In the paper, we study the problem of estimating linear response statistics under external perturbations using time series of unperturbed dynamics. A standard approach to this estimation problem is to employ the Fluctuation-Dissipation Theory, which, in turn, requires the knowledge of the functional form of the underlying unperturbed density that is not available in general. To overcome this issue, we consider a nonparametric density estimator formulated by the kernel embedding of distribution. To avoid the computational expense arises using radial type kernels, we consider the “Mercer-type” kernels constructed based on the classical orthogonal bases defined on non-compact domains, such as the Hermite and Laguerre polynomials. By studying the orthogonal polynomial approximation in the reproducing kernel Hilbert space (RKHS) setting, we establish the uniform convergence of the estimator, which justifies the use of the estimator for interpolation. Given a target function with a specific decaying property that can be quantified using the available data, our study allows one to choose the appropriate hypothesis space (an RKHS) that is “rich” enough for consistent estimation. In terms of linear response estimation, our study provides practical conditions for the well-posedness of not only the estimator but also the well-posedness of the underlying response statistics. Given a well-posed estimator, we provide a theoretical guarantee for the convergence of the estimator to the underlying actual linear response statistics. Finally, we provide a statistical error bound for the density estimation that accounts for the Monte-Carlo averaging over non-i.i.d time series and biases due to finite basis truncation. This error bound provides a mean to understand the feasibility as well as limitation of the kernel embedding with Mercer-type kernel. Numerically, we verify the effectiveness of the kernel embedding linear response estimator on two stochastic dynamics with known, yet, non-trivial equilibrium densities.
1 Introduction

Estimating the linear response statistics of dynamical systems under external forces is a problem of broad interest. This forward uncertainty quantification problem has many critical applications. For example, in climate dynamics, the linear response can be used as a proxy that quantifies the climate change statistics corresponding to exogenous forcing such as the volcanic eruptions or even the anthropogenic factor such as the human activities \[12\]. In statistical mechanics, the linear response provides a simple route to determine transport coefficients from microscopic fluctuations \[3\], such as viscosity, diffusion coefficients, and heat conductivity via Green-Kubo type of formulas \[4, 5\]. One of the popular approaches to quantify the linear response statistics is using the Fluctuation-Dissipation theory (FDT), which roughly states that the leading order (linear) statistical response to small perturbations can be approximated by a two-point statistic of the unperturbed dynamics. In this paper, we consider computing linear response in the context of ergodic stochastic differential equations, which validity was studied in \[6\].

In practice, while the relevant two-point statistics can be numerically estimated by a Monte-Carlo average over samples of unperturbed dynamics at equilibrium state, the integrand (or the function to be averaged) depends on the explicit expression of the equilibrium density of the unperturbed dynamical system which is unknown in general. One well-known example in statistical mechanics is non-equilibrium steady states, e.g., a planar Couette flow in the study of the rheology of complex fluids \[7\]. Although some general properties associated with the linear response around steady states have been identified \[8, 9, 10\], the explicit form of the probability density function is still difficult to obtain. On the other hand, the response approach shows a significant advantage in the regime of low strain rate, which is highly challenging for direct simulations due to the vanishing signal to noise ratio \[11\].

In this paper, we consider a nonparametric formulation, known as the kernel embedding of distributions \[12\], as an estimator to the unknown equilibrium density of the unperturbed dynamics, which in turn, allows us to compute the linear response statistics via the FDT theory. We should point out that the concept of kernel embedding of distribution was introduced \[12\] to characterize probability distributions with the kernel mean embedding, which are nothing but statistical quantities of relevant feature map corresponds to a reproducing kernel Hilbert space (RKHS). In this paper, we use kernel embedding to estimate probability density function. In particular, the estimator will be represented as a linear superposition of the RKHS basis functions with the kernel mean embedding as the expansion coefficients.

For this application, the direct use of the kernel embedding estimator with radial-type kernels is not practical. In particular, given a training data set of size \(N\), which can be of order \(10^7\) or larger depending on applications, the estimator will be defined as a linear superposition of radial functions \(k(x, x_i) = h(\|x - x_i\|)\), where \(\|\cdot\|\) denotes, e.g, the \(d\)-dimensional Euclidean norm for some \(h > 0\). With such estimator, computing the linear response statistics will require evaluating the norm of the distances between pairs of training data points roughly \(N^2/2\) times in addition to evaluating \(h\) on each of these \(N^2/2\) distances. Such a method is the same cost as the standard kernel density estimation \[13\]. In this paper, we consider ”Mercer-type” kernels constructed using the classical orthogonal polynomials of weighted \(L^2\)-space. Such representation allows us to conveniently consider a hypothesis model with finitely many expansion coefficients, \(M \ll N\), and thus, arrives at a parametric model and a simple theoretical error bound. Computationally, the calculation of linear response statistics amounts to evaluating \(M\) polynomial basis functions (instead of \(N/2\) radial basis functions) on \(N\) training data points.

To mathematically understand the proposed approach, we need to ”properly” construct the RKHS based on the Mercer-type kernels such that its components inherit all the “nice” properties of the kernel, such as boundedness and smoothness. This “proper” construction is needed because these desirable properties, boundedness, and smoothness, are not automatically inherited by the kernel definition alone when its domain is not a compact metric space, which leads us to call the constructed kernel as the ”Mercer-type”. We should point out that while the resulting estimator is not different from the polynomial chaos expansion (e.g., with Hermite polynomials), the RKHS representation guarantees uniform convergence of the estimator as \(M \to \infty\), which is stronger than the classical \(L^2\)-convergence of the polynomial chaos that relies on Cameron-Martin theorem (see e.g., \[14, 15\]). Once the framework for constructing the hypothesis (RKHS) space is developed, we would like to understand how ”large” is the resulting RKHS space in order to guarantee that the estimator can consistently approximate the target density function. To understand this, we generalize the notion of \(c_0\)-universality of the kernel that was introduced in \[16, 17\] on space of continuous functions on \(\mathbb{R}^d\) with appropriate decay rate. Since the target density is a positive function defined on a non-compact domain, \(\mathbb{R}^d\), we need to specify appropriate conditions for the well-posedness on the estimator to avoid admitting negative values. Once the well-posed estimator is conceived, we provide a theoretical guarantee for the consistency in the sense that, in the limit of sample size, the estimator converges to the underlying true linear response statistics. Finally, we also provide a statistical error bound for the density estimation that accounts for the Monte-Carlo discretization, averaging over non-i.i.d time series with \(\alpha\)-mixing property \[18, 19\]. This error bound provides a mean to understand the feasibility as well as limitation of the kernel
embedding with Mercer-type kernel in general problems. To complement this theoretical study, we also numerically demonstrate the effectiveness of the proposed estimator in producing accurate linear response statistics on two classical types of SDEs with known densities for verification.

Outline and Main Contributions We close this introduction with an outline of the rest of the paper, summarizing the main contributions of each section. Main results:

• In Section 2, we provide a quick review of the FDT linear response theory and relevant results on kernels and RKHS. To have a well-defined estimation problem, we deduce sufficient conditions to guarantee that the underlying FDT linear response operator is bounded uniformly in time (see Lemma 2.1). The main novel contribution in this section is the generalization of the \(c_0\)-universality of kernels to weighted \(c_0\)-universalities, which will be used to characterize the denseness of a given RKHS in the space of continuous function of a certain decay rate. We derive the connection between \(c_0\)-universal kernels and weighted \(c_0\)-universal kernels (see Lemma 2.8) so that the principals in \(c_0\)-universality can be shifted to the weighted scenario.

• In Section 3, we discuss a framework for constructing RKHS from classical orthogonal polynomials of weighted \(L^2\)-space. The main contribution is summarized in Proposition 3.4. In Section 3.1.1, we study the RKHS constructed using the Hermite polynomials. In this case, the resulting kernel is the well-known Mehler kernel [20]. We specify the regularity of the resulting RKHS in Corollary 3.5. In Section 3.1.2, we also study the RKHS constructed using the Laguerre polynomials. We show the boundedness of the resulting kernel, which is named as the Hille-Hardy kernel, in Lemma 3.6. In Section 3.2, we show that the RKHS associated with the Mehler kernel is "rich enough" to approximate any continuous density function with Gaussian (or faster) decay-rate of arbitrary variance (see Corollary 3.7 and Remark 3.8).

• In Section 4, we introduce the kernel embedding approximation to the linear response statistics. To simplify the discussion and provide a concrete error bound; we only present results based on the Mehler kernel. The same overall conclusion holds with different constants in error bound and different weighted \(L^2\)-space if the same technique is applied on the Hille-Hardy kernel. Based on the RKHS induced by the Mehler kernel, we consider the kernel embedding estimates of the target equilibrium distribution function of an ergodic Itô diffusion. Consequently, we define the kernel embedding linear response operator as the FDT response operator formula with the kernel embedding density estimate. The well-posedness is discussed before the Proposition 4.1 that summarizes the consistency of the proposed estimator. Using the regularity of the functions in RKHS induced by the Mehler kernel, we specify sufficient conditions for the external forces to admit a well-defined FDT response operator for the class of target function in the RKHS (see Remark 4.2). In Proposition 4.3, we provide an error bound for the Monte-Carlo approximation under non-i.i.d data and discuss the implication of this result.

• In Section 5, we numerically validate the kernel embedding linear response on two ergodic SDEs with known analytical equilibrium densities. We will demonstrate the effectiveness of the Hermite and Laguerre polynomials to approximate densities with symmetric and non-symmetric decaying tails, respectively.

• In Section 6, we close this paper with a summary and discussion on open problems and future research plans that stem from this study.

Some proofs are reported in the Appendices to improve the readability.

2 Preliminary on the theory of linear response and RKHS

In the current Section, we first review the linear response theory, which provides the motivation of learning the equilibrium density of SDEs from the observations. Then we include a short survey on RKHS and related results. We refer readers to [2][12][21] for more comprehensive discussions.

2.1 Linear response theory

The Fluctuation-Dissipation Theory (FDT) is a mathematical framework for quantifying the linear response of a dynamical system subjected to small external forcing [11]. The linear response statistics, determined based on two-point equilibrium statistics of the unperturbed dynamics, provide estimates for the non-equilibrium properties. In statistical mechanics literature, FDT is known as the linear response approach [11], which is the foundation for defining transport coefficients, e.g., viscosity, diffusion constant, heat conductivity, etc.
The review will be presented in the context of the \(d\)-dimensional (time-homogeneous) SDEs, also known as the Itô diffusions \([22]\). The SDEs, together with its perturbed dynamics, are written as follows,

\[
\begin{align*}
\dot{X} &= b(X) + \sigma(X) \dot{W}_t, \\
\dot{X}^\delta &= b(X^\delta) + c(X^\delta) \delta f(t) + \sigma(X^\delta) \dot{U}_t,
\end{align*}
\]

respectively, where \(W_t\) and \(U_t\) are standard Wiener processes. In the unperturbed system \([1]\), the vector field \(b(X)\) denotes the drift and \(\sigma(X)\) is the diffusion tensor; while in the perturbed system \([2]\), an order-\(\delta\) (\(\delta \ll 1\)) external perturbation is introduced, in the form of \(f(x, t) = c(x) \delta f(t)\).

We assume the system governed by Eq. \((1)\) is ergodic with a positive equilibrium density \(p_{eq}(x)\), where the system is initiated at the equilibrium state of the unperturbed dynamics \((1)\).

