

DENSITY ESTIMATION IN RKHS WITH APPLICATION TO KOROBOV SPACES IN HIGH DIMENSIONS

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Abstract. A kernel method for estimating a probability density function (pdf) from an i.i.d. sample drawn from such density is presented. Our estimator is a linear combination of kernel functions, the coefficients of which are determined by a linear equation. An error analysis for the mean integrated squared error is established in a general reproducing kernel Hilbert space setting. The theory developed is then applied to estimate pdfs belonging to weighted Korobov spaces, for which a dimension independent convergence rate is established. Under a suitable smoothness assumption, our method attains a rate arbitrarily close to the optimal rate. Numerical results support our theory.

Key words. Density estimation, High-dimensional approximation, Kernel methods

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1. Introduction. In this paper, we propose and analyse a kernel-based method to approximate probability density functions on a domain of an arbitrary dimension. Density approximations have a long history [29, 34]. However, these classical methods typically suffer from the so-called curse of dimensionality, i.e. their error convergence rates deteriorate in dimension, and thus their practical use is limited to relatively low-dimensional settings; see for example [29, 34] for more details. Over the past decade there has been increasing interest in studying random variables taking values in high-dimensional spaces. For instance, in Uncertainty Quantification applications one is typically interested to study statistics of the solution of a complex differential model that contains random components; see for example [3, 7, 24]. Our work is partly inspired by this type of applications.

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and (D, \mathcal{B}) be a measurable space. Given independent random variables $Y_1, \dots, Y_M: \Omega \rightarrow D$ that follow an identical distribution defined by a density f with respect to a measure μ on \mathcal{B} , we aim to approximate f with a positive definite kernel $K(\cdot, \cdot): D \times D \rightarrow \mathbb{R}$. In particular, we seek for an approximation of the form

$$(1.1) \quad f(\cdot) \approx \sum_{k=1}^N c_k(\omega) K(x_k, \cdot),$$

where N is a positive integer, $X := \{x_k \mid k = 1, \dots, N\}$ is a pre-selected point set in D , and the (random) coefficients $c_1(\omega), \dots, c_N(\omega) \in \mathbb{R}$, which depend on the sample $\mathbf{Y}(\omega) := (Y_1(\omega), \dots, Y_M(\omega))$, are determined by solving a linear equation. More precisely, we denote the approximate density of the form (1.1) by $f_{M,N;\mathbf{Y}}^\lambda$ and construct it as the solution of the following problem: Find $f_{M,N;\mathbf{Y}}^\lambda \in V_N$ such that

$$(1.2) \quad \langle f_{M,N;\mathbf{Y}}^\lambda, v \rangle_{L_\mu^2(D)} + \lambda \langle f_{M,N;\mathbf{Y}}^\lambda, v \rangle_K = \frac{1}{M} \sum_{m=1}^M v(Y_m) \quad \text{for all } v \in V_N,$$

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where $\lambda > 0$ is a “regularization” parameter, and

$$V_N := V_N(X) := \text{span}\{K(x_k, \cdot) \mid k = 1, \dots, N\}.$$

Here, $\langle \cdot, \cdot \rangle_{L^2_\mu(D)}$ is the L^2 -inner product with respect to the measure μ on (D, \mathcal{B}) , and $\langle \cdot, \cdot \rangle_K$ is the inner product of the reproducing kernel Hilbert space (RKHS) \mathcal{N}_K defined by K . The set of points $X := \{x_k\}_{k=1}^N \subset D$ determines the approximation space $V_N(X)$, and they should be chosen carefully. More details will be discussed in Section 2.

The approximation of type (1.2) is a variant of what Hegland et al. proposed in [20], in which a standard finite element space was considered as the approximation space. As such, the method proposed in [20] becomes infeasible when the dimension of D is large. Peherstorfer et al. [27] considered sparse-grid basis functions instead of the standard finite element basis functions in the method of [20], to deal with larger dimensions, but the approximation error and its dependence on the dimension is not investigated. Roberts and Bolt [28] considered a method in the same vein as [27], but without the regularization term. They outline an error analysis, but their claimed estimates will result in a mean integrated squared error (MISE) decaying as $\mathcal{O}_d(|\log M|^{2d} M^{-4/5})$ with a constant exponentially increasing in d . Another class of density estimators that have been developed e.g. in [19, 36] is the MAP estimator. The methods in [19, 36] involve minimising a non-linear functional via Newton’s method, whereas our method only involves solving the linear equation (1.2). Moreover, the method in [19] is limited to three dimension as the dimension of the domain of the target density, and in [36] the approximation error is not investigated. In contrast to these works, as we will see later in Section 4, under suitable smoothness/periodicity assumptions on the density f we will establish a faster, *dimension-independent* error decay in terms of MISE.

To analyse the error of our method, we first derive a general theory in a RKHS setting. Under the assumption that the target density function is in the RKHS associated with the kernel K , we will establish an MISE bound. It turns out that the bias can be bounded by an orthogonal projection error plus a regularization term, while the variance decays at a rate arbitrarily close to M^{-1} provided that f is sufficiently “smooth”. More precisely, we have

$$(\text{MISE}) \leq \|\mathcal{P}_N f - f\|_{L^2_\mu(D)}^2 + \mathcal{O}(\lambda^2 + M^{-1}\lambda^{-\tau}),$$

where \mathcal{P}_N is the \mathcal{N}_K -orthogonal projection onto V_N , and given that f is in a sufficiently small RKHS, $\tau \in (0, 1]$ can be taken arbitrarily small; see Theorem 3.6. Since a large number of projection error estimates are readily available for various kernels, this estimate will directly provide estimates on the MISE. For f smooth, the projection error typically decays fast in N . Hence, in such cases, for the optimal choice of N and λ depending on the sample size M , the MISE decays at a rate arbitrarily close to M^{-1} . Such a rate may be called *near-optimal*, since, in view of the lower bound in [5], the rate M^{-1} is optimal.

We will demonstrate the strength of this theory through an example. We will apply the theory to the so-called Korobov kernel and the corresponding space, which is, roughly speaking, a Sobolev space with periodicity. Given that the target density is in this space, it turns out that the bias can be bounded by the interpolation error up to a regularization term, where the interpolation points are $\{x_k\}_{k=1}^N$. Note that the kernel interpolation is optimal among all approximations that use only the same function values of f , in the sense that it gives the least possible worst-case error in any norm that is no stronger than the RKHS-norm; see for example [Theorem 2, 23] for a proof of this optimality result for the same setting as this paper. As such, the interpolation error can be bounded by the approximation error delivered by other algorithms that use evaluations at the same set of points $\{x_k\}_{k=1}^N$. Approximation errors in Korobov spaces by kernel interpolation have been extensively studied [38, 37, 23]. In this paper,

following [23], as $\{x_k\}_{k=1}^N$ we choose the so-called rank-1 lattice points. Moreover, like [23], we consider target (density) functions with a favourable anisotropy structure by assuming that they are in a *weighted* space. By exploiting this structure, we establish convergence-rate estimates that are *independent of the dimension*. When the smoothness parameter of the Korobov space is an even integer, the rate established turns out to be *asymptotically minimax* up to an arbitrarily small $\epsilon > 0$. Moreover, the lattice structure gives a circulant matrix for the linear equation, which makes solving the equation fast. Numerical results support our theory.

Random variables having a periodic density function arise for example as circular observations. Although they are important in many applications such as biology, geology, and political science [21, 1, 15, 25], estimating such density function in high dimensional setting remains a challenge [11]. Moreover, we note that, if the target density is compactly supported and smooth, then we can always normalize the sample domain and assume a periodic extension. We mention several other theoretical results, although for methods different from ours, on periodic density estimations; see for example [10, Chapter 12], [32], and as a special case, compactly supported density functions [33]. In particular, periodic Sobolev density functions have been considered in [32] for the one dimensional case, where the author suggests that in many applications it might be preferable to assume the true density has compact support and to scale the data to the interior of $[0, 1]$. We note that the paper [32] briefly addresses the multi-dimensional case. Their results do not exploit the anisotropic structure of the target density function, and the MISE rate proved there severely suffers from the curse of dimensionality, unlike ours.

In passing, we note that our approximation (1.1) does not, in general, give a non-negative density function nor does it integrate to 1. We remind the reader that satisfying these conditions is already an issue in the standard kernel density estimation in one dimension; see for example [31] for discussions on relaxing these conditions to obtain a MISE convergence rate faster than $O(M^{-4/5})$, where M is the sample size.

The rest of the paper is organized as follows. Section 2 introduces the problem setting and our method. An error analysis in a RKHS setting is presented in Section 3. Then in Section 4 we will apply this theory to the Korobov space setting, and establish a dimension independent MISE decay rate. Numerical results in Section 5 support our theory, and Section 6 concludes the paper.

2. Density approximation using kernels.

2.1. Reproducing kernel Hilbert space. Let (D, \mathcal{B}, μ) be a measure space, and let $(\mathcal{N}_K, \langle \cdot, \cdot \rangle_K, \|\cdot\|_K)$ denote the reproducing kernel Hilbert space (RKHS) associated with the positive definite kernel $K: D \times D \rightarrow \mathbb{R}$, i.e., $K(x, x') = K(x', x)$ for all $x, x' \in D$, and for any $m \in \mathbb{N}$, $t_j, t_k \in \mathbb{R}$, and $x_j, x_k \in D$, $j, k = 0, \dots, m$, we have $\sum_{j,k=0}^m t_j K(x_j, x_k) t_k \geq 0$. This kernel may possibly be unbounded, but we assume $\int_D \sqrt{K(x, x)} d\mu(x) < \infty$ and $\int_D K(x, x) d\mu(x) < \infty$. The first condition ensures

$$\begin{aligned} \int_D |K(x, x')| d\mu(x') &= \int_D |\langle K(\cdot, x), K(\cdot, x') \rangle_K| d\mu(x') \\ &\leq \sqrt{K(x, x)} \int_D \sqrt{K(x', x')} d\mu(x') \quad \text{for any } x \in D \end{aligned}$$

so that we have $f_{M,N;Y}^\lambda \in L_\mu^1(D)$, while the second ensures that every $g \in \mathcal{N}_K$ is μ -square integrable:

$$\int_D |g(x)|^2 d\mu(x) \leq \|g\|_K^2 \int_D \|K(\cdot, x)\|_K^2 d\mu(x) = \|g\|_K^2 \int_D K(x, x) d\mu(x) < \infty.$$

Moreover, throughout this paper we will assume that K admits a representation

$$(2.1) \quad K(x, x') = \sum_{\ell=0}^{\infty} \beta_{\ell} \varphi_{\ell}(x) \varphi_{\ell}(x') \quad x, x' \in D,$$

with a positive sequence $(\beta_{\ell})_{\ell=0}^{\infty} \subset (0, \infty)$ converging to 0, and a complete orthonormal system $\{\sqrt{\beta_{\ell}} \varphi_{\ell}\}$ of \mathcal{N}_K such that the series is absolutely (point-wise) convergent and that $\{\varphi_{\ell}\}$ is an orthonormal system of $L_{\mu}^2(D)$. Then, the inner product for \mathcal{N}_K may be represented by

$$\langle f, g \rangle_K = \sum_{\ell=0}^{\infty} \frac{\langle f, \varphi_{\ell} \rangle_{L_{\mu}^2(D)} \langle g, \varphi_{\ell} \rangle_{L_{\mu}^2(D)}}{\beta_{\ell}},$$

where we used the notation $\langle u, w \rangle_{L_{\mu}^2(D)} := \int_D u(x)v(x)d\mu(x)$ for the $L_{\mu}^2(D)$ -inner product.

For example, suppose that (D, \mathcal{B}) is a Hausdorff topological space with the corresponding Borel σ -algebra, μ is strictly positive, i.e. $\mu(O) > 0$ for any nonempty open set $O \subset D$, and that $K: D \times D \rightarrow \mathbb{R}$ is continuous. Then, the kernel K admits a representation (2.1) with an absolutely convergent series. Indeed, the condition $\int_D K(x, x)d\mu(x) < \infty$ ensures that \mathcal{N}_K is compactly embedded into $L_{\mu}^2(D)$ [30, Lemma 2.3]. In turn, [30, Lemma 2.2] implies that the integral operator $T_K: L_{\mu}^2(D) \rightarrow L_{\mu}^2(D)$ defined by

$$T_K g := \int_D K(\cdot, x)g(x) d\mu(x), \quad g \in L_{\mu}^2(D)$$

is compact, and thus we can use representatives of the corresponding eigensystem to construct the representation (2.1) (see [30, Lemma 2.12] and [30, Corollary 3.5]). We defer to [30] for more general conditions that imply the representation (2.1).

