pair: [i, j] Error: [Lambda=0   Lambda=0.1 Lambda=1]
digits pair: [0, 1] error: [0.541      1.006      1.710]
digits pair: [0, 2] error: [2.921      4.689      7.584]
digits pair: [0, 3] error: [1.601      3.386      5.841]
digits pair: [0, 4] error: [1.285      2.610      4.019]
digits pair: [0, 5] error: [2.567      4.957      8.226]
digits pair: [0, 6] error: [2.969      5.239      8.359]
digits pair: [0, 7] error: [1.218      2.808      4.810]
digits pair: [0, 8] error: [2.541      3.725      5.526]
digits pair: [0, 9] error: [2.031      3.726      5.482]
digits pair: [1, 2] error: [2.487      3.699      7.220]
digits pair: [1, 3] error: [1.644      2.688      4.913]
digits pair: [1, 4] error: [1.221      2.089      3.552]
digits pair: [1, 5] error: [1.455      2.860      4.904]
digits pair: [1, 6] error: [1.615      2.438      3.913]
digits pair: [1, 7] error: [2.157      3.693      5.689]
digits pair: [1, 8] error: [2.468      3.571      7.486]
digits pair: [1, 9] error: [1.441      2.513      3.941]
digits pair: [2, 3] error: [4.713      7.853     13.253]
digits pair: [2, 4] error: [2.998      5.602      9.525]
digits pair: [2, 5] error: [2.711      5.471     10.491]
digits pair: [2, 6] error: [3.287      5.917     10.519]
digits pair: [2, 7] error: [4.836      6.930     10.530]
digits pair: [2, 8] error: [5.080      8.460     13.531]
digits pair: [2, 9] error: [2.958      5.335      8.763]
digits pair: [3, 4] error: [1.783      3.847      6.880]
digits pair: [3, 5] error: [6.822     10.129     17.565]
digits pair: [3, 6] error: [2.017      3.887      7.088]
digits pair: [3, 7] error: [3.184      5.486      8.963]
digits pair: [3, 8] error: [5.345      9.766     16.442]
digits pair: [3, 9] error: [3.909      6.494     10.330]
digits pair: [4, 5] error: [2.254      4.871      8.757]
digits pair: [4, 6] error: [2.878      4.793      7.396]
digits pair: [4, 7] error: [3.711      7.036     11.015]
digits pair: [4, 8] error: [3.488      5.615      8.888]
digits pair: [4, 9] error: [10.199    11.587     18.058]
digits pair: [5, 6] error: [5.014      7.716     12.682]
digits pair: [5, 7] error: [2.537      4.683      8.268]
digits pair: [5, 8] error: [5.868      9.587     16.261]
digits pair: [5, 9] error: [4.562      6.578     10.935]
digits pair: [6, 7] error: [1.114      2.864      4.894]
digits pair: [6, 8] error: [4.102      5.954      9.265]
digits pair: [6, 9] error: [1.267      2.944      4.935]
digits pair: [7, 8] error: [3.197      5.623      9.093]
digits pair: [7, 9] error: [6.598     10.841     17.252]
digits pair: [8, 9] error: [4.640      7.673     12.070]
```