The FDT formulates the linear response operator, \(k_A(t)\) in \([4]\), as the following two-point statistics:

\[
k_A(t) := \mathbb{E}_{p_{eq}} \left[ A(X(t)) \otimes B(X(0)) \right], \quad B_i(t) := -\frac{\partial X_i}{\partial c_i} \left( \frac{c_i(X) p_{eq}(X)}{p_{eq}(X)} \right),
\]

where \(B_i\) and \(c_i\) denote the \(i\)th components of \(B\) and \(c\), respectively. In \([1]\), the variable \(B\) is called the conjugate variable to the external forcing. The significance of FDT is that the response operator is defined without involving the perturbed density \(p^\delta(x, t)\). Rather, it can be evaluated at equilibrium of the unperturbed dynamics. For a given \(t \geq 0\), the value of \(k_A(t)\) can be computed using a Monte-Carlo sum based on the time series of the unperturbed system \([1]\) at \(p_{eq}\). For example, let \([X_n = X(t_n)]_{n=1}^N\) be the time series generated at \(p_{eq}\) with step length \(\Delta t = t_{n+1} - t_n\), then for \(t = s\Delta t\), the Monte-Carlo approximation can be written as

\[
k_A(t) \approx \frac{1}{N-s} \sum_{n=1}^{N-s} A(X_{n+s}) \otimes B(X_n).
\]

In practice, the computation of \((6)\) can be done more efficiently using the block averaging algorithm \([24]\).

In applications, the major issue comes from the conjugate variable \(B\) in the linear response operator \([5]\). Since \(B\) depends on the explicit formula of \(p_{eq}\), which may not be available, one cannot directly apply the Monte-Carlo approximation in \((6)\) given only the time series of \([X_n]_{n=1}^N\) at \(p_{eq}\). Thus, it is natural to ask how to learn the density function \(p_{eq}\) from the observed time series, so that, the conjugate variable \(B\) can be defined via the estimated density, \(\hat{p}_{eq}\). To guarantee a well-posed estimation problem, the following lemma provides conditions on observables \(A\) and \(B\) such that the two-point statistics \(k_A(t)\) in \([4]\) is bounded \(\forall t \geq 0\).

**Lemma 2.1.** Let \(X\) be the solution of \((1)\) initiated at the equilibrium. Assume that \(A\) and \(B\) in \((5)\) have finite second moments with respect to \(p_{eq}\), then the linear response operator \(k_A(t)\) in \((5)\) is well-defined. In particular, we have

\[
k_A(t) \leq \mathbb{E}_{p_{eq}} \left[ A^2(X) \right]^{1/2} \otimes \mathbb{E}_{p_{eq}} \left[ B^2(X) \right]^{1/2}, \quad \forall t \geq 0.
\]

**Proof.** Let \(\mathcal{L}\) be the generator of the Itô diffusion \((1)\) \([23]\), and \(e^{t\mathcal{L}}\) be the corresponding semi-group. Introduce the transition kernel of \((1)\)

\[
p(x, t|y, 0) = e^{t\mathcal{L}^*} \delta(x-y), \quad t \geq 0,
\]

where \(\mathcal{L}^*\), acting on \(x\), is the adjoint operator of \(\mathcal{L}\) in the standard \(L^2(\mathbb{R}^d)\) space. The transition kernel \(p(x, t|y, 0)\) as the solution of the Fokker-Planck equation \((1)\) with initial condition \(\delta(x-y)\) can be interpreted as a density function of \(x\). With these definitions, \(k_A(t)\) in \((5)\) can be specified as a double integral \([22]\)

\[
k_A(t) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} A(x) \otimes B(y) p(x, t|y, 0) p_{eq}(y) \, dx \, dy.
\]
Using Cauchy-Schwarz inequality, we have

\[ k_A(t) \leq \left( \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} A^2(x) p(x, t|y, 0) p_{eq}(y) \, dx \, dy \right)^{1/2} \otimes \left( \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} B^2(y) p(x, t|y, 0) p_{eq}(y) \, dx \, dy \right)^{1/2} \]

\[ = \left( \int_{\mathbb{R}^d} \left( e^{11} A^2(x) \right) \int_{\mathbb{R}^d} \delta(x - y) p_{eq}(y) \, dy \, dx \right)^{1/2} \otimes \left( \int_{\mathbb{R}^d} B^2(y) p_{eq}(y) \int_{\mathbb{R}^d} p(x, t|y, 0) \, dx \, dy \right)^{1/2} \]

\[ = \left( \int_{\mathbb{R}^d} \left( e^{11} A^2(x) \right) p_{eq}(x) \, dx \right)^{1/2} \otimes \left( \int_{\mathbb{R}^d} B^2(y) p_{eq}(y) \, dy \right)^{1/2} = \mathbb{E}_{p_{eq}} \left[ A^2(X) \right]^{1/2} \otimes \mathbb{E}_{p_{eq}} \left[ B^2(X) \right]^{1/2}. \]  

We should point out that the validity of the linear response theory for SDE has been discussed in [6] under a very general setting. Here, Lemma 2.1 is to guarantee that the linear response operator in [5], which is the central object that we wish to approximate in this article, is bounded uniformly in time. The boundedness of the second moment of the observable \( A \) with respect to \( p_{eq} \) is fulfilled in many applications. As for the conjugate function \( B \), since it is related to the function \( c(\cdot) \) in the external forcing through the formula in [5], the Lemma provides a condition for admissible external forcing. In Section 3 for a specific class of \( p_{eq} \), we will provide a more concrete condition on \( c(\cdot) \) such that \( B \) has a bounded second moment with respect to \( p_{eq} \). (see Remark 3.2)

It is worthwhile to mention that learning the distribution function from the observations is a classical problem in the field of statistics and machine learning. In general, there are two types of approaches: parametric and nonparametric. The kernel embedding formulation, which is the focus of this paper, belongs to the nonparametric category. However, direct use of the kernel embedding formulation with radial-type kernels, e.g., \( k(x, y) = h(||x - y||) \) to approximate \( p_{eq} \) is computationally expensive for this application. In particular, if the length of training data is \( N \), the Monte-Carlo integral in (9) will require computing the \( \| \cdot \| \) norm in the kernel function \( N(N - s) \) times, since evaluation of \( B \) (as defined in (5)) on each sample point \( X_t \) requires the computation of \( h(||X_t - X_j||) \), for all \( j = 1, \ldots, N \). This computational cost is similar to using the kernel density estimation with radial-type kernels. To overcome this practical issue, we will consider the Mercer-type kernels, constructed using a set of orthogonal polynomials. With such kernel, the resulting kernel embedding approximation on \( B \) (or effectively \( p_{eq} \)) becomes a parametric model since the number of parameters is smaller than the size of the data, thanks to the orthogonality.

To facilitate a self-contained discussion, we now provide a quick review of the relevant background material on RKHS.

### 2.2 Kernels and RKHS

In the current subsection, we introduce the notions of kernel, feature space, feature map, and RKHS. Then we summarize a few useful results which will be used in the later proofs. All unlisted proofs can be found in Chapter 4 of [21]. We will restrict ourselves in the real domain, since it provides simpler notations and is adequate for our application.

**Definition 2.2.** Let \( X \) be a non-empty set. A function \( k: X \times X \to \mathbb{R} \) is called a kernel on \( X \) if there exists a \( \mathbb{R} \)-Hilbert space \( H \) and a map \( \Phi: X \to H \) such that \( \forall x, y \in X \) we have

\[ k(x, y) = \langle \Phi(x), \Phi(y) \rangle_H, \]  

where \( \langle \cdot, \cdot \rangle_H \) denotes the inner product of \( H \). We call \( \Phi \) a feature map and \( H \) a feature space of \( k \).

By Eq. (8), for any fixed \( x_1, x_2, \ldots, x_n \in X \), the \( n \times n \) Gram matrix

\[ \begin{aligned} K_n := \{ k(x_i, x_j) \}_{1 \leq i, j \leq n} \end{aligned} \]  

is symmetric positive definite (SPD), that is, \( \forall a = (a_1, a_2, \ldots, a_n)^T \in \mathbb{R}^n \), the bilinear form

\[ a^T K_n a = \sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j k(x_i, x_j) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j \langle \Phi(x_i), \Phi(x_j) \rangle_H \]

\[ = \sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j \Phi(x_i) \Phi(x_j) \| \sum_{i=1}^{n} a_i \Phi(x_i) \|_H^2 \geq 0. \]

We say that a function \( k: X \times X \to \mathbb{R} \) is SPD if \( \forall n \geq 1 \), and \( (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n \) the corresponding Gram matrix (9) is SPD. An important result (stated in the next lemma) states that the symmetry and positive definiteness are not only necessary for \( k \) to be a kernel but also sufficient.
Lemma 2.3. A function \( k : X \times X \to \mathbb{R} \) is a kernel if and only if it is SPD.

The lemma above is useful for checking whether a given function is a kernel. With the concept of kernel, we now define the RKHS.

Definition 2.4. Let \( X \) be a non-empty set and \( \mathcal{H} \) be a \( \mathbb{R} \)-Hilbert function space over \( X \), i.e., a \( \mathbb{R} \)-Hilbert space that consists of functions mapping from \( X \) into \( \mathbb{R} \). Then \( \mathcal{H} \) is called an RKHS with kernel \( k \), if \( k(\cdot, x) \in \mathcal{H} \), \( \forall x \in X \), and we have the reproducing property

\[
    f(x) = \langle f(\cdot), k(\cdot, x) \rangle_{\mathcal{H}}
\]

holds for all \( f \in \mathcal{H} \) and all \( x \in X \). In particular, we call such \( k(\cdot, \cdot) \) a reproducing kernel of \( \mathcal{H} \).

From Definition 2.4 it seems that the reproducing kernel is a result of RKHS. However, there is a one-to-one correspondence between the RKHS and kernel. (see Theorem 4.20 and 4.21 of [21]) In Section 3 when we construct the RKHS used for our kernel embedding linear response, we will first define a kernel, then build an RKHS to “promote” such kernel to a reproducing kernel.

In the rest of the Section, \( \mathcal{H} \) always denotes as an RKHS with kernel \( k \). The RKHS has the remarkable property that the norm convergence implies the pointwise convergence. More precisely, consider \( f_n \to f \) in \( \mathcal{H} \), that is, \( \| f_n - f \|_{\mathcal{H}} \to 0 \) as \( n \to \infty \). Then, \( \forall x \in X \), we have

\[
    |(f_n - f)(x)| = |\langle f_n - f, k(\cdot, x) \rangle_{\mathcal{H}}| \leq \| f_n - f \|_{\mathcal{H}} \| k(\cdot, x) \|_{\mathcal{H}} \to 0,
\]

as \( n \to \infty \). Eq. (11) also suggests that if \( \| k(\cdot, x) \|_{\mathcal{H}} \) is bounded uniformly in \( x \in X \), we will have the uniform convergence of \( f_n \) to \( f \). We arrive at the following lemma.

Lemma 2.5. Let \( X \) be a topological space and \( k \) be a kernel on \( X \) with RKHS \( \mathcal{H} \). If \( k \) is bounded in the sense that

\[
    \| k \|_{\infty} := \sup_{x \in X} \sqrt{k(x, x)} < \infty.
\]

and \( k(\cdot, x) : X \to \mathbb{R} \) is continuous \( \forall x \in X \), then \( \mathcal{H} \subset C_0(X) \) (space of bounded and continuous function on \( X \)), and the inclusion \( \text{id} : \mathcal{H} \to C_0(X) \) is continuous with \( \| \text{id} : \mathcal{H} \to C_0(X) \| = \| k \|_{\infty} \).