For later use, we introduce the notation

$$(2.2) \quad \langle u, w \rangle_{\lambda} := \langle u, w \rangle_{L_{\mu}^2(D)} + \lambda \langle u, w \rangle_K \quad \text{for } u, w \in \mathcal{N}_K,$$

where $\lambda > 0$ is a parameter. The bilinear form $\langle \cdot, \cdot \rangle_{\lambda}$ is an inner product on \mathcal{N}_K and $\|\cdot\|_{\lambda} := \sqrt{\langle \cdot, \cdot \rangle_{\lambda}}$ is equivalent to $\|\cdot\|_K$: for $v, w \in \mathcal{N}_K$ we have $\langle v, v \rangle_{\lambda} \geq \lambda \|v\|_K$ and $|\langle v, w \rangle_{\lambda}| \leq (\sup_{\ell \geq 0} \beta_{\ell} + \lambda) \|v\|_K \|w\|_K$.

We also introduce a continuum scale of nested Hilbert spaces related to \mathcal{N}_K . For $\tau > 0$ we denote by \mathcal{N}_K^{τ} the normed space $\mathcal{N}_K^{\tau} := \{v \in L_{\mu}^2(D) \mid \|v\|_{\mathcal{N}_K^{\tau}} < \infty\}$ with $\|v\|_{\mathcal{N}_K^{\tau}} := (\sum_{\ell=0}^{\infty} \beta_{\ell}^{-\tau} |\langle v, \varphi_{\ell} \rangle_{L_{\mu}^2(D)}|^2)^{1/2}$, where $(\beta_{\ell})_{\ell=0}^{\infty} \subset (0, \infty)$ is as in (2.1). Note that if $\tau > 0$ is such that

$$(2.3) \quad \sum_{\ell=0}^{\infty} \beta_{\ell}^{\tau} \varphi_{\ell}(x)^2 < \infty \quad \text{for all } x \in D$$

then the series $\sum_{\ell=0}^{\infty} \langle v, \varphi_{\ell} \rangle_{L_{\mu}^2(D)} \varphi_{\ell}(x)$ for $v \in \mathcal{N}_K^{\tau}$ is (point-wise) absolutely convergent for any $x \in D$. In this case, we understand $v \in \mathcal{N}_K^{\tau} \subset L_{\mu}^2(D)$ as the representative of the corresponding equivalence class in $L_{\mu}^2(D)$ specified by this series. Then, we have $\mathcal{N}_K^1 = \mathcal{N}_K$.

We denote by $(\mathcal{N}_K^{\tau})'$ the topological dual space of \mathcal{N}_K^{τ} . Moreover, we consider the normed space

$$\mathcal{N}_K^{-\tau} := \left\{ \Psi: \mathcal{N}_K^{\tau} \rightarrow \mathbb{R}, \Psi(v) := \sum_{\ell=0}^{\infty} \Psi_{\ell} \langle \varphi_{\ell}, v \rangle_{L_{\mu}^2(D)} \mid \begin{array}{l} (\Psi_{\ell})_{\ell \geq 0} \subset \mathbb{R} \text{ such that} \\ \|\Psi\|_{\mathcal{N}_K^{-\tau}} < \infty \end{array} \right\},$$

where $\|\Psi\|_{\mathcal{N}_K^{-\tau}} := (\sum_{\ell=0}^{\infty} \beta_{\ell}^{\tau} \Psi_{\ell}^2)^{1/2}$. We will use the following characterisation of $(\mathcal{N}_K^{\tau})'$.

PROPOSITION 2.1. For $\tau \in (0, 1]$, the dual space $(\mathcal{N}_K^\tau)'$ equipped with the functional norm is isometrically isomorphic to $\mathcal{N}_K^{-\tau}$.

Proof. First, we show that $\mathcal{N}_K^{-\tau}$ is a vector subspace of $(\mathcal{N}_K^\tau)'$. Indeed, for $\Psi \in \mathcal{N}_K^{-\tau}$ and $v \in \mathcal{N}_K^\tau$ we have

$$(2.4) \quad |\Psi(v)| \leq \left(\sum_{\ell=0}^{\infty} \beta_\ell^\tau \Psi_\ell^2 \right)^{1/2} \|v\|_{\mathcal{N}_K^\tau} = \|\Psi\|_{\mathcal{N}_K^{-\tau}} \|v\|_{\mathcal{N}_K^\tau} < \infty,$$

so that $\|\Psi\|_{(\mathcal{N}_K^\tau)'} \leq \|\Psi\|_{\mathcal{N}_K^{-\tau}}$ and $\mathcal{N}_K^{-\tau} \subset (\mathcal{N}_K^\tau)'$. Next, take $\Phi \in (\mathcal{N}_K^\tau)'$ and $v = \sum_{\ell=0}^{\infty} \langle v, \varphi_\ell \rangle_{L_\mu^2(D)} \varphi_\ell \in \mathcal{N}_K^\tau$ arbitrarily, where we note that $v \in \mathcal{N}_K^\tau$ implies that this series is convergent in \mathcal{N}_K^τ . Then, the continuity of Φ implies $\Phi(v) = \sum_{\ell=0}^{\infty} \Phi(\varphi_\ell) \langle v, \varphi_\ell \rangle_{L_\mu^2(D)} \in \mathbb{R}$. To show $\Phi \in \mathcal{N}_K^{-\tau}$, we note that for any $L \in \mathbb{N}$ we have

$$\begin{aligned} 0 \leq \sum_{\ell=0}^L \beta_\ell^\tau |\Phi(\varphi_\ell)|^2 &= \sum_{\ell=0}^L \beta_\ell^\tau \Phi(\varphi_\ell) \Phi(\varphi_\ell) = \Phi \left(\sum_{\ell=0}^L \beta_\ell^\tau \Phi(\varphi_\ell) \varphi_\ell \right) \\ &\leq \|\Phi\|_{(\mathcal{N}_K^\tau)'} \left\| \sum_{\ell=0}^L \beta_\ell^\tau \Phi(\varphi_\ell) \varphi_\ell \right\|_{\mathcal{N}_K^\tau} \\ &= \|\Phi\|_{(\mathcal{N}_K^\tau)'} \left(\sum_{\ell=0}^L \beta_\ell^{-\tau} |\beta_\ell^\tau \Phi(\varphi_\ell)|^2 \right)^{1/2}, \end{aligned}$$

and thus $\|\Phi\|_{\mathcal{N}_K^{-\tau}} = \left(\sum_{\ell=0}^{\infty} \beta_\ell^\tau |\Phi(\varphi_\ell)|^2 \right)^{1/2} \leq \|\Phi\|_{(\mathcal{N}_K^\tau)'} < \infty$. Together with (2.4), we conclude $(\mathcal{N}_K^\tau)' = \mathcal{N}_K^{-\tau}$ and $\|\cdot\|_{\mathcal{N}_K^{-\tau}} = \|\cdot\|_{(\mathcal{N}_K^\tau)'}$, and thus the identity operator is the sought isomorphism. \square

2.2. The kernel estimator. Let $Y_1, \dots, Y_M: \Omega \rightarrow D$ be independent random variables that follow the distribution defined by a density $f \in \mathcal{N}_K$ with respect to μ , i.e. Y_j follows $\mathbb{P}_Y(A) = \int_A f(y) d\mu(y)$, $A \in \mathcal{B}$. We are after an approximation to f of the form $f(\cdot) \approx \sum_{n=1}^N c_n K(x_n, \cdot)$ with $K(\cdot, \cdot)$ given by (2.1), where $X = \{x_1, \dots, x_N\} \subset D$ is a set of carefully chosen points. The choice of X is important, since given $K(\cdot, \cdot)$, it determines the approximation space

$$(2.5) \quad V_N := V_N(X) := \text{span}\{K(x_j, \cdot) \mid j = 1, \dots, N\}.$$

The starting point of our method is the following ideal minimization problem:

$$(2.6) \quad f_N^\lambda := \arg \min_{v \in V_N} \tilde{J}_\lambda(v) := \arg \min_{v \in V_N} \left[\frac{1}{2} \|v - f\|_{L_\mu^2(D)}^2 + \frac{\lambda}{2} \|v\|_K^2 \right].$$

This method is not practical as the evaluation of \tilde{J}_λ requires full knowledge of the target density f . Let us rewrite \tilde{J}_λ as

$$\begin{aligned} \tilde{J}_\lambda(v) &= \frac{1}{2} \|v\|_{L_\mu^2(D)}^2 - \langle v, f \rangle_{L_\mu^2(D)} + \frac{1}{2} \|f\|_{L_\mu^2(D)}^2 + \frac{\lambda}{2} \|v\|_K^2 \\ &= J_\lambda(v) + \frac{1}{2} \|f\|_{L_\mu^2(D)}^2, \end{aligned}$$

with $J_\lambda(v) = \frac{1}{2} \|v\|_{L_\mu^2(D)}^2 - \langle v, f \rangle_{L_\mu^2(D)} + \frac{\lambda}{2} \|v\|_K^2$. Then, since $\frac{1}{2} \|f\|_{L_\mu^2(D)}^2$ is a constant function in v , we have

$$f_N^\lambda = \arg \min_{v \in V_N} \tilde{J}_\lambda(v) = \arg \min_{v \in V_N} J_\lambda(v).$$

Now we approximate $J_\lambda(v)$ using the i.i.d. sample $\mathbf{Y} := (Y_1, \dots, Y_M) \sim f d\mu$, which yields

$$f_{M,N;\mathbf{Y}}^\lambda := \arg \min_{v \in V_N} J_{M,\lambda}(v) := \arg \min_{v \in V_N} \left[\frac{1}{2} \|v\|_{L_\mu^2(D)}^2 + \frac{\lambda}{2} \|v\|_K^2 - \frac{1}{M} \sum_{m=1}^M v(Y_m) \right].$$

This is the minimization problem we solve, which can be equivalently written as: Find $f_{M,N;\mathbf{Y}}^\lambda \in V_N$ such that

$$(2.7) \quad \langle f_{M,N;\mathbf{Y}}^\lambda, v \rangle_\lambda = \frac{1}{M} \sum_{m=1}^M v(Y_m) \quad \text{for all } v \in V_N,$$

where $\langle \cdot, \cdot \rangle_\lambda$ is as in (2.2); see for example [6, Theorem 6.1-1] for this equivalence. To see that this problem is well defined, note that $\Delta_{\mathbf{Y}}: \mathcal{N}_K \rightarrow \mathbb{R}$ defined by

$$(2.8) \quad \Delta_{\mathbf{Y}(\omega)}(v) := \frac{1}{M} \sum_{m=1}^M v(Y_m)$$

is a linear continuous functional on \mathcal{N}_K , hence on V_N , for any $\omega \in \Omega$, since $\Delta_{\mathbf{Y}(\omega)}$ is the sum of point evaluation functionals on the RKHS \mathcal{N}_K . Hence, in view of the Riesz representation theorem, the solution $f_{M,N;\mathbf{Y}}^\lambda$ exists and is unique in V_N . The corresponding coefficients $\mathbf{c} = (c_1, \dots, c_n)^\top$ satisfy the linear system

$$(2.9) \quad \mathbf{A}\mathbf{c} = \mathbf{b},$$

where the matrix \mathbf{A} is given by $\mathbf{A}_{jk} = \langle K(x_j, \cdot), K(x_k, \cdot) \rangle_{L_\mu^2(D)} + \lambda K(x_j, x_k)$, for $j, k = 1, \dots, N$ and the vector \mathbf{b} is given by $\mathbf{b}_j = \frac{1}{M} \sum_{m=1}^M K(x_j, Y_m(\omega))$, for $j = 1, \dots, N$. Notice that, as we mentioned before, the solution of (2.7) exists uniquely in V_N , and thus \mathbf{b} is in the columns space of \mathbf{A} . Nevertheless, the equation (2.9) may not be uniquely solvable if the functions $K(x_j, \cdot)$, $j = 1, \dots, N$ are linearly dependent. In such a case where \mathbf{A} is singular, we take $\mathbf{c} \in \mathbb{R}^N$ such that $\mathbf{c} \in (\text{null}(\mathbf{A}))^\perp$, where the orthogonal complement is taken with respect the Euclidean inner product.

The resulting mapping $\mathbf{b} \mapsto \mathbf{c}$ is continuous, and since $\omega \mapsto \mathbf{b}(\omega)$ is $\mathcal{F}/\mathcal{B}(\mathbb{R}^N)$ -measurable, where $\mathcal{B}(\mathbb{R}^N)$ is the Borel σ -algebra of \mathbb{R}^N , $\omega \mapsto \mathbf{c}(\omega)$ is also $\mathcal{F}/\mathcal{B}(\mathbb{R}^N)$ -measurable.

Taking the expectation on both sides of (2.7) leads to

$$(2.10) \quad \langle \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda], v \rangle_\lambda = \mathbb{E}[v(Y_1)] = \int_D f(y)v(y)d\mu(y) \quad \text{for all } v \in V_N,$$

and thus $f_{M,N;\mathbf{Y}}^\lambda$ is an estimator such that its expectation is the solution to the variational problem (2.6), i.e. $\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] = f_N^\lambda$.

3. General error estimate. We measure the error in terms of the mean integrated squared error (MISE):

$$(3.1) \quad \mathbb{E} \left[\int_D |f_{M,N;\mathbf{Y}}^\lambda(x) - f(x)|^2 d\mu(x) \right] = \|\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f\|_{L_\mu^2(D)}^2 + \mathbb{E}[\|f_{M,N;\mathbf{Y}}^\lambda - \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda]\|_{L_\mu^2(D)}^2].$$

In the following, we will analyse the first term (hereafter called the *squared bias* term) and the second term (hereafter called the *variance* term) separately.

3.1. Bias estimate. To study the bias, we introduce the \mathcal{N}_K -orthogonal projection $\mathcal{P}_N g$ of g from \mathcal{N}_K onto V_N and relate the bias with the projection error. If K is a strictly positive definite kernel, the kernel interpolation $\mathcal{I}_N g \in V_N$ of $g \in \mathcal{N}_K$ that interpolates g at distinct x_1, \dots, x_N can be uniquely determined, and it is well known that $\mathcal{I}_N g = \mathcal{P}_N g$. Since a large number of interpolation error estimates are readily available for various kernels, this will directly provide estimates on the bias. For more details on the kernel interpolation, see for example [35].

Trivially, we have

$$(3.2) \quad \begin{aligned} \|\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f\|_{L_\mu^2(D)}^2 &= \langle \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f, \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \rangle_{L_\mu^2(D)} \\ &\quad + \langle \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f, \mathcal{P}_N f - f \rangle_{L_\mu^2(D)}, \end{aligned}$$

the second term of which can be bounded as

$$(3.3) \quad \begin{aligned} &\langle \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f, \mathcal{P}_N f - f \rangle_{L_\mu^2(D)} \\ &\leq \frac{1}{2} \|\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f\|_{L_\mu^2(D)}^2 + \frac{1}{2} \|\mathcal{P}_N f - f\|_{L_\mu^2(D)}^2. \end{aligned}$$

Bounding the first term is more involved.

LEMMA 3.1. *Let $\{x_1, \dots, x_N\} \subset D$ be arbitrary and let V_N be the corresponding space (2.5). Then, for the \mathcal{N}_K -orthogonal projection $\mathcal{P}_N: \mathcal{N}_K \rightarrow V_N$, we have*

$$\langle \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f, \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \rangle_{L_\mu^2(D)} \leq \frac{1}{2} \lambda \|f\|_K^2.$$

Proof. From $\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \in V_N$, the equation (2.10) implies

$$\begin{aligned} &\langle \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda], \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \rangle_{L_\mu^2(D)} \\ &\quad + \lambda \langle \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f + f, \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \rangle_K = \langle f, \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \rangle_{L_\mu^2(D)}, \end{aligned}$$

and thus

$$(3.4) \quad \begin{aligned} &\langle \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f, \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \rangle_{L_\mu^2(D)} \\ &\quad + \lambda \langle \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f, \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \rangle_K = -\lambda \langle f, \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \rangle_K. \end{aligned}$$

Since \mathcal{P}_N is the \mathcal{N}_K -orthogonal projection, we have $\langle \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f, \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \rangle_K = \|\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f\|_K^2$, and thus the Young's inequality implies

$$\langle \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f, \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \rangle_{L_\mu^2(D)} + \frac{1}{2} \lambda \|\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f\|_K^2 \leq \frac{1}{2} \lambda \|f\|_K^2.$$

This completes the proof. \square

Hence, we obtain an estimate of the squared bias.

PROPOSITION 3.2. *Let the assumptions of Lemma 3.1 hold. Then, the solution $f_{M,N;\mathbf{Y}}^\lambda$ to (2.7) satisfies*

$$\|\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f\|_{L_\mu^2(D)}^2 \leq \|\mathcal{P}_N f - f\|_{L_\mu^2(D)}^2 + \lambda \|f\|_K^2.$$

By exploiting a stronger smoothness of f , we can establish a bound that is of second order in λ .

PROPOSITION 3.3. *Let $\{x_1, \dots, x_N\} \subset D$ be arbitrary and let V_N be the corresponding space (2.5). Suppose $f \in \mathcal{N}_K^2$. Then, the solution $f_{M,N;\mathbf{Y}}^\lambda$ to (2.7) satisfies*

$$\|\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f\|_{L_\mu^2(D)}^2 \leq 3\|\mathcal{P}_N f - f\|_{L_\mu^2(D)}^2 + 8\lambda^2\|f\|_{\mathcal{N}_K^2}^2.$$

Proof. From (3.4) we have

$$\begin{aligned} & \langle \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f, \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \rangle_{L_\mu^2(D)} + \lambda \|\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f\|_K^2 \\ &= -\lambda \langle f, \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f \rangle_K \\ &\leq \lambda \|f\|_{\mathcal{N}_K^2} \|\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f\|_{L_\mu^2(D)} \\ &\leq 2\lambda^2 \|f\|_{\mathcal{N}_K^2}^2 + \frac{1}{8} \|\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - \mathcal{P}_N f\|_{L_\mu^2(D)}^2 \\ &\leq 2\lambda^2 \|f\|_{\mathcal{N}_K^2}^2 + \frac{1}{4} \|\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f\|_{L_\mu^2(D)}^2 + \frac{1}{4} \|f - \mathcal{P}_N f\|_{L_\mu^2(D)}^2. \end{aligned}$$

Thus, (3.2) and (3.3) imply

$$\left(\frac{1}{2} - \frac{1}{4}\right) \|\mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda] - f\|_{L_\mu^2(D)}^2 \leq \left(\frac{1}{2} + \frac{1}{4}\right) \|\mathcal{P}_N f - f\|_{L_\mu^2(D)}^2 + 2\lambda^2 \|f\|_{\mathcal{N}_K^2}^2.$$

Now the proof is complete. \square

3.2. Variance estimate. Now we bound the variance $\mathbb{E}[\|f_{M,N;\mathbf{Y}}^\lambda - \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda]\|_{L_\mu^2(D)}^2]$ in (3.1). Taking the difference of (2.7) and (2.10) yields

$$(3.5) \quad \langle f_{M,N;\mathbf{Y}}^\lambda - \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda], v \rangle_\lambda = \Delta_{\mathbf{Y}}(v) - F(v) \quad \text{for all } v \in V_N,$$

where $\Delta_{\mathbf{Y}}$ is defined in (2.8), and we used the notation

$$(3.6) \quad F(v) := \int_D v(y) f(y) d\mu(y).$$

Then, we have $F \in (\mathcal{N}_K)'$, and as point-evaluation functionals are continuous on \mathcal{N}_K , we also have $\Delta_{\mathbf{Y}} \in (\mathcal{N}_K)'$.

If f is smooth and thus accordingly K is taken to be smooth, the corresponding space \mathcal{N}_K may be smaller than necessary for $\Delta_{\mathbf{Y}}$ to be continuous. Namely, in such cases $\Delta_{\mathbf{Y}}$ is continuous on larger spaces \mathcal{N}_K^τ , $\tau \in (\tau_0, 1)$ for some $\tau_0 \geq 0$. We will exploit this observation in the variance estimate and assess the variance of $\Delta_{\mathbf{Y}} - F$ in $\mathcal{N}_K^{-\tau}$.

LEMMA 3.4. *Suppose that for some $\tau \in (0, 1]$ we have $\Delta_{\mathbf{Y}} \in \mathcal{N}_K^{-\tau}$, and that f satisfies $\langle K_\tau(\cdot, \cdot), f \rangle_{L_\mu^2(D)} := \int_D K_\tau(x, x) f(x) d\mu(x) < \infty$ with $K_\tau(x_1, x_2) := \sum_{\ell=0}^{\infty} \beta_\ell^\tau \varphi_\ell(x_1) \varphi_\ell(x_2)$. Then, the equality*

$$\mathbb{E}[\|\Delta_{\mathbf{Y}} - F\|_{\mathcal{N}_K^{-\tau}}^2] = \frac{\langle K_\tau(\cdot, \cdot), f \rangle_{L_\mu^2(D)} - \|F\|_{\mathcal{N}_K^{-\tau}}^2}{M}$$

holds, where F is defined in (3.6).

Proof. We have

$$(3.7) \quad \mathbb{E}[\|\Delta_{\mathbf{Y}} - F\|_{\mathcal{N}_K^{-\tau}}^2] = \mathbb{E}[\|\Delta_{\mathbf{Y}}\|_{\mathcal{N}_K^{-\tau}}^2] - 2\mathbb{E}[\langle \Delta_{\mathbf{Y}}, F \rangle_{\mathcal{N}_K^{-\tau}}] + \|F\|_{\mathcal{N}_K^{-\tau}}^2.$$

For the second term, first notice that for any $L \in \mathbb{N}$ we have

$$\begin{aligned}
\mathbb{E} \left[\left| \sum_{\ell=0}^L \beta_\ell^\tau \Delta_{\mathbf{Y}}(\varphi_\ell) F(\varphi_\ell) \right| \right] &\leq \mathbb{E} \left[\frac{1}{M} \sum_{m=1}^M \sum_{\ell=0}^L \beta_\ell^\tau |\varphi_\ell(Y_m)| |\langle f, \varphi_\ell \rangle_{L_\mu^2(D)}| \right] \\
&= \frac{1}{M} \sum_{m=1}^M \sum_{\ell=0}^L \beta_\ell^\tau \mathbb{E}[|\varphi_\ell(Y_m)|] |\langle f, \varphi_\ell \rangle_{L_\mu^2(D)}| \\
&\leq \frac{1}{M} \sum_{m=1}^M \sum_{\ell=0}^L \beta_\ell^\tau \sqrt{\mathbb{E}[|\varphi_\ell(Y_m)|^2]} |\langle f, \varphi_\ell \rangle_{L_\mu^2(D)}| \\
&= \sum_{\ell=0}^L \beta_\ell^\tau \sqrt{\langle \varphi_\ell^2, f \rangle_{L_\mu^2(D)}} |\langle f, \varphi_\ell \rangle_{L_\mu^2(D)}| \\
&\leq \sqrt{\sum_{\ell=0}^L \langle \beta_\ell^\tau \varphi_\ell^2, f \rangle_{L_\mu^2(D)}} \sqrt{\sum_{\ell=0}^L \beta_\ell^\tau |\langle f, \varphi_\ell \rangle_{L_\mu^2(D)}|^2} \\
&\leq \sqrt{\langle K_\tau(\cdot, \cdot), f \rangle_{L_\mu^2(D)}} \|F\|_{\mathcal{N}_K^{-\tau}} < \infty,
\end{aligned}$$

where in the last equality we used the non-negativity of $\beta_\ell^\tau \varphi_\ell^2 f$, and in view of Proposition 2.1 the slight abuse of notation $\|F\|_{\mathcal{N}_K^{-\tau}}$ should be unambiguous. Hence, we can use the dominated convergence theorem to conclude

$$-2\mathbb{E}[\langle \Delta_{\mathbf{Y}}, F \rangle_{\mathcal{N}_K^{-\tau}}] = -2 \sum_{\ell=0}^{\infty} \beta_\ell \mathbb{E}[\Delta_{\mathbf{Y}}(\varphi_\ell)] F(\varphi_\ell) = -2\|F\|_{\mathcal{N}_K^{-\tau}}.$$

The first term in the right-hand side of (3.7) can be rewritten as

$$\begin{aligned}
\mathbb{E}[\|\Delta_{\mathbf{Y}}\|_{\mathcal{N}_K^{-\tau}}^2] &= \frac{1}{M^2} \sum_{m=1}^M \mathbb{E}[\|\delta_{Y_m}\|_{\mathcal{N}_K^{-\tau}}^2] + \frac{1}{M^2} \sum_{m=1}^M \sum_{\substack{k=1 \\ k \neq m}}^M \mathbb{E}[\langle \delta_{Y_m}, \delta_{Y_k} \rangle_{\mathcal{N}_K^{-\tau}}] \\
&= \frac{1}{M} \sum_{\ell=0}^{\infty} \beta_\ell^\tau \mathbb{E}[\varphi_\ell(Y_1)^2] + \frac{1}{M^2} \sum_{m=1}^M \sum_{\substack{k=1 \\ k \neq m}}^M \sum_{\ell=0}^{\infty} \beta_\ell^\tau \mathbb{E}[\varphi_\ell(Y_m)] \mathbb{E}[\varphi_\ell(Y_k)] \\
&= \frac{\langle K_\tau(\cdot, \cdot), f \rangle_{L_\mu^2(D)}}{M} + \frac{M-1}{M} \|F\|_{\mathcal{N}_K^{-\tau}}^2,
\end{aligned}$$

where we used the notation $\delta_{Y_m}(v) := v(Y_m)$ for $m = 1, \dots, M$. Hence, we conclude

$$\mathbb{E}[\|\Delta_{\mathbf{Y}} - F\|_{\mathcal{N}_K^{-\tau}}^2] = \frac{\langle K_\tau(\cdot, \cdot), f \rangle_{L_\mu^2(D)} - \|F\|_{\mathcal{N}_K^{-\tau}}^2}{M}. \quad \square$$

We arrive at the variance estimate of our density approximation. The proof is inspired by [2, Theorem 2].