Here, to see the connection between \( \| k \|_{\infty} \) and \( \| k(\cdot, x) \|_{\mathcal{H}} \), simply notice that \( k(\cdot, x) \in \mathcal{H} \), and with the reproducing property we have

\[
    \| k(\cdot, x) \|_{\mathcal{H}}^2 = \langle k(\cdot, x), k(\cdot, x) \rangle_{\mathcal{H}} = k(x, x).
\]

Thus, \( \| k \|_{\infty} \) is the upper bound of \( \| k(\cdot, x) \|_{\mathcal{H}} \), and \( \forall f \in \mathcal{H} \),

\[
    \| f(x) \| = |\langle f(\cdot), k(\cdot, x) \rangle_{\mathcal{H}}| \leq \| f \|_{\mathcal{H}} \| k(\cdot, x) \|_{\mathcal{H}} = \| f \|_{\mathcal{H}} k^\frac{1}{2}(x, x), \quad \forall x \in X,
\]

that is, \( f(x) \) yields the same decay rate as \( k^\frac{1}{2}(x, x) \). In this paper, we focus on the RKHS with a bounded kernel.

As a subspace of \( C_0(X) \), it is natural to ask whether the RKHS \( \mathcal{H} \) is dense in the Banach space \( C_0(X) \) equipped with the uniform norm. The density of \( \mathcal{H} \) in \( C_0(X) \) is equivalent to the \( \epsilon \)-universality [17] of the corresponding kernel \( k \), which has been discussed by Steinwart [25] for compact \( X \). In this paper, we are interested in the case where \( X \) is non-compact, e.g., \( X = \mathbb{R}^d \), and the target \( f \) is a continuous density function which vanishes at infinity. For a locally compact Hausdorff (LCH) space \( X \), let \( C_0(X) \) denote the space of all continuous functions on \( X \) which vanish at infinity, that is, \( \forall \epsilon > 0 \) the set \( \{ x \in X \mid |f(x)| \geq \epsilon \} \) is compact \( \forall f \in C_0(X) \). \( C_0(X) \), like \( C_0(X) \), is a Banach space with respect to the infinite-norm \( \| \cdot \|_{\infty} \). As an analog of the \( \epsilon \)-universal kernel, the concept of \( C_0 \)-universal was introduced by Sriperumbudur et al. in [17].

Definition 2.6. \((C_0 \text{-universal}) \) Let \( X \) be an LCH space with the kernel \( k \) being bounded and \( k(\cdot, x) \in C_0(X) \), \( \forall x \in X \). The kernel \( k \) is said to be \( C_0 \)-universal if the RKHS, \( \mathcal{H} \), induced by \( k \) is dense in \( C_0(X) \) with respect to the uniform norm, that is, \( \forall g \in C_0(X) \) and \( \forall \epsilon > 0 \), there exist \( \hat{g} \in \mathcal{H} \) such that \( \| g - \hat{g} \|_{\infty} < \epsilon \).

A series of characterizations of \( C_0 \)-universality for different types of kernels has been developed in [16] [17] based on the Hahn-Banach theorem and Riesz representation theorem. When \( X = \mathbb{R}^d \), a typical example of \( C_0 \)-universal kernel is the Gaussian kernel \( k(x, y) = \exp(-\theta \| x - y \|^2) \), \( x, y \in \mathbb{R}^d \), for some \( \theta > 0 \). To facilitate the applications in this paper (see Section 3), we generalize the concept of \( C_0 \)-universality to a weighted \( C_0 \)-space.

Lemma 2.7. Let \( X \) be an LCH space, and \( q \) be a bounded positive continuous function on \( X \). Then we have the following results.

1. The set of functions

\[
    C_0(X, q^{-1}) := \{ f \in C(X) \mid f q^{-1} \in C_0(X) \}
\]

defines a vector space.
2. The map \( \| \cdot \|_{C_0(q^{-1})} : C_0(X, q^{-1}) \rightarrow \mathbb{R} \) defined as
\[
\| f \|_{C_0(q^{-1})} := \| f q^{-1} \|_\infty, \quad f \in C_0(X, q^{-1}),
\]
is a norm. Moreover, \( C_0(X, q^{-1}) \), equipped with the norm \( \| \cdot \|_{C_0(q^{-1})} \), is a Banach space.

3. The Banach spaces \( C_0(X, q^{-1}) \) and \( C_0(X) \) are isometrically isomorphic.

Proof. It is straightforward to check \( C_0(X, q^{-1}) \) is a norm space with respect to the norm \( \| \cdot \|_{C_0(q^{-1})} \). To see \( C_0(X, q^{-1}) \) is closed under the topology induced by \( \| \cdot \|_{C_0(q^{-1})} \), we introduce the linear bijection \( Q : C_0(X) \rightarrow C_0(X, q^{-1}) \) defined as \( Q : g \mapsto g q \). The bijection \( Q \) is norm-preserving in the sense that \( \forall g \in C_0(X) \),
\[
\| Q g \|_{C_0(q^{-1})} = \| g q \|_{\infty}.
\]

Therefore, for any Cauchy sequence \( \{ f_n \} \) in \( C_0(X, q^{-1}) \), \( \{ g_n := Q^{-1} f_n \} \) defines a Cauchy sequence in Banach space \( C_0(X) \). Let \( g_n \rightarrow g^* \) in \( C_0(X) \), then \( f^* := Q g^* \in C_0(X, q^{-1}) \) and \( f_n \rightarrow f^* \) in \( C_0(X, q^{-1}) \). With \( C_0(X, q^{-1}) \) being a Banach space, the operator \( Q \) becomes an isometrical isomorphism. \( \Box \)

In practice, we use the weight function \( q \) to characterize the decay rate of continuous functions. For example, take \( X = \mathbb{R}^d \), and \( q \propto \exp(-\theta \|x\|^2) \) for some \( \theta > 0 \), then the functions in \( C_0(\mathbb{R}^d, q^{-1}) \) are continuous with a Gaussian decay rate. Motivated by the decay rate \( \| \cdot \|_{1,3} \) of functions in \( \mathcal{H} \), the following lemma provides conditions for \( \mathcal{H} \) being dense in \( C_0(X, q^{-1}) \).

**Lemma 2.8.** (weighted \( c_0 \)-universal) Let \( X \) and \( q \) be the same as in Lemma 2.7 and the kernel \( k \), satisfying \( k(\cdot, x) \in C_0(X, q^{-1}) \), \( \forall x \in X \). Then, \( k(x, y) := k(x, y) q^{-1}(x) q^{-1}(y) \) defines a kernel on \( X \), and the RKHS, \( \mathcal{H} \) induced by \( k \) is dense in \( C_0(X, q^{-1}) \) if and only if the kernel \( k \) is \( c_0 \)-universal.

Proof. To begin with, by Lemma 2.3 \( \tilde{k} \) defines a kernel, and \( \tilde{k}(\cdot, x) = q^{-1}(x) k(\cdot, x) q^{-1}(\cdot) \in C_0(X) \), \( \forall x \in X \) since \( k(\cdot, x) \in C_0(X, q^{-1}) \), \( \forall x \in X \).

By Definition 2.6 it is enough to show that \( \mathcal{H} \) dense in \( C_0(X, q^{-1}) \) is equivalent to \( \tilde{\mathcal{H}} \), the RKHS induced by \( \tilde{k} \), dense in \( C_0(X) \). Recall that, by Lemma 2.7 the Banach spaces \( C_0(X, q^{-1}) \) and \( C_0(X) \) are isometrically isomorphic with \( Q : C_0(X) \rightarrow C_0(X, q^{-1}) \), defined as \( Q : g \mapsto g q \), being the isomorphism. Following the same idea, we take
\[
\tilde{\mathcal{H}} := \{ f q^{-1} \mid f \in \mathcal{H} \}
\]
with the inner product
\[
\langle g_1, g_2 \rangle_{\tilde{\mathcal{H}}} := \langle g_1 q, g_2 q \rangle_{\mathcal{H}}, \quad \forall g_1, g_2 \in \tilde{\mathcal{H}}.
\]

Since \( \mathcal{H} \) is a Hilbert space, \( \tilde{\mathcal{H}} \) equipped with the inner product \( \langle \cdot, \cdot \rangle_{\tilde{\mathcal{H}}} \) is also a Hilbert space. With \( \tilde{k}(\cdot, x) = q^{-1}(x) k(\cdot, x) q^{-1}(\cdot) \), and \( k(\cdot, x) \in \mathcal{H} \), \( \forall x \in X \), we have \( \tilde{k}(\cdot, x) \in \tilde{\mathcal{H}} \), \( \forall x \in X \).

In terms of the reproducing property, \( \forall g = f q^{-1} \in \tilde{\mathcal{H}} \) with \( f \in \mathcal{H} \), we have
\[
\langle g, \tilde{k}(\cdot, x) \rangle_{\tilde{\mathcal{H}}} = \langle f, \tilde{k}(\cdot, x) q^{-1}(\cdot) \rangle_{\mathcal{H}} = \langle f, k(\cdot, x) \rangle_{\mathcal{H}} q^{-1}(x) = f(x) q^{-1}(x) = g(x), \quad \forall x \in X.
\]

Thus, \( \tilde{\mathcal{H}} \) indeed is the RKHS induced by \( \tilde{k} \) satisfying \( Q(\tilde{\mathcal{H}} \cap C_0(\mathbb{R}^d)) = \mathcal{H} \cap C_0(\mathbb{R}^d, q^{-1}) \). Finally, by the fact that \( Q \) defines an isometrical isomorphism between \( C_0(X) \) and \( C_0(X, q^{-1}) \), we reach the equivalence. \( \Box \)

Our next lemma characterizes how the differentiability of a kernel is inherited by the functions of its RKHS. In particular, we take \( X \subset \mathbb{R}^d \) to be an open subset, and introduce the multi-index notation \( \vec{m} = (m_1, m_2, \ldots, m_d) \) with \( m_i \) being nonnegative integers. Then, we say that the kernel \( k \) is \( M \)-times continuously differentiable if \( \partial^{\vec{m}} k : X \times X \rightarrow \mathbb{R} \) exist and are continuous for all multi-indexes \( \vec{m} \) with \( \| \vec{m} \|_1 := \sum m_i \leq M \). Recall that
\[
\partial^{\vec{m}} k(x, y) := \frac{\partial^{\vec{m}}}{\partial x^{\vec{m}}} \frac{\partial^{\vec{m}}}{\partial y^{\vec{m}}} k(x, y), \quad x, y \in \mathbb{R}^d.
\]

**Lemma 2.9.** Let \( X \) be an open subset of \( \mathbb{R}^d \), and kernel \( k \) be an \( M \)-times continuously differentiable kernel. Then every \( f \in \mathcal{H} \) is \( M \)-times continuously differentiable in \( X \), and \( \forall \| \vec{m} \|_1 \leq M \), we have
\[
\| \partial^{\vec{m}} f(x) \| \leq f \| _{\mathcal{H}} \cdot \left( \partial^{\vec{m}} k(x, x) \right)^{\frac{1}{2}}, \quad \forall x \in \mathbb{R}^d.
\]

From Lemma 2.3 and 2.5 we have learned the importance of constructing reproducing kernel \( k \) with certain “nice” properties. In practice, we construct the bounded kernel using \( \Phi \) based on a feature map \( \Phi : X \rightarrow H \), where \( H \) is a simple Hilbert space (e.g., \( \ell^2 \)-space). Then, we define the corresponding RKHS \( \mathcal{H} \) as a subspace of \( C_0(\mathbb{R}^d) \) such that \( \mathcal{H} \) yields the reproducing property. In the next section, we are going to follow this procedure of constructing RKHS by using the orthogonal polynomials to define the feature map.
3 From orthogonal polynomials to RKHS

In Section 2 we have reviewed the linear response theory, as our motivation of using kernel embedding to learn the equilibrium densities $p_{eq}$ from the observed time series, as well as the general theory of RKHS, to which we are going to embed the target distribution function. In practice, such RKHS should be well selected such that:

1. The corresponding reproducing kernel $k$ has all good properties in Lemma 2.4 and 2.9 so that we can derive convergence results of the estimates. We will show examples of RKHSs constructed from Hermite and Laguerre polynomials, respectively. \( \text{(see Section 3.1)} \)

2. The RKHS is rich enough in the sense of Lemma 2.6 to contain good estimates of $p_{eq}$ with a certain decaying rate. \( \text{(see Section 3.2)} \)

3.1 Constructing RKHS via orthogonal polynomials

Inspired by the Mercer’s theorem \[21\] and reproducing kernel weighted Hilbert space used in \[26, 27, 28, 23\], we consider the orthonormal polynomials with respect to a weighted $L^2$-space, $L^2(\mathbb{R}^d, W)$, to construct our kernel and RKHS. Here, $L^2(\mathbb{R}^d, W)$ denotes the product space $\prod_{i=1}^{d} L^2(\mathbb{R}, W_i)$, and $W(x) = \prod_{i=1}^{d} W_i(x_i)$ for $x = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$.