PROPOSITION 3.5. *Suppose that for some $\tau \in (0, 1]$ we have $\Delta_{\mathbf{Y}} \in \mathcal{N}_K^{-\tau}$, and that f satisfies $\langle K_\tau(\cdot, \cdot), f \rangle_{L_\mu^2(D)} < \infty$ with $K_\tau(x_1, x_2) = \sum_{\ell=0}^{\infty} \beta_\ell^\tau \varphi_\ell(x_1) \varphi_\ell(x_2)$. Then, for any $\lambda \in (0, 1]$ we have*

$$\mathbb{E}[\|f_{M,N;\mathbf{Y}}^\lambda - \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda]\|_\lambda^2] \leq \frac{\langle K_\tau(\cdot, \cdot), f \rangle_{L_\mu^2(D)}}{M\lambda^\tau}.$$

Proof. For $\tau \in (0, 1]$ such that $\Delta_{\mathbf{Y}} \in \mathcal{N}_K^{-\tau}$, choosing $v = f_{M,N;\mathbf{Y}}^\lambda - \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda]$ in (3.5) and taking the expectation on both sides yields

$$\begin{aligned} \mathbb{E}[\|f_{M,N;\mathbf{Y}}^\lambda - \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda]\|_\lambda^2] \\ \leq \lambda^{-\tau/2} \mathbb{E}[\|\Delta_{\mathbf{Y}} - F\|_{\mathcal{N}_K^{-\tau}} \lambda^{\tau/2} \|f_{M,N;\mathbf{Y}}^\lambda - \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda]\|_{\mathcal{N}_K^\tau}]. \end{aligned}$$

For any $v \in \mathcal{N}_K$, from $1/\tau \in [1, \infty)$ we have

$$\begin{aligned} \lambda^\tau \|v\|_{\mathcal{N}_K^\tau}^2 &= \lambda^\tau \sum_{\ell=0}^{\infty} \frac{1}{\beta_\ell^\tau} \langle v, \varphi_\ell \rangle_{L_\mu^2(D)}^{2(\tau+(1-\tau))} \\ &\leq \lambda^\tau \left(\sum_{\ell=0}^{\infty} \frac{1}{\beta_\ell^{\tau \frac{1}{\tau}}} \langle v, \varphi_\ell \rangle_{L_\mu^2(D)}^2 \right)^\tau \left(\sum_{\ell=0}^{\infty} \langle v, \varphi_\ell \rangle_{L_\mu^2(D)}^2 \right)^{1-\tau} \\ &= \lambda^\tau \|v\|_{\mathcal{N}_K}^{2\tau} \|v\|_{L_\mu^2(D)}^{2(1-\tau)} \leq \tau \lambda \|v\|_{\mathcal{N}_K}^2 + (1-\tau) \|v\|_{L_\mu^2(D)}^2 \leq \|v\|_\lambda^2, \end{aligned}$$

and thus

$$\|v\|_{\mathcal{N}_K^\tau} \leq \lambda^{-\tau/2} \|v\|_\lambda.$$

Hence, we obtain

$$\begin{aligned} \mathbb{E}[\|f_{M,N;\mathbf{Y}}^\lambda - \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda]\|_\lambda^2] &\leq \lambda^{-\tau/2} \mathbb{E}[\|\Delta_{\mathbf{Y}} - F\|_{\mathcal{N}_K^{-\tau}} \|f_{M,N;\mathbf{Y}}^\lambda - \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda]\|_\lambda] \\ &\leq \lambda^{-\tau/2} \sqrt{\frac{\langle K_\tau(\cdot, \cdot), f \rangle_{L_\mu^2(D)}}{M}} \sqrt{\mathbb{E}[\|f_{M,N;\mathbf{Y}}^\lambda - \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda]\|_\lambda^2]}, \end{aligned}$$

and thus

$$\mathbb{E}[\|f_{M,N;\mathbf{Y}}^\lambda - \mathbb{E}[f_{M,N;\mathbf{Y}}^\lambda]\|_\lambda^2] \leq \frac{\langle K_\tau(\cdot, \cdot), f \rangle_{L_\mu^2(D)}}{M\lambda^\tau}.$$

The proof is now complete. \square

3.3. MISE estimate.

We summarise the discussions so far as a theorem.

THEOREM 3.6. *Let $f \in \mathcal{N}_K$ be the target density function and let $f_{M,N;\mathbf{Y}}^\lambda \in V_N$ satisfy (2.7). Moreover, let $\mathcal{P}_N: \mathcal{N}_K \rightarrow V_N$ be the \mathcal{N}_K -orthogonal projection. Suppose that for some $\tau \in (0, 1]$ we have $\Delta_{\mathbf{Y}} \in \mathcal{N}_K^{-\tau}$, and that f satisfies $\langle K_\tau(\cdot, \cdot), f \rangle_{L_\mu^2(D)} < \infty$ with $K_\tau(x_1, x_2) = \sum_{\ell=0}^{\infty} \beta_\ell^\tau \varphi_\ell(x_1) \varphi_\ell(x_2)$. Then, we have the MISE estimate*

$$(3.8) \quad \mathbb{E} \left[\int_D |f_{M,N;\mathbf{Y}}^\lambda(x) - f(x)|^2 d\mu(x) \right] \leq \|\mathcal{P}_N f - f\|_{L_\mu^2(D)}^2 + \lambda \|f\|_K^2 + \frac{\langle K_\tau(\cdot, \cdot), f \rangle_{L_\mu^2(D)}}{M\lambda^\tau}.$$

Suppose furthermore $f \in \mathcal{N}_K^2$. Then we also have

$$(3.9) \quad \begin{aligned} \mathbb{E} \left[\int_D |f_{M,N;\mathbf{Y}}^\lambda(x) - f(x)|^2 d\mu(x) \right] \\ \leq 3 \|\mathcal{P}_N f - f\|_{L_\mu^2(D)}^2 + 8\lambda^2 \|f\|_{\mathcal{N}_K^2}^2 + \frac{\langle K_\tau(\cdot, \cdot), f \rangle_{L_\mu^2(D)}}{M\lambda^\tau}. \end{aligned}$$

3.4. Limiting case $N \rightarrow \infty$ and link with kernel density estimation. In principle, the projection error in the right hand side of (3.8) and (3.9) is independent of the other two

terms. Thus, it may be natural to pose the problem in \mathcal{N}_K rather than in V_N : Find $f_{M;\mathbf{Y}}^\lambda \in \mathcal{N}_K$ such that

$$\langle f_{M;\mathbf{Y}}^\lambda, v \rangle_\lambda = \frac{1}{M} \sum_{m=1}^M v(Y_m) \quad \text{for all } v \in \mathcal{N}_K.$$

Then, from

$$\langle f_{M;\mathbf{Y}}^\lambda, \varphi_\ell \rangle_{L_\mu^2(D)} + \frac{\lambda}{\beta_\ell} \langle f_{M;\mathbf{Y}}^\lambda, \varphi_\ell \rangle_{L_\mu^2(D)} = \frac{1}{M} \sum_{m=1}^M \varphi_\ell(Y_m) \quad \text{for } \ell \geq 0,$$

the solution is given by a linear combination

$$f_{M;\mathbf{Y}}^\lambda = \frac{1}{M} \sum_{m=1}^M K_\lambda^*(Y_m, \cdot)$$

of the kernel $K_\lambda^*(x, x') := \sum_{\ell=0}^{\infty} \frac{\beta_\ell}{\beta_\ell + \lambda} \varphi_\ell(x) \varphi_\ell(x')$, $x, x' \in D$, which is of the form similar to the standard kernel density estimation; see for example [29]. Note that we indeed have $f_{M;\mathbf{Y}}^\lambda \in \mathcal{N}_K$: from

$$\frac{\beta_\ell}{\beta_\ell + \lambda} \langle \varphi_\ell(Y_m(\omega)) \varphi_\ell, \varphi_\ell \rangle_{L_\mu^2(D)} = \frac{\beta_\ell}{\beta_\ell + \lambda} \varphi_\ell(Y_m(\omega))$$

provided $\lambda > 0$, for any realization $\mathbf{y} = (y_1, \dots, y_M) = \mathbf{Y}(\omega)$ we have

$$\|f_{M;\mathbf{y}}^\lambda\|_K^2 = \sum_{\ell=0}^{\infty} \frac{\beta_\ell}{(\beta_\ell + \lambda)^2} \frac{1}{M} \sum_{m=1}^M \varphi_\ell(y_m)^2 \leq \frac{1}{\lambda^2} \frac{1}{M} \sum_{m=1}^M K(y_m, y_m) < \infty.$$

Notice however that $f_{M;\mathbf{Y}}^\lambda$ is not a linear combination of the kernel K , and in general the kernel K_λ^* cannot be given in a closed form, even if K is. Hence, in practice it is much more computationally efficient to seek the approximation in V_N .

The problem posed in \mathcal{N}_K in the discussion above can be seen as a limiting case of our finite dimensional setting with $N \rightarrow \infty$ and a dense subset $X = \{x_j\}_{j \in \mathbb{N}}$ of D in the following sense. Suppose that D is a separable metric space, \mathcal{B} is a corresponding Borel σ -algebra, and that μ is a σ -finite measure on (D, \mathcal{B}) . Then, the Hilbert space of equivalence classes of square integrable functions $L_\mu^2(D)$ is separable; see for example [12, p. 92]. Moreover, assume that the positive definite kernel $K: D \times D \rightarrow \mathbb{R}$ is continuous. Then, there exists a dense subset $\{q_j\}_{j \in \mathbb{N}} \subset D$ such that $\overline{\text{span}\{\{K(q_j, \cdot)\}_{j \in \mathbb{N}}\}} = \mathcal{N}_K$, in particular \mathcal{N}_K is separable as shown in the next proposition.

PROPOSITION 3.7. *Under the assumptions above on (D, \mathcal{B}, μ) , there exists a subset $\{q_j\}_{j \in \mathbb{N}} \subset D$ such that $\overline{\text{span}\{\{K(q_j, \cdot)\}_{j \in \mathbb{N}}\}} = \mathcal{N}_K$, where the closure is taken with respect to the \mathcal{N}_K -norm.*

Proof. Since D is assumed to be separable, there exists a subset $\{q_j\}_{j \in \mathbb{N}} \subset D$ that approximates all $x \in D$. Consider the subset $\{K(q_j, \cdot)\}_{j \in \mathbb{N}} \subset \mathcal{N}_K$. Let $\mathcal{M} := \overline{\text{span}\{\{K(q_j, \cdot)\}_{j \in \mathbb{N}}\}} \subset \mathcal{N}_K$. Since \mathcal{M} is a closed subspace of \mathcal{N}_K , we have $\mathcal{N}_K = \mathcal{M} \oplus \mathcal{M}^\perp$. We will show $\mathcal{M}^\perp = \{0\}$. Indeed, for $g \in \mathcal{M}^\perp$, we have

$$0 = \langle g, K(q_j, \cdot) \rangle_K = g(q_j) \quad \text{for any } j \in \mathbb{N}.$$

Now, observe that the continuity of the kernel implies that all elements in \mathcal{N}_K are (sequentially) continuous on D . Therefore, we have $g(x) = 0$ for all $x \in D$. Hence, $\mathcal{M}^\perp = \{0\}$. \square

4. Application to densities in weighted Korobov spaces. In this section, we will apply the theory established in Section 3 to the case where the kernel defines the so-called Korobov space. Throughout this section, we assume that the density function f is defined on the d -dimensional unit hypercube $[0, 1]^d \subset \mathbb{R}^d$, and that the density is with respect to the uniform measure. This choice of reference measure is due to the definition of the Korobov space, whose norm is based on the standard L^2 -inner product with respect to the uniform measure. Since in this section $D = [0, 1]^d$ is a subset of \mathbb{R}^d , we will use the bold symbol \mathbf{x} to denote a point in $[0, 1]^d$.