For a more substantial discussion, we begin our analyses with the following class of one-dimensional weight functions that satisfy the following lemma.

**Lemma 3.1.** Let $W = e^{-2Q}$, where $Q : \mathbb{R} \to \mathbb{R}$ is an even $C^2$-function. We assume that $Q > 0$ in $(0, \infty)$, and there exist real numbers $B \geq A > 1$, such that

$$ A \leq \frac{(xQ'(x))^2}{Q(x)} \leq B, \quad \forall x \in (0, \infty). \quad \text{(14)} $$

Then the orthonormal polynomials \{p_n\} on $L^2(\mathbb{R}, W)$ satisfy

$$ C_1 n^\frac{1}{2} \frac{1}{\alpha} \leq \sup_{x \in \mathbb{R}} \left| p_n(x) \right| W^\frac{1}{2}(x) \leq C_2 n^\frac{1}{2} \frac{1}{\alpha}, \quad n = 0, 1, \ldots, \quad \text{(15)} $$

where $C_1$ and $C_2$ are positive constants independent of $n$.

**Proof.** Eq. \[15\] is a combination of Corollary 1.4 and Lemma 5.2 in \[29\].

A typical type of functions satisfying the conditions in Lemma 3.1 is $Q_m(x) = |x|^m$ for $m > 1$, and we have

$$ \frac{(xQ_m'(x))^2}{Q_m(x)} = m. $$

Let $W_m = e^{-2Q_m}$, and \[15\] leads to

$$ \sup_{x \in \mathbb{R}} \left| p_n(x) \right| W_m^\frac{1}{2}(x) \sim n^\frac{1}{2} \frac{1}{\alpha}. $$

With the control of the $L^\infty$-norm of the orthonormal polynomials in \[15\], the following lemma defines the bounded kernel we need to build our RKHS.

**Lemma 3.2.** Let $W$ and $p_n(x)$ be as in Lemma 3.1. Given a sequence of monotonically decreasing positive real numbers \{\lambda_n\}_{n=0}^{\infty} satisfying

$$ \sum_{n=0}^{\infty} \lambda_n n^\frac{1}{2} \frac{1}{\alpha} < \infty, \quad \text{(16)} $$

then, for $\beta \geq \frac{1}{2}$, the bivariate function $k_\beta(\cdot, \cdot) : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ defined by,

$$ k_\beta(x, y) := \sum_{n=0}^{\infty} \lambda_n p_n(x) p_n(y) W^\beta(x) W^\beta(y), \quad \text{(17)} $$

is a well-defined bounded continuous function. Moreover, $k_\beta$ is a kernel.
Proof. Notice that by the uniform bound \( [15] \) in Lemma 3.1, we have
\[
\left| \lambda_n p_n(x) p_n(y) W^\beta(x) W^\beta(y) \right| \leq C_2^2 \lambda_n n^{\frac{1}{2} - \frac{1}{2}} W^\beta(x) W^\beta(y),
\]
and combining with the condition \( [10] \), we reach the uniform convergence of the summation in \( [17] \). Thus, \( k_\beta(x, y) \) in \( [17] \) is a well-defined continuous function on \( \mathbb{R}^2 \) with a decay rate,
\[
|k_\beta(x, y)| \leq C_3 W^\beta(x) W^\beta(y), \quad C_3 := C_2^2 \sum_{n=0}^{\infty} \lambda_n n^{\frac{1}{2} - \frac{1}{2}}. \tag{18}
\]
To show that \( k_\beta \) is a kernel, we define the feature map \( \Phi_\beta : \mathbb{R} \rightarrow \ell^2 \) as
\[
\Phi_\beta(x) := \left( \sqrt{\lambda_0} p_0(x) W^\beta(x), \sqrt{\lambda_1} p_1(x) W^\beta(x), \ldots, \sqrt{\lambda_n} p_n(x) W^\beta(x), \ldots \right), \quad x \in \mathbb{R}.
\]
With \( k_\beta(x, y) = \langle \Phi_\beta(x), \Phi_\beta(y) \rangle_{\ell^2} \), by Definition 2.2, \( k_\beta \) is a kernel. \( \square \)

To generalize Lemma 3.2 to the \( d \)-dimensional case, consider the orthonormal polynomial in \( L^2(\mathbb{R}^d, W) \) of the form
\[
p_{\vec{m}}(x) := \prod_{i=1}^{d} p_{m_i}(x_i), \quad x \in \mathbb{R}^d,
\]
where \( \vec{m} = (m_1, m_2, \ldots, m_d) \) is a multi-index and \( \{p_n\} \) are the orthonormal polynomials on \( L^2(\mathbb{R}, W) \). Following Lemma 3.2, we define
\[
k_\beta(x, y) := \sum_{\vec{m} \geq 0} \lambda_{\vec{m}} p_{\vec{m}}(x) p_{\vec{m}}(y) W^\beta(x) W^\beta(y), \quad x, y \in \mathbb{R}^d, \lambda_{\vec{m}} := \prod_{i=1}^{d} \lambda_{m_i}, \tag{19}
\]
for \( \beta \geq \frac{1}{2} \), as the \( d \)-dimensional generalization of the kernel \( k_\beta \) in Eq. \( [17] \). Here, \( \lambda_n \) satisfies the condition in Lemma 3.2. The function \( k_\beta(x, y) \) in \( [19] \) is well-defined since
\[
\sum_{\vec{m} \geq 0} \lambda_{\vec{m}} p_{\vec{m}}(x) p_{\vec{m}}(y) W^\beta(x) W^\beta(y) = \prod_{i=1}^{d} \left( \sum_{m_i=0}^{\infty} \lambda_{m_i} p_{m_i}(x_i) p_{m_i}(y_i) W^\beta(x_i) W^\beta(y_i) \right) < \infty.
\]
Moreover, similar to \( [18] \), \( k_\beta(x, y) \) yields the following decay rate
\[
|k_\beta(x, y)| \leq C_3^d W^\beta(x) W^\beta(y), \tag{20}
\]
where \( C_3 \) is the same constant as in \( [18] \).

Formally, one can always define a kernel by the infinite sum in \( [17] \). In Lemma 3.2, the uniform convergence of the summation in \( [17] \) is proved based on the asymptotic behavior of a class of orthogonal polynomials (see Lemma 3.1). In practice, one can also rely on existing identities to show the boundedness of the kernel defined by \( [17] \). (See Section 3.1.2 below)

Our next task is to define the RKHS, denoted by \( \mathcal{H}_\beta \), such that the bounded kernel \( k_\beta \) in \( [19] \) is the reproducing kernel of \( \mathcal{H}_\beta \). A crucial observation is that, by Definition 2.4, a necessary condition for \( \mathcal{H}_\beta \) is \( k_\beta(\cdot, x) \in \mathcal{H}_\beta, \forall x \in \mathbb{R}^d \). Thus, we shall first study the function space containing \( \{k_\beta(\cdot, x), x \in \mathbb{R}^d \} \). We have the following lemma.

Lemma 3.3. Let \( W(x), p_n(x) \), and \( \{\lambda_n\} \) be as in Lemma 3.2. The kernel \( k_\beta \) defined by \( [19] \) satisfies \( \forall x \in \mathbb{R}^d, k_\beta(\cdot, x) \in L^2(\mathbb{R}^d, W^{1-2\beta}) \cap C_0(\mathbb{R}^d) \).

Proof. First notice that \( \forall x \in \mathbb{R}^d, k_\beta(\cdot, x) \in C_0(\mathbb{R}^d) \) is a direct result of the decay rate \( [20] \). Introduce \( \{\Psi_{\vec{m}, \vec{n}} := p_{\vec{m}} W^\beta\} \), which defines an orthonormal basis on \( L^2(\mathbb{R}^d, W^{1-2\beta}) \), and we rewrite the kernel \( k_\beta(x, y) \) in \( [19] \) as
\[
k_\beta(x, y) = \sum_{\vec{m} \geq 0} \lambda_{\vec{m}} \Psi_{\vec{m}, \vec{m}}(x) \Psi_{\vec{m}, \vec{m}}(y). \tag{21}
\]
In particular, by the orthogonality of \( \{\Psi_{\vec{m}, \vec{n}}\} \), we have
\[
\int_{\mathbb{R}^d} k_\beta^2(y, y) W^{1-2\beta}(y) \, dy = \sum_{\vec{m} \geq 0} \lambda_{\vec{m}}^2 \Psi_{\vec{m}, \vec{m}}^2(x) \leq \lambda_0 k_\beta(x, x) \leq \lambda_0 \|k_\beta\|_{L^2}^2, \quad \forall x \in \mathbb{R}^d.
\]
Thus, \( \{k_\beta(\cdot, x), x \in \mathbb{R}^d\} \subset L^2(\mathbb{R}^d, W^{1-2\beta}) \cap C_0(\mathbb{R}^d) \). \( \square \)
We shall emphasize that $L^2(\mathbb{R}^d, W^{1,2-\beta}) \cap C_0(\mathbb{R}^d)$ is the set consisting all continuous functions vanishing at the infinity which are $W^{1,2-\beta}$-weighted $L^2$-integrable, while each element in $L^2(\mathbb{R}^d, W^{1,2-\beta})$ represents an equivalent class of functions due to the difference of their topologies. With the topology induced by the weighted $L^2$-norm $\| \cdot \|_{L^2(W^{1,2-\beta})}$, the expansion formula for $f \in L^2(\mathbb{R}^d, W^{1,2-\beta})$ given by

$$f = \sum_{m \geq 0} \hat{f}_m \Psi_{\beta,m}, \quad \hat{f}_m = \int_{\mathbb{R}^d} f(x)\Psi_{\beta,m}(x) W^{1,2-\beta}(x) \, dx = \int_{\mathbb{R}^d} f(x)p_{\beta,m}(x) W^{1,\beta}(x) \, dx,$$

is valid in the sense that

$$\lim_{M \to \infty} \| f - f_M \|_{L^2(W^{1,2-\beta})} = 0, \quad f_M := \sum_{\|m\| \leq M} \hat{f}_m \Psi_{\beta,m},$$

which is relatively weak since most of the properties of $f_M$ no longer exist after passing thought the limit. The following proposition, as the main result of the current section, defines the RKHS, $\mathcal{H}_\beta \subset L^2(\mathbb{R}^d, W^{1,2-\beta}) \cap C_0(\mathbb{R}^d)$, corresponding to the kernel $k_\beta$ in [19], such that $\forall f \in \mathcal{H}_\beta$, the expansion [22] holds pointwisely and $f_M$ converges uniformly to $f$ in $C_0(\mathbb{R}^d)$.