Let a smoothness parameter $\alpha > 1$ be given. For non-negative parameters $\gamma = \{\gamma_{\mathbf{u}}\}_{\mathbf{u} \subset \mathbb{N}}$, which we call *weights*, we consider the Korobov kernel

$$(4.1) \quad K_{\alpha}^{\text{kor}}(\mathbf{x}, \mathbf{x}') = \sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^{-1} e^{2\pi i \mathbf{h} \cdot (\mathbf{x} - \mathbf{x}')}, \quad \mathbf{x}, \mathbf{x}' \in [0, 1]^d,$$

where $\mathbf{h} \cdot \mathbf{x}$ denotes the Euclidean inner product $\mathbf{h} \cdot \mathbf{x} = \sum_{j=1}^d h_j x_j$, and

$$r(\mathbf{h}, \gamma) := \begin{cases} 1, & \text{if } \mathbf{h} = (0, \dots, 0) \\ \gamma_{\text{supp}(\mathbf{h})}^{-1} \prod_{\text{supp}(\mathbf{h})} |h_j|^{\alpha}, & \text{if } \mathbf{h} \neq (0, \dots, 0) \end{cases},$$

with $\text{supp } \mathbf{h} := \{1 \leq j \leq d \mid h_j \neq 0\}$. We take $\gamma_{\emptyset} := 1$, so that the norm of a constant function in the corresponding reproducing kernel Hilbert space matches its L^2 norm. We denote the corresponding reproducing kernel Hilbert space by $\mathcal{N}_{\text{kor}, \alpha}$, which consists of 1-periodic functions on \mathbb{R}^d with a suitable smoothness governed by the parameter $\alpha > 1$. This kernel can be rewritten as

$$K_{\alpha}^{\text{kor}}(\mathbf{x}, \mathbf{x}') = 1 + \sum_{\emptyset \neq \mathbf{u} \subseteq \{1, \dots, d\}} \gamma_{\mathbf{u}} K_{\alpha}^{\text{kor}}(\mathbf{x}_{\mathbf{u}}, \mathbf{x}'_{\mathbf{u}}),$$

with

$$K_{\alpha}^{\text{kor}}(\mathbf{x}_{\mathbf{u}}, \mathbf{x}'_{\mathbf{u}}) = \prod_{j \in \mathbf{u}} \left(\sum_{h \in \mathbb{Z} \setminus \{0\}} \frac{e^{2\pi i h(x_j - x'_j)}}{|h|^{\alpha}} \right) = \prod_{j \in \mathbf{u}} 2 \sum_{h=1}^{\infty} \frac{\cos(2\pi h(x_j - x'_j))}{h^{\alpha}}.$$

For $\alpha > 1$, the kernel K_{α}^{kor} is well defined for all $\mathbf{x}, \mathbf{x}' \in [0, 1]^d$ and satisfies $\sup_{\mathbf{x}, \mathbf{x}' \in [0, 1]^d} K_{\alpha}^{\text{kor}}(\mathbf{x}, \mathbf{x}') < \infty$, and with

$$\langle v, e^{2\pi i \mathbf{h} \cdot \cdot} \rangle_{L^2([0, 1]^d)} := \int_{[0, 1]^d} v(\mathbf{x}) e^{-2\pi i \mathbf{h} \cdot \mathbf{x}} d\mathbf{x},$$

the corresponding norm is given by

$$\|v\|_{\text{kor}, \alpha} = \left(\sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma) |\langle v, e^{2\pi i \mathbf{h} \cdot \cdot} \rangle_{L^2([0, 1]^d)}|^2 \right)^{1/2},$$

where the series is absolutely convergent.

If α is an even integer, the expression of the kernel and the norm simplifies. First, the reproducing kernel $K_{\alpha}^{\text{kor}}(\mathbf{x}, \mathbf{x}')$ is related to the Bernoulli polynomials B_{α} : for α even, we have

$$B_{\alpha}(x) = \frac{(-1)^{\frac{\alpha}{2}+1} \alpha!}{(2\pi)^{\alpha}} \sum_{h \in \mathbb{Z} \setminus \{0\}} \frac{e^{2\pi i h x}}{|h|^{\alpha}} \quad \text{for any } x \in [0, 1],$$

so that

$$K_{\alpha}^{\text{kor}}(\mathbf{x}, \mathbf{x}') = 1 + \sum_{\emptyset \neq \mathbf{u} \subseteq \{1, \dots, d\}} \gamma_{\mathbf{u}} \left(\frac{(2\pi)^{\alpha}}{(-1)^{\frac{\alpha}{2}+1} \alpha!} \right)^{|\mathbf{u}|} \prod_{j \in \mathbf{u}} B_{\alpha}(|\{x_j - x'_j\}|),$$

where $\{x\}$ denotes the fractional part of x . Moreover, the norm $\|\cdot\|_{\text{kor},\alpha}$ can be rewritten as the norm in an “unanchored” weighted Sobolev space of dominating mixed smoothness of order $\alpha/2$,

$$\begin{aligned} & \|v\|_{\text{kor},\alpha} \\ &= \sqrt{\sum_{\mathbf{u} \subseteq \{1, \dots, d\}} \frac{1}{(2\pi)^{\alpha|\mathbf{u}|} \gamma_{\mathbf{u}}} \int_{[0,1]^{|\mathbf{u}|}} \left| \int_{[0,1]^{d-|\mathbf{u}|}} \left(\prod_{j \in \mathbf{u}} \frac{\partial^{\alpha/2}}{\partial x_j^{\alpha/2}} \right) v(\mathbf{x}) \, d\mathbf{x}_{-\mathbf{u}} \right|^2 \, d\mathbf{x}_{\mathbf{u}}}, \end{aligned}$$

where $\mathbf{x}_{\mathbf{u}}$ denotes the components of \mathbf{x} with indices that belong to the subset \mathbf{u} , and $\mathbf{x}_{-\mathbf{u}}$ denotes the components that do not belong to \mathbf{u} , and $|\mathbf{u}|$ denotes the cardinality of \mathbf{u} . See for example [26] for more details on weighted Korobov spaces.

We note that if the weights $\gamma_{\mathbf{u}}$ are of the product form, i.e.

$$\gamma_{\mathbf{u}} = \prod_{j \in \mathbf{u}} \gamma_j \quad \text{for some positive } \gamma_j, \quad \text{for } j = 1, \dots, d,$$

then the kernel $K_{\alpha}^{\text{kor}}(\cdot, \cdot)$ can be written as the product of kernels:

$$(4.2) \quad K_{\alpha}^{\text{kor}}(\mathbf{x}, \mathbf{x}') = \prod_{j=1}^d K_{1, \alpha, \gamma_j}^{\text{kor}}(x_j, x'_j),$$

with $K_{1, \alpha, \gamma_j}^{\text{kor}}(x, x') = 1 + \gamma_j \sum_{h \in \mathbb{Z} \setminus \{0\}} \frac{e^{2\pi i h(x-x')}}{|h|^{\alpha}}$.

Under this setting, the equation (2.7) is equivalent to the following: Find $f_{M, N; \mathbf{Y}}^{\lambda} = \sum_{n=1}^N c_n K(\mathbf{x}_n, \cdot)$ such that

$$\langle f_{M, N; \mathbf{Y}}^{\lambda}, K_{\alpha}^{\text{kor}}(\mathbf{x}_k, \cdot) \rangle_{L^2([0,1]^d)} + \lambda f_{M, N; \mathbf{Y}}^{\lambda}(\mathbf{x}_k) = \frac{1}{M} \sum_{m=1}^M K_{\alpha}^{\text{kor}}(\mathbf{x}_k, Y_m(\omega))$$

for $k = 1, \dots, N$. The linear system for $\mathbf{c} = (c_1, \dots, c_N)^{\top}$ is given by (2.9), which can be written in a closed form for α even. Indeed, we have

$$\langle K_{\alpha}^{\text{kor}}(\mathbf{x}_j, \cdot), K_{\alpha}^{\text{kor}}(\mathbf{x}_k, \cdot) \rangle_{L^2([0,1]^d)} = \tilde{K}_{\alpha}^{\text{kor}}(\mathbf{x}_j, \mathbf{x}_k)$$

with

$$(4.3) \quad \tilde{K}_{\alpha}^{\text{kor}}(\mathbf{x}, \mathbf{x}') := \sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^{-2} e^{2\pi i \mathbf{h} \cdot (\mathbf{x} - \mathbf{x}')},$$

which can be written in a closed form with $B_{2\alpha}$.

As the point set $\{\mathbf{x}_k\}_{k=1}^N$, we will consider the so-called *rank-1 lattice* points. A rank-1 lattice point set $\{\mathbf{x}_k\}_{k=1}^N$ is given by

$$(4.4) \quad \mathbf{x}_k = \left\{ \frac{k\mathbf{z}}{N} \right\} \quad \text{for } k = 1, \dots, N,$$

where $\mathbf{z} \in \{1, \dots, N\}^d$, and the braces around the vector of length d indicate that each component of the vector is to be replaced by its fractional part. Because of the lattice structure of these points, the left-hand side of the equation (2.9) but with K_{α}^{kor} in place of K becomes a circulant

matrix, and thus the equation can be solved fast using the Fast Fourier Transform. See [23, Section 2.2] for an analogous argument.

As stated in Proposition 3.2, the squared bias can be bounded by the $\mathcal{N}_{\text{kor},\alpha}$ -orthogonal projection error to the space spanned by N functions $K_\alpha^{\text{kor}}(\mathbf{x}_k, \cdot)$, $k = 1, \dots, N$. Under the setting of this section, the projection is given by the kernel interpolation. Notice that, given N , the integer vector \mathbf{z} completely determines the lattice points (4.4), and thus the corresponding kernel interpolant. In [23], the present authors and co-authors obtained the following result on the choice of \mathbf{z} and the resulting interpolation error, which we re-state here in our context.

PROPOSITION 4.1. *Given $d \geq 1$, $\alpha > 1$, weights $(\gamma_{\mathbf{u}})_{\mathbf{u} \in \mathbb{N}}$ with $\gamma_\emptyset = 1$, and prime N , a generating vector \mathbf{z} can be constructed by a greedy algorithm called the component-by-component construction [8, 9] so that the L^2 -approximation error of the kernel interpolant $\mathcal{I}_N f$ of the density $f \in \mathcal{N}_{\text{kor},\alpha}$ using \mathbf{z} satisfies*

$$\|\mathcal{I}_N f - f\|_{L^2([0,1]^d)} \leq C_{\alpha,\delta,d} \|f\|_{\text{kor},\alpha} \frac{1}{N^{\alpha/4-\delta}} \quad \text{for every } \delta \in (0, \frac{\alpha}{4}),$$

with $C_{\alpha,\delta,d} := C_{\alpha,\delta,d}((\gamma_{\mathbf{u}})_{\mathbf{u} \in \mathbb{N}}) := (\sum_{\mathbf{u} \subset \{1, \dots, d\}} \max(|\mathbf{u}|, 1) \gamma_{\mathbf{u}}^{\frac{1}{\alpha-4\delta}} [2\zeta(\frac{\alpha}{\alpha-4\delta})]^{|\mathbf{u}|})^{\alpha-4\delta}$. Here, $\zeta(x) := \sum_{k=1}^{\infty} k^{-x}$, $x > 1$, denotes the Riemann zeta function. The constant $C_{\alpha,\delta,d}$ depends on δ but can be bounded independently of d provided that the weights satisfy

$$(4.5) \quad \sum_{\substack{\mathbf{u} \subset \mathbb{N} \\ |\mathbf{u}| < \infty}} \max(|\mathbf{u}|, 1) \gamma_{\mathbf{u}}^{\frac{1}{\alpha-4\delta}} [2\zeta(\frac{\alpha}{\alpha-4\delta})]^{|\mathbf{u}|} < \infty.$$

We now apply the variance estimate, Proposition 3.5. Let $\mathcal{N}_{\text{kor},\alpha}^\tau$ be the normed subspace of $L^2([0,1]^d)$ defined by

$$\mathcal{N}_{\text{kor},\alpha}^\tau := \{v \in L^2([0,1]^d) \mid \|v\|_{\mathcal{N}_{\text{kor},\alpha}^\tau} < \infty\},$$

with $\|v\|_{\mathcal{N}_{\text{kor},\alpha}^\tau} := (\sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^\tau |\langle v, e^{2\pi i \mathbf{h} \cdot} \rangle_{L^2([0,1]^d)}|^2)^{1/2} < \infty$, and let $\mathcal{N}_{\text{kor},\alpha}^{-\tau}$ be the vector space of continuous linear functionals on $\mathcal{N}_{\text{kor},\alpha}^\tau$. Note that, following an argument analogous to the proof of Proposition 2.1, for $\Phi \in \mathcal{N}_{\text{kor},\alpha}^{-\tau} = (\mathcal{N}_{\text{kor},\alpha}^\tau)'$ we have

$$\|\Phi\|_{\mathcal{N}_{\text{kor},\alpha}^{-\tau}} = \left(\sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^{-\tau} |\Phi(e^{2\pi i \mathbf{h} \cdot})|^2 \right)^{1/2}.$$

To be able to invoke Proposition 3.5, we first derive a lower bound for τ such that $\Delta_{\mathbf{Y}}$ is in $\mathcal{N}_{\text{kor},\alpha}^{-\tau}$.