**Proposition 3.4.** Let $W(x)$, $p_n(x)$, and $\{\lambda_n\}$ be as in Lemma [3.2] then, for any fixed $\beta \geq \frac{1}{2}$, we have the following results.

i) For any sequence $\{\hat{f}_m\} \in \ell^2$ satisfying

$$\sum_{m \geq 0} \hat{f}_m^2 \lambda_m \Psi_{\beta,m} < \infty,$$

where $\lambda_m$ is defined in [19], the sequence of functions

$$f_n := \sum_{\|m\| \leq n} \hat{f}_m \Psi_{\beta,m}, \quad n \geq 0,$$

converge uniformly in $C_0(\mathbb{R}^d)$. Moreover, the limit, denoted as $f^*$, satisfies $f^* \in L^2(\mathbb{R}^d, W^{1,2-\beta}) \cap C_0(\mathbb{R}^d)$.

ii) The function space

$$\mathcal{H}_\beta := \left\{ f = \sum_{m \geq 0} \hat{f}_m \Psi_{\beta,m} \bigg| \sum_{m \geq 0} \hat{f}_m^2 \lambda_m \Psi_{\beta,m} < \infty \right\},$$

is a well-defined subspace of $L^2(\mathbb{R}^d, W^{1,2-\beta}) \cap C_0(\mathbb{R}^d)$. Further, define the map $\langle \cdot, \cdot \rangle : \mathcal{H}_\beta \times \mathcal{H}_\beta \to \mathbb{R}$ as

$$\langle f, g \rangle := \sum_{m \geq 0} \hat{f}_m \hat{g}_m \lambda_m^{-1}, \quad f = \sum_{m \geq 0} \hat{f}_m \Psi_{\beta,m}, g = \sum_{m \geq 0} \hat{g}_m \Psi_{\beta,m} \in \mathcal{H}_\beta.$$

Then $\langle \cdot, \cdot \rangle$ defines an inner product, and $\mathcal{H}_\beta$, equipped with the inner product $\langle \cdot, \cdot \rangle$, is a Hilbert space.

iii) $\mathcal{H}_\beta$ is the RKHS with reproducing kernel $k_\beta$ in [19].

See Appendix A for the proofs. Notice that the kernel $k_\beta$ is bounded, by Lemma [2.5] we know that the norm convergence in $\mathcal{H}_\beta$ implies the uniform convergence in $C_0(\mathbb{R}^d)$. In particular, $\forall f \in \mathcal{H}_\beta$, the expansion formula [22] converges uniformly, that is, there is a one-to-one correspondence between the function $f \in \mathcal{H}_\beta$ and the sequence of expansion coefficients $\{\hat{f}_m\} \in \ell^2$ satisfies [24]. Since the condition [24] is independent of $\beta$, which means that the class of RKHS $(\mathcal{H}_\beta)$ defined in Proposition 3.4 are isometrically isomorphic to each other. In particular, $\forall \beta_1, \beta_2 > \frac{1}{2}$, the linear map $I_{\beta_1, \beta_2} : \mathcal{H}_{\beta_1} \to \mathcal{H}_{\beta_2}$ given by

$$I_{\beta_1, \beta_2} f = f \cdot W^{\beta_2 - \beta_1}, \quad \forall f \in \mathcal{H}_{\beta_1},$$

defines the isometrical isomorphism between $\mathcal{H}_{\beta_1}$ and $\mathcal{H}_{\beta_2}$, with $I_{\beta_1, \beta_2}^{-1} = I_{\beta_2, \beta_1}$.

To connect the kernel $k_\beta$ in [19] with Mercer’s theorem, we define the integral operator $T_{k_\beta} : L^2(\mathbb{R}^d, W^{1,2-\beta}) \to L^2(\mathbb{R}^d, W^{1,2-\beta})$ as follows

$$(T_{k_\beta} f)(x) := \int_{\mathbb{R}^d} k_\beta(y, x) f(y) W^{1,2-\beta}(y) \, dy.$$  

Replace $f$ by $\psi_{\beta,n}$ in [26], and we have

$$\left(T_{k_\beta} \Psi_{\beta,m}\right)(x) = \sum_{n \geq 0} \lambda_n \Psi_{\beta,m}(x) \int_{\mathbb{R}^d} \Psi_{\beta,n}(y) \Psi_{\beta,n}(y) W^{1,2-\beta}(y) \, dy = \lambda_n \Psi_{\beta,m}(x).$$
where we have used the fact that the convergence in (19) is uniform to switch the order of integration and summation. Thus, $\lambda_{\hat{m}}$ and $\Psi_{\hat{m}}$ correspond to the eigenvalue and eigenfunction of $T_{k_\rho}$, respectively.

So far we have introduced a framework to construct RKHS as a subspace of $L^2(\mathbb{R}^d, \mathcal{W}^{1-2\beta}) \cap C_b(\mathbb{R}^d)$. The resulting RKHS extracts features of both $L^2(\mathbb{R}^d, \mathcal{W}^{1-2\beta})$ and $C_b(\mathbb{R}^d)$, e.g., the expansion formula (22) makes sense not only in $L^2(\mathbb{R}^d, \mathcal{W}^{1-2\beta})$ but also holds pointwisely in terms of the function value. The main advantage with the representation in (25) over the radial-type kernel is as follows. In practice, for data $\{X_n\}_{n=1}^N$ sampled from the target density $f$, we will choose a function in $\mathcal{H}_f$ with a finite sum, $\|\hat{m}\|_1 \leq M$, where $M \ll N$, as an estimator for $f$.

While the choice of $M$ allows us to specify the theoretical "bias" or "approximation error", thanks to the orthogonal representation (see Section 4), the resulting hypothesis function becomes a parametric model and the evaluation of $f$ on a new $x \in \mathbb{R}^d$ amounts to evaluating $\binom{M+d}{M}$ components of $\{\Psi_{\hat{m},\hat{n}}(x) \mid \|\hat{m}\|_1 \leq M\}$. This is computationally much cheaper than using the radial-type kernel as a feature, that is, $f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}_f}$, where $k(x, y) = h(\|x-y\|)$ for some positive function $h$, since the computation of the inner product requires evaluating $h(\|X_n - x\|)$, for all $n = 1, \ldots, N$.

In the remaining of this subsection, we discuss two examples, the classes of Mercer-type kernels based on the Hermite and Laguerre polynomials.

### 3.1.1 Hermite polynomials

Let $W$ be the $d$-dimensional standard Gaussian distribution, that is, $W(x) = (2\pi)^{-\frac{d}{2}} \exp\left(-\frac{1}{2}\|x\|^2\right)$. As a result, the corresponding orthonormal polynomials are the normalized Hermite polynomials, denoted by $\{\psi_n\}$. To satisfy the condition in Lemma 3.2, we take $\lambda_n = \rho^n$ with $\rho \in (0, 1)$. Following (19), we define the kernel

$$k_{\beta,\rho}(x, y) := \sum_{n=0}^\infty \rho^n \psi_n(x)\psi_n(y), \quad \forall x, y \in \mathbb{R}^d, \|\psi_{\hat{m},\hat{n}}\|_2 \leq M. \tag{27}$$

For this special case, we do have an explicit expression for $k_{\beta,\rho}$. When $d = \beta = 1$, the kernel $k_{1,1}$ in (27) is known as the Mehler kernel

$$k_{1,1}(x, y) = \sum_{n=0}^\infty \rho^n \psi_n(x)\psi_n(y) = \sum_{n=0}^\infty \rho^n \exp\left(-\frac{1}{2(1-\rho^2)}\right). \tag{28}$$

For general $d$-dimensional case, we have

$$k_{\beta,\rho}(x, y) = (2\pi)^{-\frac{d}{2}} \exp\left(-\frac{1}{2(1-\rho^2)}\right) \sum_{n=0}^\infty \rho^n \exp\left(-\frac{1}{2(1-\rho^2)}\right), \tag{29}$$

and

$$\|k_{\beta,\rho}\|_\infty = (2\pi)^{-\frac{d}{2}} \left(1-\rho^2\right)^{-\frac{d}{2}}. \tag{30}$$

For $\beta \in \left[\frac{d}{2}, \infty\right)$ and $\rho \in (0, 1)$, we will call the kernel $k_{\beta,\rho}$ in (29) and the corresponding RKHS

$$\mathcal{H}_{\beta,\rho} := \left\{ f = \sum_{n=0}^\infty \hat{f}_n \psi_n(x) : \sum_{n=0}^\infty \rho^n \hat{f}_n^2 \hat{m}_n \leq \infty \right\}, \tag{31}$$

following Proposition 3.4 the $d$-dimensional Mehler kernel and Mehler RKHS, respectively. The explicit formula of the Mehler kernel (29) is convenient for verifying the properties of the Mehler RKHS. For example, since the kernel $k_{\beta,\rho}$ is smooth, by Lemma 3.3 we have the following regularity result.

**Corollary 3.5.** Every function $f \in \mathcal{H}_{\beta,\rho}$ is smooth, and $\forall \hat{m} \geq 0$,

$$\left| \partial^n \hat{m} f(x) \right| \leq \| f \|_{\mathcal{H}_{\beta,\rho}} \cdot \left| \partial^n \hat{m} k_{\beta,\rho}(x, x) \right|^{\frac{1}{2}} \tag{32}$$

In particular, the first order partial derivative of $f \in \mathcal{H}_{\beta,\rho}$ satisfies

$$\left| \frac{\partial}{\partial x_i} f(x) \right| \leq \| f \|_{\mathcal{H}_{\beta,\rho}} \cdot \left| \frac{\partial}{\partial x_i} k_{\beta,\rho}(x, x) \right| \tag{33}$$

When $\hat{m} = \hat{0}$, Corollary 3.5 reduces to (13), which means the functions in $\mathcal{H}_{\beta,\rho}$ yields the same decay rate as $k_{\beta,\rho}(x, x)$. In particular, $\forall f \in \mathcal{H}_{\beta,\rho}$,

$$\left| f(x) \right| \leq (2\pi)^{-\frac{d}{2}} \left(1-\rho^2\right)^{-\frac{d}{2}} \| f \|_{\mathcal{H}_{\beta,\rho}} \exp\left(-\frac{1}{2(1+\rho)}\right) \tag{34}$$
3.1.2 Laguerre polynomials

The normalized Laguerre polynomials, denoted by \( \ell^{(\beta)}_{\tilde{m}}(x) \), are the orthonormal polynomials with respect to the Gamma distribution \( G(x;\theta) \propto x^{\beta} e^{-x}, \) for \( \theta = 0, 1, \ldots, \) and \( x \geq 0 \). Following [19], we introduce the \( d \)-dimensional Gamma distribution and corresponding normalized Laguerre polynomials

\[
G(x;\tilde{\theta}) = \prod_{i=1}^{d} \frac{1}{(\theta_i + 1)} x_i^{\beta_i} e^{-x_i}, \quad \ell^{(\beta)}_{\tilde{m}}(x) := \prod_{i=1}^{d} \ell^{(\beta_i)}_{m_i}(x_i), \quad x \in [0,\infty)^d, \quad \tilde{\theta} \in [0,1,\ldots)^d,
\]

respectively, and the eigenfunction \( \Psi_{\tilde{\beta},\tilde{m}} \) defined as

\[
\Psi_{\tilde{\beta},\tilde{m}}(x) := \ell^{(\beta)}_{\tilde{m}}(x)G^{\tilde{\beta}}(x;\tilde{\theta}), \quad \tilde{m} \geq 0
\]

form an orthonormal basis on \( L^2 \left( [0,\infty)^d; G^{1-2\tilde{\beta}}(\cdot;\tilde{\theta}) \right) \).