PROPOSITION 4.2. *Let $\alpha > 1$ and $\tau \in (0, 1]$ be given. Then, the point evaluation functional $\delta_{\mathbf{x}}(v) = v(\mathbf{x})$ satisfies $\delta_{\mathbf{x}} \in \mathcal{N}_{\text{kor},\alpha}^{-\tau}$ for all $\mathbf{x} \in [0, 1]^d$ if and only if $\tau > \frac{1}{\alpha}$.*

Proof. For $v \in \mathcal{N}_{\text{kor},\alpha}^\tau$ we have

$$\begin{aligned} |\delta_{\mathbf{x}}(v)| &= \left| \sum_{\mathbf{h} \in \mathbb{Z}^d} \langle v, e^{2\pi i \mathbf{h} \cdot} \rangle_{L^2([0,1]^d)} e^{2\pi i \mathbf{h} \cdot \mathbf{x}} \right| \\ &\leq \left(\sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^{-\tau} \right)^{1/2} \left(\sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^\tau |\langle v, e^{2\pi i \mathbf{h} \cdot} \rangle_{L^2([0,1]^d)}|^2 \right)^{1/2} \\ &= \left(\sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^{-\tau} \right)^{1/2} \|v\|_{\mathcal{N}_{\text{kor},\alpha}^\tau}, \end{aligned}$$

but for $\alpha\tau > 1$ the first factor is bounded:

$$\sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^{-\tau} = 1 + \sum_{\emptyset \neq \mathbf{u} \subseteq \{1, \dots, d\}} \gamma_{\mathbf{u}}^{\tau} \left(\sum_{h \in \mathbb{Z} \setminus \{0\}} \frac{1}{|h|^{\alpha\tau}} \right)^{|\mathbf{u}|} < \infty,$$

and thus if $\tau > \frac{1}{\alpha}$, then $\delta_{\mathbf{x}} \in \mathcal{N}_{\text{kor}, \alpha}^{-\tau}$ for any $\mathbf{x} \in [0, 1]^d$. Suppose now $\tau \leq \frac{1}{\alpha}$. If $\delta_{\mathbf{x}}$ is continuous on $\mathcal{N}_{\text{kor}, \alpha}^{\tau}$, then from Riesz representation theorem there exists $\Phi_{\mathbf{x}} \in \mathcal{N}_{\text{kor}, \alpha}^{\tau}$ such that

$$v(\mathbf{x}) = \sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^{\tau} \langle \Phi_{\mathbf{x}}, e^{2\pi i \mathbf{h} \cdot \cdot} \rangle_{L^2([0, 1]^d)} \overline{\langle v, e^{2\pi i \mathbf{h} \cdot \cdot} \rangle_{L^2([0, 1]^d)}} \text{ for any } v \in \mathcal{N}_{\text{kor}, \alpha}^{\tau},$$

where we let $\overline{\langle v, e^{2\pi i \mathbf{h} \cdot \cdot} \rangle_{L^2([0, 1]^d)}} := \int_{[0, 1]^d} v(\mathbf{y}) e^{2\pi i \mathbf{h} \cdot \mathbf{y}} d\mathbf{y}$. Choosing $v(\mathbf{x}) = e^{2\pi i \tilde{\mathbf{h}} \cdot \mathbf{x}}$, $\tilde{\mathbf{h}} \in \mathbb{Z}^d$ yields $e^{2\pi i \tilde{\mathbf{h}} \cdot \mathbf{x}} = r(\tilde{\mathbf{h}}, \gamma)^{\tau} \langle \Phi_{\mathbf{x}}, e^{2\pi i \tilde{\mathbf{h}} \cdot \cdot} \rangle_{L^2([0, 1]^d)}$, and thus $1 = r(\tilde{\mathbf{h}}, \gamma)^{2\tau} |\langle \Phi_{\mathbf{x}}, e^{2\pi i \tilde{\mathbf{h}} \cdot \cdot} \rangle_{L^2([0, 1]^d)}|^2$. Hence, we obtain

$$\sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^{-\tau} = \sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^{\tau} |\langle \Phi_{\mathbf{x}}, e^{2\pi i \mathbf{h} \cdot \cdot} \rangle_{L^2([0, 1]^d)}|^2.$$

From $\Phi_{\mathbf{x}} \in \mathcal{N}_{\text{kor}, \alpha}^{\tau}$, the right hand side is convergent, whereas for $\tau\alpha \leq 1$ the left hand side is divergent, a contradiction. Hence, $\delta_{\mathbf{x}}$ is not continuous on $\mathcal{N}_{\text{kor}, \alpha}^{\tau}$. \square

Indeed, for $\alpha\tau > 1$ the space $\mathcal{N}_{\text{kor}, \alpha}^{\tau}$ is a reproducing kernel Hilbert space. To see this, let

$$\begin{aligned} K_{\alpha; \tau}^{\text{kor}}(\mathbf{x}, \mathbf{x}') &:= \sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^{-\tau} e^{2\pi i \mathbf{h} \cdot (\mathbf{x} - \mathbf{x}')} \\ &= 1 + \sum_{\emptyset \neq \mathbf{u} \subseteq \{1, \dots, d\}} \gamma_{\mathbf{u}}^{\tau} K_{\alpha; \tau}(\mathbf{x}_{\mathbf{u}}, \mathbf{x}'_{\mathbf{u}}), \end{aligned}$$

where

$$K_{\alpha; \tau}^{\text{kor}}(\mathbf{x}_{\mathbf{u}}, \mathbf{x}'_{\mathbf{u}}) = \prod_{j \in \mathbf{u}} \left(\sum_{h \in \mathbb{Z} \setminus \{0\}} \frac{e^{2\pi i h(x_j - x'_j)}}{|h|^{\alpha\tau}} \right).$$

If $\alpha\tau > 1$, the series is uniformly absolutely-convergent and thus the kernel is continuous on $[0, 1]^d$; if $\alpha\tau \leq 1$, then the series $K_{\alpha; \tau}(\mathbf{0}, \mathbf{0})$ is divergent. Hence, $K_{\alpha; \tau}^{\text{kor}}(\mathbf{x}, \mathbf{x}')$ is a reproducing kernel if and only if $\alpha\tau > 1$.

We conclude this section with the following estimates.

THEOREM 4.3. *Let $\alpha > 1$. Fix $\delta \in (0, \frac{\alpha}{4})$ and $\tau \in (\frac{1}{\alpha}, 1]$ arbitrarily. Let the weights $(\gamma_{\mathbf{u}})_{\mathbf{u} \subset \mathbb{N}}$ satisfy $\gamma_{\emptyset} = 1$. Then, for $f \in \mathcal{N}_{\text{kor}, \alpha}$ we have*

$$\begin{aligned} \mathbb{E} \left[\int_{[0, 1]^d} |f_{M, N; \mathbf{Y}}^{\lambda}(\mathbf{x}) - f(\mathbf{x})|^2 d\mathbf{x} \right] \\ \leq C_{\alpha, \delta, \tau, d} \left(\|f\|_{\text{kor}, \alpha}^2 \frac{1}{N^{\alpha/2 - 2\delta}} + \lambda \|f\|_{\text{kor}, \alpha}^2 + \frac{\|f\|_{L^2([0, 1]^d)}}{M\lambda^{\tau}} \right), \end{aligned}$$

where the constant $C_{\alpha, \delta, \tau, d} = C_{\alpha, \delta, \tau, d}((\gamma_{\mathbf{u}})_{\mathbf{u} \subset \mathbb{N}}) > 0$ depends on α, δ, τ but can be bounded independently of d provided that (4.5) holds. Moreover, if f is in the RKHS $(\mathcal{N}_{\text{kor}, \alpha}^{\sim}, \|\cdot\|_{\text{kor}, \alpha}^{\sim})$ associated with the kernel (4.3), then the bound improves to

$$\begin{aligned} \mathbb{E} \left[\int_{[0, 1]^d} |f_{M, N; \mathbf{Y}}^{\lambda}(\mathbf{x}) - f(\mathbf{x})|^2 d\mathbf{x} \right] \\ \leq \tilde{C}_{\alpha, \delta, \tau, d} \left(\|f\|_{\text{kor}, \alpha}^2 \frac{1}{N^{\alpha/2 - 2\delta}} + \lambda^2 \|f\|_{\text{kor}, \alpha}^{\sim 2} + \frac{\|f\|_{L^2([0, 1]^d)}}{M\lambda^{\tau}} \right), \end{aligned}$$

where the constant $\tilde{C}_{\alpha,\delta,\tau,d} = \tilde{C}_{\alpha,\delta,\tau,d}((\gamma_{\mathbf{u}})_{\mathbf{u} \subset \mathbb{N}}) > 0$ depends on α, δ, τ but can be bounded independently of d provided that the weights corresponding to the kernel (4.3) satisfy the summability condition analogous to (4.5).

Proof. From (3.8) in Theorem 3.6, Proposition 4.1 implies

$$\begin{aligned} & \mathbb{E} \left[\int_{[0,1]^d} |f_{M,N;\mathbf{Y}}^\lambda(\mathbf{x}) - f(\mathbf{x})|^2 d\mathbf{x} \right] \\ & \leq C_{\alpha,\delta}^2 \|f\|_{\text{kor},\alpha}^2 \frac{1}{N^{\alpha/2-2\delta}} + \lambda \|f\|_{\text{kor},\alpha}^2 + \frac{\langle K_{\alpha;\tau}^{\text{kor}}(\cdot, \cdot), f \rangle_{L^2([0,1]^d)}}{M\lambda^\tau}, \end{aligned}$$

for any $\delta \in (0, \frac{\alpha}{4})$ and $\tau \in (\frac{1}{\alpha}, 1]$, where we note that

$$\langle K_{\alpha;\tau}^{\text{kor}}(\cdot, \cdot), f \rangle_{L^2([0,1]^d)} \leq \|f\|_{L^2([0,1]^d)} \sum_{\mathbf{h} \in \mathbb{Z}^d} r(\mathbf{h}, \gamma)^{-\tau} < \infty.$$

The proof for the second claim follows from an analogous argument using (3.9). \square

Given that the density is sufficiently smooth, we obtain the MISE convergence rate arbitrarily close to $M^{-1/(1+\frac{1}{\alpha})}$, independently of the dimension d .

COROLLARY 4.4. *Let $\alpha > 1$. Fix $\delta \in (0, \frac{\alpha}{4})$ and $\epsilon \in (0, 1 - \frac{1}{\alpha}]$ arbitrarily. Suppose that weights $(\gamma_{\mathbf{u}})_{\mathbf{u} \subset \mathbb{N}}$ satisfy $\gamma_\emptyset = 1$. Then, for $f \in \mathcal{N}_{\text{kor},\alpha}$, choosing $\lambda^* = M^{-1/(1+\frac{1}{\alpha}+\epsilon)}$, $N^* = \mathcal{O}(M^{1/(\frac{\alpha}{2}(1+\epsilon)+\frac{1}{2}-\frac{\delta}{2}(1+\frac{1}{\alpha}+\epsilon)))}$, and $\tau^* = \frac{1}{\alpha} + \epsilon$ in Theorem 4.3 yields*

$$\mathbb{E} \left[\int_{[0,1]^d} |f_{M,N;\mathbf{Y}}^\lambda(\mathbf{x}) - f(\mathbf{x})|^2 d\mathbf{x} \right] \leq C_{\alpha,\delta,d} \|f\|_{\text{kor},\alpha}^2 M^{-1/(1+\frac{1}{\alpha}+\epsilon)}.$$

Moreover, if f is in the RKHS $(\mathcal{N}_{\text{kor},\alpha}, \|\cdot\|_{\text{kor},\alpha})$ associated with the kernel (4.3), then by choosing $\tau^* = \frac{1}{\alpha} + 2\epsilon$, $\lambda^* = M^{-1/(2+\frac{1}{\alpha}+2\epsilon)}$, and $N^* = \mathcal{O}(M^{1/(\frac{\alpha}{2}(1+\epsilon)+1-\frac{\delta}{2}(1+\frac{1}{2\alpha}+\epsilon)))}$ in Theorem 4.3, we have a rate asymptotically faster in α

$$\mathbb{E} \left[\int_{[0,1]^d} |f_{M,N;\mathbf{Y}}^\lambda(\mathbf{x}) - f(\mathbf{x})|^2 d\mathbf{x} \right] \leq C_{\alpha,\delta,d} \|f\|_{\text{kor},\alpha}^2 M^{-1/(1+\frac{1}{2\alpha}+\epsilon)}.$$

The constant $C_{\alpha,\delta,d} = C_{\alpha,\delta,d}((\gamma_{\mathbf{u}})_{\mathbf{u} \subset \mathbb{N}}) > 0$ can be bounded independently of d provided that (4.5) holds.