Notice that the Laguerre weight function \( G(x,\theta) \) does not satisfy the hypothesis of Lemma 3.1 so we cannot use Lemma 3.2 to verify the boundedness of the Mercer-type kernel analogous to Eq. (27). Nevertheless, we can still verify the boundedness of the kernel using existing identities and summarize the result as follows.

**Lemma 3.6.** (Hille-Hardy kernel) Let \( G(x;\tilde{\theta}), \ell^{(\beta)}_{\tilde{m}}(x) \), and \( \Psi_{\tilde{\beta},\tilde{m}}(x) \) be the same as in Eq. (34) and (35). For \( \rho \in (0,1) \), and \( \beta \in \left( \frac{1}{2}, \infty \right) \),

\[
k_{\tilde{\beta},\rho}(x,y) := \sum_{m=0}^{\infty} \rho^m \Psi_{\tilde{\beta},m}(x)\Psi_{\tilde{\beta},m}(y), \quad x,y \in [0,\infty)^d,
\]

defines a bounded kernel. In particular, we have the following \( d \)-dimensional generalized Hille-Hardy formula [30]

\[
k_{\tilde{\beta},\rho}(x,y) = \frac{\rho^{-\frac{1}{2}}}{(1-\rho)^d} \exp \left( -\frac{1+\rho}{2(1-\rho)} \|x + y\|_1 \right) G^{\tilde{\beta} - \frac{1}{2}}(x;\tilde{\theta})G^{\tilde{\beta} - \frac{1}{2}}(y;\tilde{\theta}) \prod_{i=1}^{d} I_{\tilde{\theta}_i} \left( \frac{2\sqrt{\|x_i\|_2}}{1-\rho} \right),
\]

where \( I_{\tilde{\theta}_i} \) denotes the modified Bessel function [31].

The Hille-Hardy formula (Eq. (37) with \( d = 1 \)) can be interpreted as a generalization of the Mehler kernel [28], since Hermite polynomials can be entirely reduced to Laguerre polynomials [32]. See Appendix B for the proof.

With Lemma 3.6 following Proposition 3.4 one can construct the RKHS corresponding to the Hille-Hardy kernel in (37) as an analogy of the Mehler RKHS in (31). One can also specify the regularity of this function space analogous to Lemma 3.5 by checking the boundedness of the derivatives of the Hille-Hardy kernel using results in [31], which we omitted here for brevity.

3.2 Universality of the Mehler RKHS

As mentioned in the introduction, for a reliable estimation, we would like to construct a hypothesis space (RKHS) that is “rich” enough to capture particular behavior of the target function. Specifically, we will use the notion of weighted \( c_0 \)-universality described in Lemma 2.8 to specify the appropriate Mehler RKHS that can capture the decaying property (Gaussian or faster) of the target density function. The key idea is to understand the “richness” of space \( \mathcal{H}_{\tilde{\beta},\rho} \) as we summarize now.

**Corollary 3.7.** For Mehler kernel \( k_{\tilde{\beta},\rho} \) in (29) and Mehler RKHS \( \mathcal{H}_{\tilde{\beta},\rho} \) in (31), let

\[
q_{\tilde{\beta},\rho}(x) := \exp \left( -\frac{1}{2(1+\rho)} + \frac{\tilde{\beta} - 1}{2} \|x\|^2 \right), \quad x \in \mathbb{R}^d,
\]

then \( \mathcal{H}_{\tilde{\beta},\rho} \) is dense in \( C_0 \left( \mathbb{R}^d; q_{\tilde{\beta},\rho}^{-1} \right) \).

**Proof.** By Lemma 2.8 we need to check the following two conditions.

1. \( k_{\tilde{\beta},\rho}(\cdot,x) \in C_0 \left( \mathbb{R}^d; q_{\tilde{\beta},\rho}^{-1} \right), \forall x \in \mathbb{R}^d, \)
2. \( \tilde{k}(x,y) := k_{\tilde{\beta},\rho}(x,y)q_{\tilde{\beta},\rho}^{-1}(x)q_{\tilde{\beta},\rho}^{-1}(y) \) is \( c_0 \)-universal.
Notice that for any fixed \( y \in \mathbb{R}^d \), as a function of \( x \),
\[
k_{\beta,\rho}(x, y) q_{\beta,\rho}^{-1}(x) \propto \exp \left[ -\frac{1}{2(1-\rho^2)} \left( \rho \|x\|^2 - 2\rho \sum_{i=1}^{d} x_i y_i \right) \right],
\]
that is, \( k_{\beta,\rho}(\cdot, y) q_{\beta,\rho}^{-1}(\cdot) \in C_0(\mathbb{R}^d) \) since \( \rho \in (0, 1) \). By the definition of \( C_0\left(\mathbb{R}^d, q_{\beta,\rho}^{-1}\right) \) (see Lemma 2.7), the first condition holds.

For the second condition, simply notice that
\[
\tilde{k}(x, y) \propto \exp \left[ -\frac{1}{2(1-\rho^2)} \left( \rho \|x\|^2 + \rho \|y\|^2 - 2\rho \sum_{i=1}^{d} x_i y_i \right) \right] = \exp \left[ -\frac{\rho}{2(1-\rho^2)} \|x - y\|^2 \right],
\]
and \( \frac{\rho}{2(1-\rho^2)} > 0 \), that is, \( \tilde{k}(x, y) \) is a Gaussian kernel which is \( c_0 \)-universal.

\[\blacksquare\]

**Remark 3.8.** Corollary 3.7 suggests that the Mehler RKHS \( \mathcal{H}_{\beta,\rho} \) is rich enough to approximate the functions in \( C_0\left(\mathbb{R}^d, q_{\beta,\rho}^{-1}\right) \). Moreover, notice that in the formula of \( q_{\beta,\rho} \) in (38), we have
\[
\left\{ \frac{1}{2(1+\rho)} + \frac{\beta - 1}{2} : \beta \in \left(\frac{1}{2}, \infty\right), \rho \in (0, 1) \right\} = (0, \infty),
\]
thus, for any target density function \( f \) which is continuous and of a Gaussian decay rate, that is, there exist constants \( \theta, C_f > 0 \) such that
\[
|f(x)| \leq C_f \exp \left(-\theta \|x\|^2\right), \quad \forall x \in \mathbb{R}^d,
\]
we can find \( \beta^* > \frac{1}{2} \) and \( \rho^* \in (0, 1) \) such that
\[
\frac{1}{2(1+\rho^*)} + \frac{\beta^* - 1}{2} < \theta,
\]
and the decay rate (39) implies \( f \in C_0\left(\mathbb{R}^d, q_{\beta^*,\rho^*}^{-1}\right) \). This means that one can approximate any continuous function that has Gaussian (or faster) decaying rate as in (39) up to any desirable accuracy using an estimator that belongs to the Mehler RKHS \( \mathcal{H}_{\beta^*,\rho^*} \), which is a space of functions with Gaussian decay rate slower than (39).

We should point out that Corollary 3.7 relies on the analytical expression of the Mehler kernel that allows us to find an isometrically isomorphic map that transforms the Mehler kernel into a radial kernel that is known to be \( c_0 \)-universal. Unfortunately this same technique is not trivially applicable for the Hille-Hardy kernel since its analytical expression, as shown in (37), is more complicated. To verify the “richness” of the Hille-Hardy RKHS, one possible approach is to develop a weighted-\( c_0 \) universality characterization based on the Proposition 12 in [17], and we leave it as an open problem.

### 4 Kernel embedding linear response

In the current section, we first define the kernel embedding estimate for distribution functions, then, as an application, we introduce the kernel embedding linear response. The consistency of the kernel embedding linear response will be demonstrated. We will close the section by addressing several issues occurred in the numerics, including an error bound for empirical kernel embedding estimates based on non-i.i.d. data. For simplicity, we only discuss the linear response estimate based on the Mehler RKHS hypothesis space. Similar proving technique can be applied to the Hille-Hardy kernel.

We assume the target \( d \)-dimensional density function \( f \) lives in the Mehler RKHS \( \mathcal{H}_{\beta,\rho} \) for some \( \rho \in (0, 1) \) and \( \beta \geq \frac{1}{2} \). Recall that, by the reproducing property and the expansion formula (22), we have
\[
f = \sum_{\hat{m} \geq 0} \hat{f}_{\hat{m}} \Psi_{\hat{m}}, \quad \hat{f}_{\hat{m}} = \int_{\mathbb{R}^d} f(x) \psi_{\hat{m}}(x) W^{1-\beta}(x) \, dx, \quad \psi_{\hat{m}} = \prod_{i=1}^{d} \psi_{m_i}, \quad (40)
\]
where \( W(x) \propto \exp\left(-\frac{1}{2}\|x\|^2\right) \), and \( \{|\psi_{m_i}\} \) are the normalized Hermite polynomials. We define the order-\( M \) kernel embedding estimates of \( f \), denoted by \( \hat{f}_M \), as the order-\( M \) truncation of Eq. (40), that is,
\[
\hat{f}_M := \sum_{|\hat{m}|_{1 \leq M} \leq M} \hat{f}_{\hat{m}} \Psi_{\hat{m}}, \quad (41)
\]
We should point out that, with this choice of basis representation, we arrive at a polynomial chaos approximation of $f$. But the convergence $f_M \to f$ as $M \to \infty$ is valid in both $L^2(\mathbb{R}^d, W^{1-\beta})$ and $C_0(\mathbb{R}^d)$. Another remark is that, although, the formula of kernel embedding estimates (41) is independent of parameter $\rho$, this parameter does affect the convergent rate of the residual error $\|f - f_M\|_{\mathcal{H}_{\rho,\rho}}$ (see Proposition 4.3).

In practice, the integral in (40) can be approximated by Monte-Carlo, that is,

$$f_M, N := \sum_{n=1}^{N} \hat{f}_{\tilde{r}, N} \Psi_{\tilde{r}, N}(X_{t_n})$$

where $\{X_{t_n}\}_{n=1}^{N}$ are sampled from the target density function $f$. One can define the order-$M$ empirical kernel embedding estimate of $f$ as

$$f_{M,N} := \sum_{n=1}^{N} \hat{f}_{\tilde{r}, N} \Psi_{\tilde{r}, N}$$

In our application, we set $f = p_{eq}$, and the sample $\{X_{t_n}\}$ corresponds to a time series of $X(t_n)$ in the unperturbed dynamics (1) generated at the equilibrium. We should point out that that error bound, to be discussed in Proposition 4.3 will account for the fact that the empirical estimator in (42) is based on non-i.i.d. data.

Let’s replace the unknown $p_{eq}$ in (3) by its order-$M$ kernel embedding estimates, denoted as $p_M$. We can naively define the order-$M$ kernel embedding linear response operator as

$$k_{\lambda}(t) := \mathbb{E}_{p_{eq}} \left[ A(X(t)) \otimes \hat{B}(X(0)) \right], \quad \hat{B}_1(X) := -\partial_{X_1} [c_1(X) p_M(X)] / p_M(X),$$

for integrable observable $A(X)$ and external forcing $c(X) \delta f(t)$. Unfortunately, Eq. (44) is not a well-defined estimator for the linear response operator $k_\lambda(t)$, since the basis function $\Psi_{\rho, \hat{r}}(x)$ in (27), as a product of normalized Hermite polynomials and the standard Gaussian distribution, can be negative. To circumvent this issue, since the problematic term is the estimator of $B$, we consider a modification to the variable $B$ in the definition of the linear response operator in (5). Given a compact set $D \subset \mathbb{R}^d$ and observables $A$ and $B$ in (5), we define the restricted linear response operator

$$k_{\lambda,D}(t) := \mathbb{E}_{p_{eq}} \left[ A(X(t)) \otimes B_D(X(0)) \right], \quad B_D := B \cdot \chi_D \quad \forall t \geq 0,$$

where $\chi_D$ denotes the characteristic function with respect to $D$. Further assume both $A(\cdot)$ and $B(\cdot)$ have finite second moments with respect to $p_{eq}$, then, $B_D$ in (45) is also of finite second moment. Thus, according to Lemma 2.1, $k_{\lambda,D}(t)$ in (45) is well-defined $\forall t \geq 0$. Moreover, replacing $B$ by $B(1 - \chi_D)$ in (7), one can show that

$$|k_\lambda(t) - k_{\lambda,D}(t)| \leq \left( \int_{\mathbb{R}^d} \bar{A}^2(x) p_{eq}(x) \, dx \right)^{\frac{1}{2}} \otimes \left( \int_{D_c} \bar{B}^2(x) p_{eq}(x) \, dx \right)^{\frac{1}{2}}, \quad \forall t \geq 0.$$

By the continuity of the integrals, we can claim that $\forall \epsilon > 0$, there exists a compact set $D_\epsilon \subset \mathbb{R}^d$ such that

$$|k_\lambda(t) - k_{\lambda,D_\epsilon}(t)| < \epsilon, \quad \forall t \geq 0.$$  

(46)

Further notice that, by Lemma 2.2 and Eq. (30), $p_M$ converges uniformly to the positive function $p_{eq}$ with

$$\|p_{eq} - p_M\|_{\infty} \leq \|\Psi_{\rho, \hat{r}}\|_{\mathcal{H}_{\rho, \rho}} \|p_{eq} - p_M\|_{\mathcal{H}_{\rho, \rho}} = (2\pi)^{-\frac{d^2}{2}} (1 - \rho^2)^{-\frac{d}{2}} \|p_{eq} - p_M\|_{\mathcal{H}_{\rho, \rho}},$$

where $\|p_{eq} - p_M\|_{\mathcal{H}_{\rho, \rho}}$ goes to zero monotonously. Thus, to ensure the positivity of $p_M$ on $D_\epsilon$, we define

$$M_\epsilon := \min \left\{ M \mid \|p_{eq} - p_M\|_{\mathcal{H}_{\rho, \rho}} < (2\pi)^{-\frac{d^2}{2}} (1 - \rho^2)^{-\frac{d}{2}} \delta \right\}, \quad \delta := \min_{x \in D_\epsilon} p_{eq}(x) > 0,$$

which suggests $\forall M \geq M_\epsilon, p_M$ is strictly positive on $D_\epsilon$, and the estimator of $k_{\lambda,D_\epsilon}$ in (45) given by

$$\hat{k}_{\lambda,D_\epsilon}(t) := \mathbb{E}_{p_{eq}} \left[ A(X(t)) \otimes \hat{B}_{D_\epsilon}(X(0)) \right],$$

(48)
Proposition 4.1. Consider a d-dimensional Itō diffusion \( \{ \} \) with a positive equilibrium distribution function \( p_{eq} \in \mathcal{H}_{\beta, \rho} \), and its perturbed dynamics \( \{ \} \). Assume both observables \( A(t) \) and the conjugate variable \( B(t) \) have finite second moment with respect to \( p_{eq} \). For the restricted linear response operator \( k_{A,D_k}(t) \) in \( \{ \} \) and its estimator \( \hat{k}_{A,D_k}(t) \) in \( \{ \} \), we have

\[
\lim_{M \to +\infty} \| k_{A,D_k}(t) - \hat{k}_{A,D_k}(t) \|_F = 0
\]

uniformly in \( t \). Here, \( \| \cdot \|_F \) denotes the Frobenius norm of matrices.

Proof. For simpler notations, without lose of generality, we assume \( c(x) \) in the perturbed dynamics \( \{ \} \) is a scalar function in our proof. As a result, following Eq. \( \{ \} \), we have

\[
B(x) = \left( \nabla p_{eq}(x)c(x) + \nabla c(x)p_{eq}(x) \right) p_{eq}^{-1}(x), \quad \hat{B}(x) = \left( \nabla p_M(x)c(x) + \nabla c(x)p_M(x) \right) p_M^{-1}(x).
\]

(50)

Under the integrability assumptions of \( A \) and \( B \), both \( k_{A,D_k}(t) \) in \( \{ \} \) and its estimator \( \hat{k}_{A,D_k}(t) \) in \( \{ \} \) are well-defined, and, by Lemma \( \{ \} \) we have

\[
| k_{A,D_k}(t) - \hat{k}_{A,D_k}(t) | \leq E_{p_{eq}} \left[ A(X(t)) \otimes (B_{D_k} - \hat{B}_{D_k})(X(0)) \right] \leq E_{p_{eq}} \left[ A(X)^2 \right] \leq E_{p_{eq}} \left[ (B_{D_k}(X) - \hat{B}_{D_k}(X))^2 \right].
\]

(51)

Furthermore we have,

\[
E_{p_{eq}} \left[ (B_{D_k}(X) - \hat{B}_{D_k}(X))^2 \right] \leq \int_{D_k} \left[ (B - \hat{B})^2(x) p_{eq}(x) \right] \, dx = \int_{D_k} \left[ (B - \hat{B}) p_M p_{eq}^{-1} + \hat{B} p_M p_{eq}^{-1} - \hat{B} \right] \, dx
\]

\[
= \int_{D_k} \left[ \left( p_{eq} - p_M \right) c + \nabla c(p_{eq} - p_M) \right] p_{eq}^{-1} \, dx + \hat{B}^2(p_M^{-1} - 1) \, dx
\]

\[
\leq 2 \int_{D_k} \left[ \left( p_{eq} - p_M \right) c + \nabla c(p_{eq} - p_M) \right]^2 \, dx + 2 \int_{D_k} \hat{B}^2 \, dx + \delta \left\| p_M - p_{eq} \right\|_2^2 \int_{D_k} \hat{B}^2 \, dx \leq 2 \delta \int_{D_k} \left[ \left( p_{eq} - p_M \right) c + \nabla c(p_{eq} - p_M) \right] \, dx + 2 \left\| p_M - p_{eq} \right\|_2^2 \int_{D_k} \hat{B}^2 \, dx,
\]

where \( \delta \) is the same as in \( \{ \} \). By Lemma \( \{ \} \) and Corollary \( \{ \} \) we have the uniform convergence of \( p_M \to p_{eq} \) and \( \nabla p_M \to \nabla p_{eq} \) as \( M \to \infty \), that is,

\[
\lim_{M \to +\infty} \int_{D_k} \left[ \left( p_{eq} - p_M \right) c + \nabla c(p_{eq} - p_M) \right] \, dx = 0.
\]

(52)

With the uniform convergence, we take \( M \) large enough such that \( \left\| p_{eq} - p_M \right\|_2 \leq \delta \), that is, \( p_M \geq \frac{\delta}{2} \) on \( D_k \), and

\[
\int_{D_k} \hat{B}^2 \, dx \leq 2 \delta^{-2} \int_{D_k} \left[ \left( p_{eq} - p_M \right) c + \nabla c(p_{eq} - p_M) \right]^2 \, dx \leq 4 \delta^{-2} \int_{D_k} \hat{B}^2 \, dx < \infty,
\]

as \( M \to \infty \). Combine \( \{ \} \) with \( \{ \} \), we reach the convergence

\[
\lim_{M \to +\infty} E_{p_{eq}} \left[ (B_{D_k}(X) - \hat{B}_{D_k}(X))^2 \right] = 0.
\]

(53)

Together, Eq. \( \{ \} \) and the square integrability of \( A \), Eq. \( \{ \} \) holds and the convergence is uniform in \( t \).

\[
\square
\]

Remark 4.2. It is worthwhile to mention that, for \( p_{eq} \in \mathcal{H}_{\beta, \rho} \), by the decay rate of \( p_{eq} \) and \( \nabla p_{eq} \), a sufficient condition for \( B \) in \( \{ \} \) to have finite second moment is that \( c(\cdot) \) is continuously differentiable and

\[
\exists \theta \in \left( 0, \frac{1}{4(1 + \rho)} + \frac{\beta - 1}{4} \right) \text{ s.t. } \sup_{x \in R^d} (|c(x)| + \|\nabla c(x)\|) \exp \left( -\theta \|x\|^2 \right) < \infty.
\]

This is a concrete condition that can be used in practice to check whether the FDT response is well-defined under external forces of the form \( f(x, t) = c(x) \delta f(t) \) for unperturbed dynamics with equilibrium density having Gaussian (or faster) decay rate of arbitrary variance.

In practice, since the sample size is finite, one can always find \( D_k \) in \( \{ \} \) for \( \epsilon \) small enough such that the sample \( \{X_n\}_{n=1}^N \subset D_k \). Thus, for \( M \) large enough, the estimator in \( \{ \} \) is well-defined and can be approximated by a Monte-Carlo integral of the form \( \{ \} \) over the entire data set \( \{X_n\}_{n=1}^N \). The following proposition addresses the Monte-Carlo error of the order-\(M\) empirical kernel embedding estimate \( \hat{f}_{MN} \).
Proposition 4.3. Given a $d$-dimensional stationary (time-homogeneous) Markov process $X(t)$ with a discretization $\{X_n := X((n - 1)\Delta t)\}_{n=1}^N$ that satisfies

1. $\{X_n\}$ yields a stationary distribution $f \in \mathcal{H}_{\beta, \rho}$ for some $\rho \in (0, 1)$ and $\beta \in \left[\frac{1}{4}, \frac{1}{1 - \rho}\right]$.
2. $\{X_n\}$ is an $\alpha$-mixing process [18] with mixing coefficient $\alpha(k)$ satisfies
   \[ C_\alpha := \sum_{k=1}^{\infty} \alpha(k) \frac{1}{k^\epsilon} < \infty, \]
   for some $\epsilon \in (0, 2)$.

Then, for $d \leq \frac{1}{2} M + 1$, we have the following error bound for the empirical kernel embedding estimate $f_{M,N}$ in $\mathcal{H}_{\beta, \rho}$:

\[ E\left[ \|f - f_{M,N}\|_{L^2(W^{1,2})}^2 \right] \leq \frac{1}{N} \left[ C_f (M + 1)^d + 24 C_\alpha C_f \beta^\frac{1}{2} M^{d-1} \left(\frac{3}{2}\right)^{M+3} \right] + \rho M^{\frac{1}{2}} \|f\|_{\mathcal{H}_{\beta, \rho}}^2, \]  

(55)

where $C_f := (2\pi)^{\frac{d-1}{2}} (1 - \rho^2)^{-\frac{d}{4}} \|f\|_{\mathcal{H}_{\beta, \rho}}$, and the expectation in (55) is defined over random variables $\{X_n\}_{n=1}^N$.

See Appendix C for the proof. The first term in the upper bound in (55) corresponds to the estimation (or Monte-Carlo) error, which consists of the variance and covariance terms. The covariance term accounts for the error due to averaging over correlated or non-i.i.d. samples. The last term in upper bound in (55) corresponds to the approximation error or bias due to finite truncation, $M$. Asymptotically, it is clear that the error vanishes as both $M, N \to \infty$.