It turns out that the rate established above is almost minimax when α is an even integer. For simplicity, let us consider the equal weights $\gamma_{\mathbf{u}} = 1$ for all $\mathbf{u} \subset \{1, \dots, d\}$. For general weights, the following inequality still holds true, up to a constant depending on $(\gamma_{\mathbf{u}})_{\mathbf{u} \subset \{1, \dots, d\}}$.

Indeed, from the classical asymptotic minimax rate for the Korobov spaces $\mathcal{N}_{\text{kor},\alpha,1}$ for $d = 1$ and α even, (see [13, Example 1], also [14], where we note that the definition of α in [13] is different from ours by a factor of 2), for M sufficiently large we have

$$\begin{aligned} C_\alpha M^{-1/(1+\frac{1}{\alpha})} & \leq \inf_f \sup_{\substack{f \in \mathcal{N}_{\text{kor},\alpha,1} \\ \|f\|_{\text{kor},\alpha,1} \leq 1}} \mathbb{E} \left[\int_{[0,1]} |\hat{f}(x) - f(x)|^2 dx \right] \\ & \leq \inf_f \sup_{\substack{f \in \mathcal{N}_{\text{kor},\alpha} \\ \|f\|_{\text{kor},\alpha} \leq 1}} \mathbb{E} \left[\int_{[0,1]^d} |\hat{f}(\mathbf{x}) - f(\mathbf{x})|^2 d\mathbf{x} \right] \\ & \leq \sup_{\substack{f \in \mathcal{N}_{\text{kor},\alpha} \\ \|f\|_{\text{kor},\alpha} \leq 1}} \mathbb{E} \left[\int_{[0,1]^d} |f_{M,N;\mathbf{Y}}^\lambda(\mathbf{x}) - f(\mathbf{x})|^2 d\mathbf{x} \right] \leq C_{\alpha,\delta,d} M^{-1/(1+\frac{1}{\alpha}+\epsilon)}, \end{aligned}$$

where the infimum is taken over all possible estimates $\hat{f} = \hat{f}(Y_1, \dots, Y_M)$. Here, the first inequality follows from [13, Example 1], in the second inequality we used that $f \in \mathcal{N}_{\text{kor},\alpha,1}$ can be seen as a function $\tilde{f} \in \mathcal{N}_{\text{kor},\alpha}$ on $[0, 1]^d$ depending only on one variable with $\|f\|_{\text{kor},\alpha,1} = \|\tilde{f}\|_{\text{kor},\alpha}$ for $\alpha/2 \in \mathbb{N}$ with equal weights, and the last inequality is from Corollary 4.4. Hence, we conclude that the rate $\mathcal{O}(M^{-1/(1+\frac{1}{\alpha}+\epsilon)})$ as in Corollary 4.4 is asymptotically minimax up to $\epsilon > 0$ for $f \in \mathcal{N}_{\text{kor},\alpha}$. Similarly, for $f \in \mathcal{N}_{\text{kor},\alpha}^{\sim}$ the rate $\mathcal{O}(M^{-1/(1+\frac{1}{2\alpha})})$ is asymptotically minimax, at least for α integer.

5. Numerical results. We consider the density function

$$(5.1) \quad f(\mathbf{y}) = \prod_{j=1}^d \left(1 + \frac{1}{j^4} B_4(y_j) \right), \quad \mathbf{y} \in [0, 1]^d,$$

with respect to the uniform measure. Notice that, from $B_4 > -1$ on $[0, 1]$ and $\int_0^1 B_4(t) dt = 0$ the function f is indeed a density function. The dimensions we consider are $d = 6$ and $d = 15$.

We generate samples $Y_m \sim \int f(\mathbf{y}) d\mathbf{y}$ using the Acceptance-Rejection method; see for example [16, Section 2.2]. The generating vector for the lattice points are obtained by the component-by-component algorithm in [8]. The experiments were implemented in Julia 1.6.0 [4]. We approximate the MISE by

$$\begin{aligned} & \mathbb{E} \left[\int_{[0,1]^d} |f_{M,N;\mathbf{Y}}^\lambda(\mathbf{x}) - f(\mathbf{x})|^2 d\mathbf{x} \right] \\ & \approx \frac{1}{S} \sum_{k=1}^S \frac{1}{100N} \sum_{n=1}^N \sum_{\ell=1}^{100} |f_{M,N;\mathbf{Y}^{(k)}}^\lambda(\{\mathbf{x}_n + \mathbf{p}_\ell\}) - f(\{\mathbf{x}_n + \mathbf{p}_\ell\})|^2, \end{aligned}$$

where \mathbf{x}_n , $n = 1, \dots, N$ are the lattice points used to determine the approximation space, \mathbf{p}_ℓ , $\ell = 1, \dots, 100$ are a set of Sobol' points generated by the Julia function `SobolSeq` [22], and the braces around the vector of length d indicate that each component of the vector is to be replaced by its fractional part. This choice of evaluation points admits a fast evaluation; see [23] for more details. The number S of Monte Carlo replications $\mathbf{Y}^{(1)}, \dots, \mathbf{Y}^{(S)}$ is chosen such that the estimated confidence interval is smaller than the estimated MISE at least by a factor of 10. As a kernel, we consider the Korobov kernel with product weights $\gamma_{\mathbf{u}} = \prod_{j \in \mathbf{u}} \frac{1}{j^\alpha}$ as in (4.2), with $\alpha \in \{2, 4\}$. Observe that f as in (5.1) satisfies $f \in \mathcal{N}_{\text{kor},\alpha}$ with $\alpha \in (1, 4]$.

Fig. 1 shows a decay of MISE for $N = 5, 7, 11$, with various values of λ between 0.8 and 0.01 for $d = 6$. Firstly, we report that increasing N beyond $N = 11$ did not help decreasing the error. We interpret this as the projection error in Theorem 4.3 being negligible, and we focus, therefore, on the other two error terms in Theorem 4.3. For the sample size M large ($M = 10^5, 10^6$), we observe that the error decreases as λ becomes smaller. This supports Theorem 4.3, where the term $\mathcal{O}(1/(M\lambda^\tau))$, $\tau \in (1/\alpha, 1)$ with large M would be negligible, and the term $\mathcal{O}(\lambda)$ would be dominant. For smaller values of M , from Theorem 4.3 we expect that the term $\mathcal{O}(1/(M\lambda^\tau))$ is dominant relative to $\mathcal{O}(\lambda)$, and that as M increases the MISE decays. This is precisely what we observe in Fig. 1. We also see that the values of α affect the decay in M only up to a constant, which again indicates the validity of our theory. We report a similar behaviour of the error for $d = 15$ in Fig. 2, which further supports our theory.

Next, we will see the behaviour of MISE for even smaller values of λ . Figs. 3 and 4 show a decay of MISE for various values of λ between 0.1 and 0.0001 with $N = 11$ and varying sample size M . Like in the previous case, we observe that the MISE decays in M with rate M^{-1} until it reaches a plateau. However, unlike in the previous case, we see that even on the plateau the

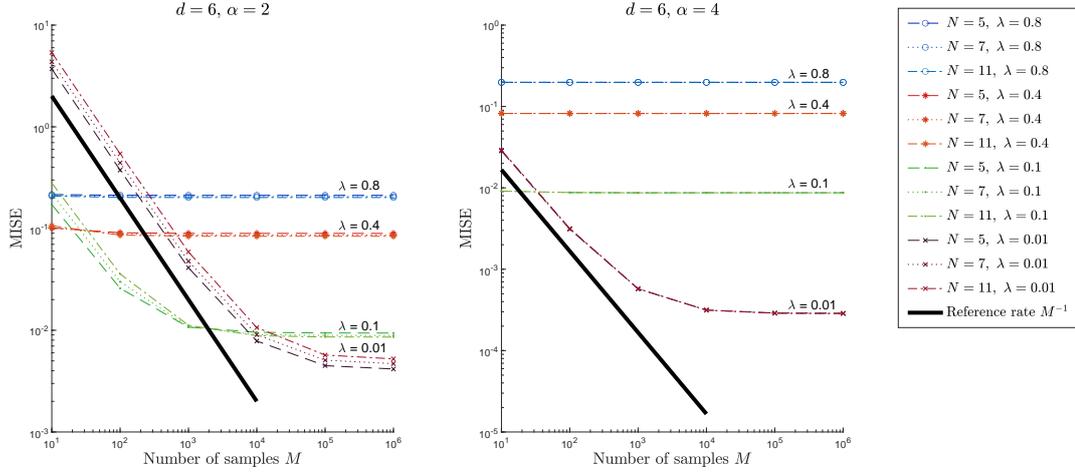


FIG. 1. Plot of MISE with $d = 6$, $\alpha = 2$ (left), 4 (right), and $\lambda = 0.8, \dots, 0.01$ with varying sample size M

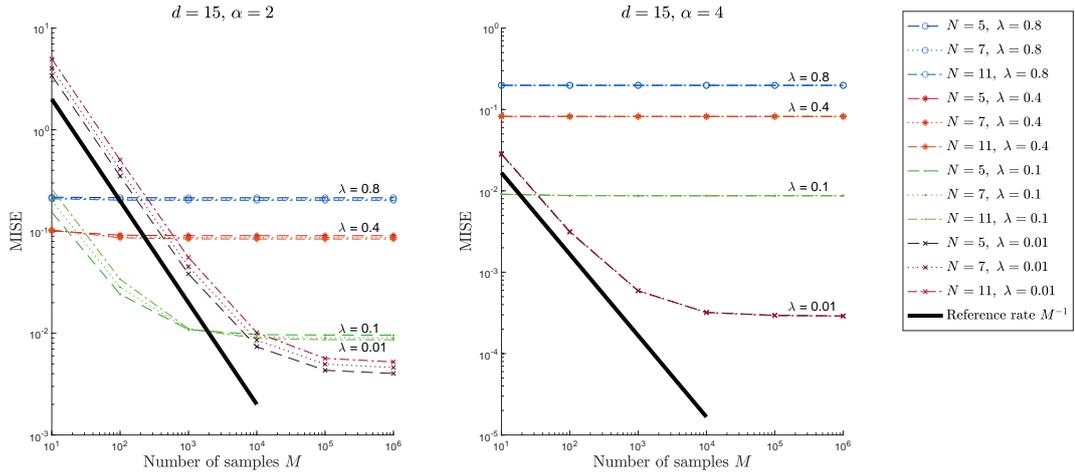


FIG. 2. Plot of MISE with $d = 15$, $\alpha = 2$ (left), 4 (right), and $\lambda = 0.8, \dots, 0.01$ with varying sample size M

error may be larger for smaller λ . To understand this observation, we next see the behaviour of the MISE in λ , with other parameters being fixed.

Figs. 5 and 6 show MISE with $N = 11$ and $M = 10^4$, with $\lambda = 0.7^k$, $k = 0, \dots, 70$ for $d = 6$ and 15.

For $d = 6$ and $\alpha = 2$, from $\lambda = 1$ to $\lambda = 0.7^9 \approx 0.04$, we see the MISE decays almost quadratically in λ ; see the graphs on the left in Fig. 5. Then, the MISE increases as λ becomes small until it reaches a plateau. Although the rate of this increase in the regime of $\lambda = 0.7^{10} \approx 0.03, \dots, 0.7^{25} \approx 0.001$ is faster than the rate $\lambda^{-1/\alpha}$ that is anticipated by Theorem 4.3, asymptotically the observed rate of increase is better than this theoretical rate. This observation may suggest that our theoretical rate is not sharp, but it is consistent with our theory.

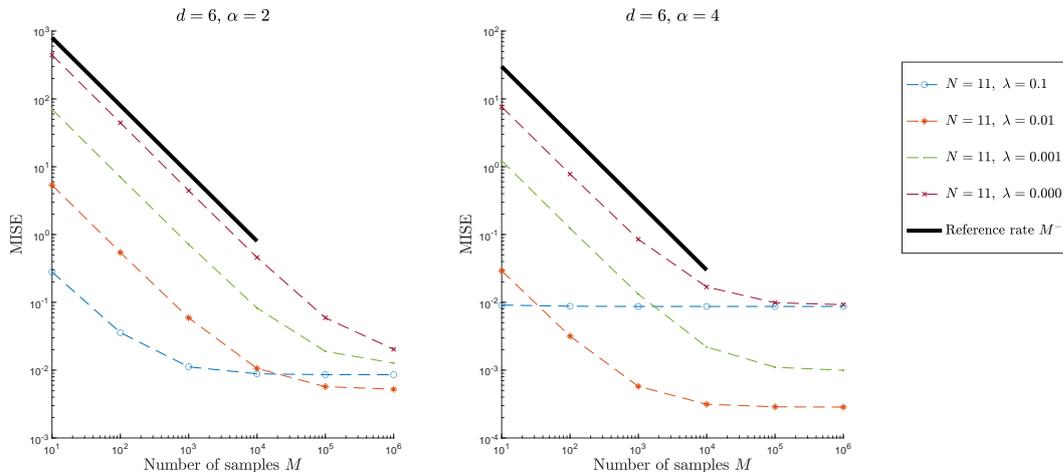


FIG. 3. Plot of MISE for $d = 6$, $\alpha = 2$ (left), 4 (right), and $\lambda = 0.1, \dots, 0.0001$ with varying sample size M .

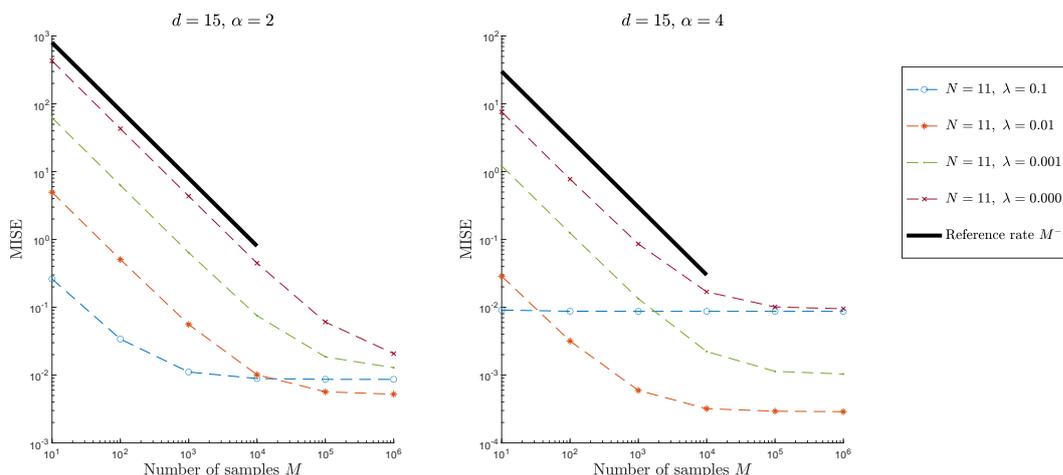


FIG. 4. Plot of MISE for $d = 15$, $\alpha = 2$ (left), 4 (right), and $\lambda = 0.1, \dots, 0.0001$ with varying sample size M .

For $\alpha = 4$ we observe a similar behaviour in the graphs on the right in Fig. 5: the MISE decays, and then increases until it reaches a plateau. This observation again supports Theorem 4.3. For $d = 15$, we observe similar results, which further supports our theory; see Fig. 6.

Finally, we show in Figs. 7 and 8 the error decay for $\lambda = \lambda(M, \alpha)$ depending on M and α as in Corollary 4.4. For $\alpha = 2$, we let $\lambda = 1000M^{-\frac{1}{1+1/\alpha}}$, and for $\alpha = 4$ we let $\lambda = 5000M^{-\frac{1}{1+1/\alpha}}$, with $M = 10^k$, $k = 3, \dots, 7$. In both Figs., we observe that the MISE decays with rate essentially $M^{-\frac{1}{1+1/\alpha}}$, which supports our theory.

6. Conclusions. In this paper, we considered a kernel method to approximate probability density functions. A major contribution of this paper is to have established a dimension-

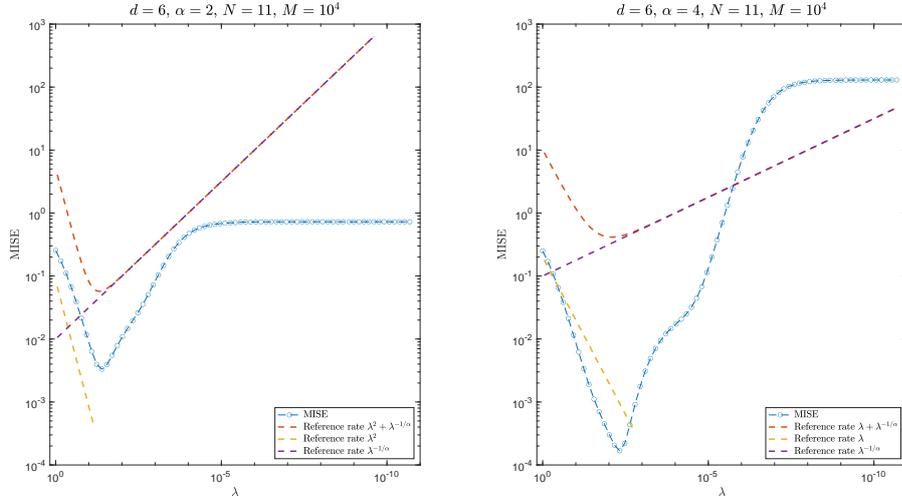


FIG. 5. Plot of MISE for $d = 6$, $\alpha = 2$ (left), 4 (right), $N = 11$, and $M = 10^4$ with $\lambda = 0.7^k$, $k = 0, \dots, 70$.

independent error convergence rate. To show this, we first developed a theory in a general RKHS setting. We then applied this theory to the Korobov-space setting, in which we established a dimension-independent error decay rate. Therein, the implied constant is also dimension independent under suitable assumptions on the underlying weights. By choosing parameters suitably, we obtained the rate in terms of the MISE arbitrarily close to 1 in the sample size, given that the target density is in the weighted Korobov space of arbitrary order. For the Korobov spaces whose order is an even integer, the rate obtained is asymptotically minimax. Numerical results supported the theory.

In closing, we discuss some possible future directions. An important point in the kernel density literature concerns the choice of the bandwidth (see for instance [18, 17] for robust adaptive selection, independent on the smoothness of the underlying density) In the present setting, our kernel is polynomial and not necessarily localised, so the problem of bandwidth selection does not really apply to our case. On the other hand, our results assume that the target density is in the RKHS corresponding to the kernel we use. Thus, a relevant question is how one should choose the weights in the kernel, as well as the regularization parameter λ , when the regularity class of the target density is not known. This topic is left for future work.

Another important point to discuss is the periodicity assumption. The full error estimates with respect to the sample size M as in Corollary 4.4 presented in this paper is limited to the weighted Korobov space setting, in which the target density is assumed to admit a smooth periodic extension. Needless to say, there is scope for further work to generalise our error bounds. In this regard, we stress that the results we established in Section 3 are general and applicable to many other kernel functions. As we demonstrated in Section 4, to obtain precise estimates as in Corollary 4.4 for such kernels, it suffices to obtain a kernel interpolation estimate. Moreover, in view of the optimality of kernel interpolation, it suffices to obtain a sampling-based approximation that gives a small error in the corresponding reproducing kernel Hilbert space. In turn, this paper provides further motivations on fully discrete approximation methods.

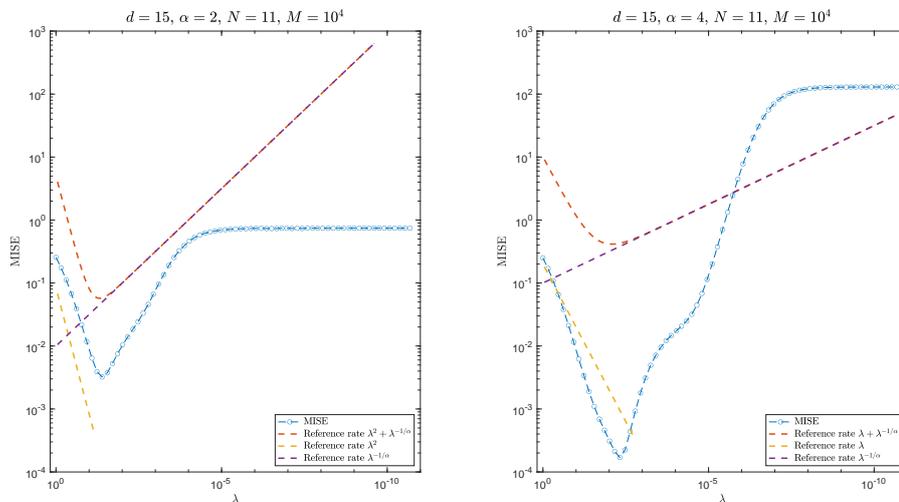


FIG. 6. Plot of MISE for $d = 15$, $\alpha = 2$ (left), 4 (right), $N = 11$, and $M = 10^4$ with $\lambda = 0.7^k$, $k = 0, \dots, 70$.

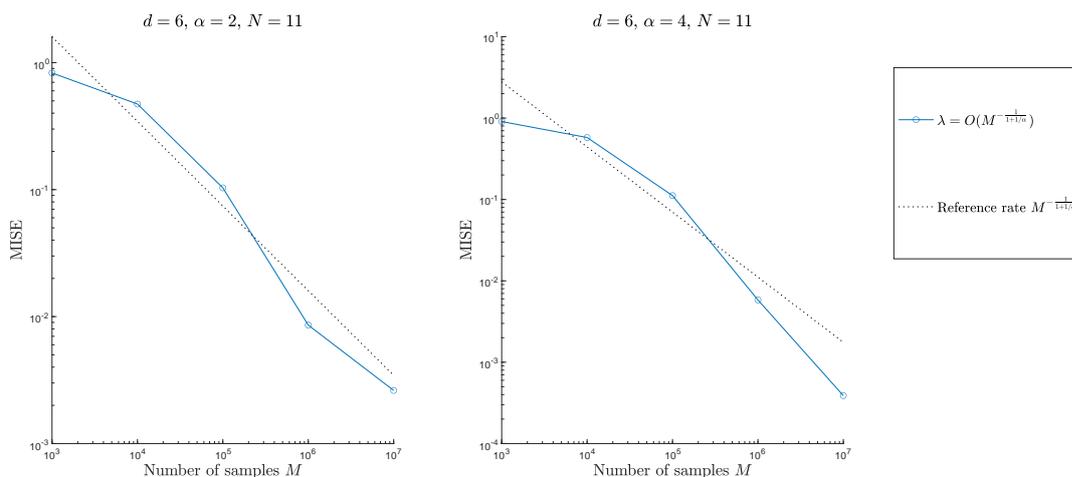


FIG. 7. Plot of MISE for $d = 6$ with $N = 11$, $\alpha = 2$ (left), 4 (right), and $\lambda = O(M^{-\frac{1}{1+1/\alpha}})$.

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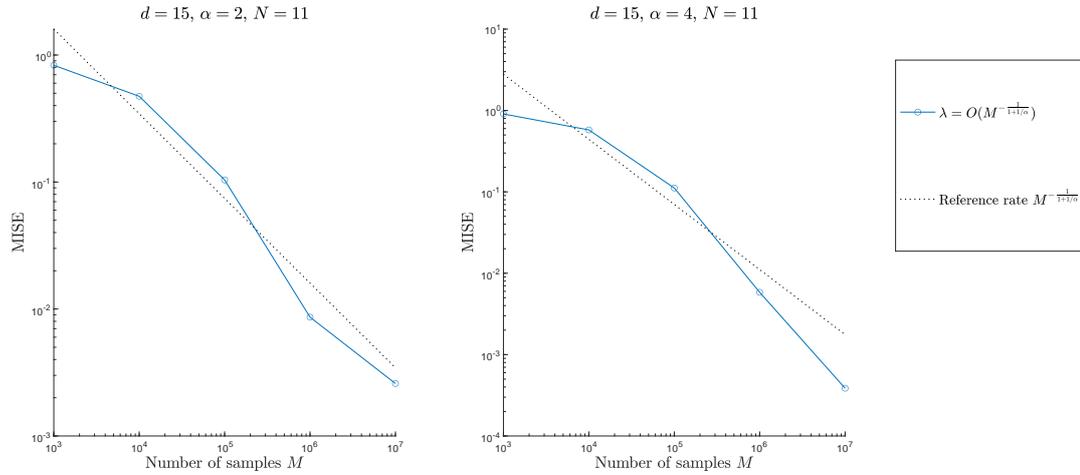


FIG. 8. Plot of MISE for $d = 15$ with $N = 11$, $\alpha = 2$ (left), 4 (right), and $\lambda = O(M^{-\frac{1}{1+\alpha}})$.

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