If $\{X_n\}_{n=1}^N$ are i.i.d. samples of $f$, the error bound (55) reduces to

\[ E\left[ \|f - f_{M,N}\|_{L^2(W^{1,2})}^2 \right] \leq \frac{C_f}{N} (M + 1)^d + \rho M^{\frac{1}{2}} \|f\|_{\mathcal{H}_{\beta, \rho}}^2, \]  

(56)

where we are left with the variance and bias terms in the upper bound. We should point out that, in this case, the assumption of $d \leq \frac{1}{2} M + 1$, which is used to obtain the upper bound for the non-i.i.d. estimation error (55), can be neglected. First, we note that the error estimate shows that the approximation error (or bias) is independent of the dimension. In fact, the approximation error in (56) decays exponentially as a function of the model parameters, $M$, since $0 < \rho < 1$. This fact is not surprising since the target function, $f \in \mathcal{H}_{\beta, \rho}$, is bounded, smooth, and has Gaussian decay. However, the estimation error depends exponentially on the dimension. This curse of dimensionality is due to the use of tensor products in the orthonormal basis. While the constants in the error bound may be different, the same curse of dimensionality issue should also be suffered by the estimation with the Hille-Hardy RKHS, and the method of proof is not different from the one presented in Appendix C.

For data points that lie on an $m$-dimensional compact manifold $\mathcal{M}$ embedded in $\mathbb{R}^d$, it was shown in [22] that the estimation error (or variance) can be improved to be exactly $M^{-1}$ using the Mercer-kernel constructed by the eigenvalues and orthonormal eigenfunctions of the Laplace-Beltrami operator, defined on functions that take values on $\mathcal{M}$. In fact, if the target function is a Sobolev class $H^s(\mathcal{M})$, one can show that the approximation error is of order $M^{-\frac{s}{d}}$, where the Weyl asymptotics for eigenvalue of the Laplace-Beltrami operator on compact manifolds [33] is used. Balancing these errors, we obtain the famous optimal bias-variance tradeoff rate of order $N^{-\frac{d}{2d-3m}}$ for linear model [34]. When the target function is smooth such as $\ell = d$, the optimal error rate of order $N^{-2/3}$ suggests that this approach overcomes the curse of dimension. While this is appealing, the numerical method in approximating the orthonormal eigenfunctions of the Laplace-Beltrami operator, such as the diffusion maps [35], which suffers from the curse of dimension with a spectral convergence rate of order $N^{-\frac{1}{d}}$ [36]. Thus, the curse of dimension is not completely avoided. The key takeaway point is that this nonparametric estimation is still feasible if the target function is supported on a low-dimensional intrinsic manifold $\mathcal{M}$.

In the next section, we will numerically verify the kernel embedding linear response based on estimator obtained from both, the Mehler RKHS and the Hille-Hardy RKHS. For applications of approximation of target functions that take data on smooth manifolds embedded in $\mathbb{R}^d$, see [26, 27].

5 Numerical Examples

In this section, we will test the methods on two models, a stochastic gradient system with a triple-well potential (Section 5.1) and a Langevin equation with the Morse potential (Section 5.2). In [37], the authors have explored...
these two model problems. Here, our goal is to demonstrate the numerical implementation of the kernel embedding linear response approach introduced in Section 2 based on different choices of orthogonal polynomials. We also stress that we picked examples with explicit equilibrium distributions so that we can verify the estimates by directly comparing to the exact linear response via the FDT reviewed in Section 2.1.

For the triple-well model, the potential function contains a quadratic retaining potential, which introduces a Gaussian tail to the density function. Thus, we will consider a two-dimensional Mehler kernel in the kernel embedding linear response.

For the Langevin equation, the marginal distribution of the velocity \(v\) is Gaussian, while the marginal distribution of the displacement \(x\), governed by the Morse potential, is asymmetric. In computing the kernel embedding linear response, to obtain the best result, the kernel will be derived based on a tensor product of Hermite (for the variable \(v\)) and Laguerre (for the variable \(x\)) polynomials.

### 5.1 A gradient system with a triple-well potential

We first consider a two-dimensional stochastic gradient system as follows,

\[
\dot{X} = -\nabla V(X) + \sqrt{2k_B T} \mathbf{W}_t, 
\]

where \(\mathbf{W}_t\) is a two-dimensional Wiener process, and \(V\), similar to the model in [38], is a triple-well potential,

\[
V(x) = -v\left(x_1^2 + x_2^2\right) - (1 - \gamma) v\left((x_1 - 2a)^2 + x_2^2\right) - (1 + \gamma) v\left((x_1 - a)^2 + (x_2 - a/\sqrt{3})^2\right) + 0.8 \left((x_1 - a)^2 + (x_2 - a/\sqrt{3})^2\right),
\]

with

\[
v(z) = 10 \exp\left(\frac{1}{z^2 - a^2}\right) \cdot \chi_{(-a,a)}(z), \quad z \in \mathbb{R},
\]

where \(\chi_{(-a,a)}\) denotes the characteristic function over the interval \((-a,a)\). The parameter \(\gamma \in (0,1)\) in (58) indicates the depth of the three wells. The additional quadratic term \(0.8[(x_1 - a)^2 + (x_2 - a/\sqrt{3})^2]\) in the triple-well potential (59) is a smooth retaining potential (also known as a confining potential). The triple-well model (57), as a stochastic gradient system [22], yields an equilibrium distribution given by

\[
p_{eq}(x) \propto \exp\left(-\frac{V(x)}{k_B T}\right) \quad x \in \mathbb{R}^2.
\]

To derive a linear response operator, we consider an external forcing that is constant in \(x\). Subsequently, the perturbed dynamics is given by,

\[
dx(t) = (-\nabla V(x) + f(t) \delta) \, dt + \sqrt{2k_B T} \, dW_t,
\]

where \(|\delta| \ll 1\). If we select \(A(x) := x\) as the observable, the corresponding linear response operator, as a 2-by-2 matrix-valued function given by (5), reads

\[
k_A(t) = -\mathbb{E}_{p_{eq}} [x(t) \otimes \nabla \log(p_{eq}(x(0)))] = \frac{1}{k_B T} \mathbb{E}_{p_{eq}} [x(t) \otimes \nabla V(x(0))].
\]

With the quadratic retaining potential in (59), \(p_{eq}\) in (59) yields a Gaussian tail. Therefore, we apply the kernel embedding linear response to the linear response operator \(k_A(t)\) in (60) based on the Hermite polynomials. Let \(\hat{p}_{eq}\) denote the kernel embedding estimate of \(p_{eq}\) in (59), and by Eq. (44), the kernel embedding linear response operator, as an estimate of \(k_A(t)\) in (60), is defined as

\[
\hat{k}_A(t) = -\mathbb{E}_{\hat{p}_{eq}} [x(t) \otimes \nabla \log(\hat{p}_{eq}(x(0)))].
\]

In the numerical experiment, we set \((a, k_B T, \gamma) = (1, 1.5, 0.25)\). To generate the data from (57), we apply the weak trapezoidal method [39] with step size \(h = 1 \times 10^{-3}\), followed by a 1/5-subsample. Figure 1 shows the order-25 \((M = 25\) in (41)) kernel embedding estimates \(\hat{p}_{eq}\) compared with the \(p_{eq}\) in (59). The estimate \(\hat{p}_{eq}\) captures the well structure of the model with a decent accuracy. Figure 2 includes the estimates of the linear response operator \(k_A(t)\) in (60) via kernel embedding linear response, compared to the true linear response. Since the unperturbed dynamics (57) is a stochastic gradient system, the off-diagonal entries of the linear response operator \(k_A(t)\) in (60) should be zero at \(t = 0\) due to the equipartition of the energy in statistical mechanics. However, the empirical estimates of \(k_A\) reported in Figure 2 is not consistent with the theory, which may be due to the Monte-Carlo error.

We observe that the linear response under a constant external forcing can be estimated accurately by the kernel embedding linear response. The discrepancies between the estimates, which are more pronounced in the non-diagonal components of the linear response operator, are due to the error in derivatives of the density estimate.
Figure 1: The equilibrium distribution of the triple-well model (57) (upper left panel) and its kernel embedding estimate (upper right panel) based on a total of $1 \times 10^7$ sample. The contour plot (lower panel) displays the absolute error of the estimate.

5.2 A Langevin equation with Morse potential

For the second example, we consider a Langevin dynamic in statistical mechanics, describing the dynamics of a particle driven by a conservative force, a damping force, and a stochastic force. In particular, we choose the conservative force based on the Morse potential

$$U(x) = U_0(a(x - x_0)), \quad U_0(x) = \epsilon(e^{-2x} - 2e^{-x} + 0.03x^2), \quad (62)$$

where the last quadratic term in $U_0$, similar to the last term in the triple-well potential (58), acts as a retaining potential, preventing the particle from moving to infinity. For this one-dimensional model, we rescale the mass to unity, and write the dynamics as follows

$$\begin{cases}
\dot{x} = v, \\
\dot{v} = -U'(x) - \gamma v + \sqrt{2\gamma k_B T} \dot{W},
\end{cases} \quad (63)$$

where $\dot{W}$ is a white noise. The smooth retaining potential $U(x)$ guarantees the ergodicity of the Langevin system in (63). (see Appendix C of [37] for the proof) Namely, there is an equilibrium distribution (also known as the Gibbs measure) $p_{eq}(x, v)$, given by

$$p_{eq}(x, v) \propto \exp \left[ -\frac{1}{k_B T} \left( U(x) + \frac{1}{2} v^2 \right) \right], \quad (64)$$

which is independent of $\gamma$. 
To derive a linear response operator in (5), introduce a constant external forcing together with a constant external velocity field, and the corresponding perturbed system is given by

\[
\begin{align*}
\dot{x} &= v + \delta f_1 \\
\dot{v} &= -U'(x) - \gamma v + \delta f_2 + \sqrt{2\gamma k_B T} \dot{W},
\end{align*}
\]

By selecting the observable \( A = (x, v)^T \), the resulting linear response operator is given by

\[
k_A(t) = -\mathbb{E}_{p_{eq}} \left[ (x(t), v(t))^T \otimes \nabla \log(p_{eq}(x(0), v(0))) \right] = \frac{1}{k_B T} \mathbb{E}_{p_{eq}} \left[ \begin{pmatrix} x(t) U'(x(0)) & x(t) v(0) \\ v(t) U'(x(0)) & v(t) v(0) \end{pmatrix} \right].
\] (65)

Here, to derive the 2-by-2 two-point statistics matrix in (65), we have used the fact that the variables \( x \) and \( v \) are independent at the equilibrium. However, in our estimation problem, we do not assume that the underlying density, \( p_{eq} \), is a product of two marginal densities. In particular, adopting the notation in Section 3.1.1 and 3.1.2, we define the order-\((M_1, M_2)\) kernel embedding estimate of \( p_{eq} \) in (64) as

\[
\hat{p}_{eq} = \sum_{m_1=0}^{M_1} \sum_{m_2=0}^{M_2} \hat{p}_{m_1 m_2} \ell_m^{(1)}(x) \psi_{m_2}(v) G(x; 1) W(v), \quad \hat{p}_{m_1 m_2} := \int_{\mathbb{R}^2} \ell_m^{(1)}(x) \psi_{m_2}(v) p_{eq}(x, v) \, dx \, dv,
\] (66)

where \( \{\ell_m^{(1)} \} \) denotes the normalized Laguerre polynomials with respect to the Gamma distribution \( G(x; 1) \propto x e^{-x} \); while \( \{\psi_{m_2} \} \) denotes the normalized Hermite polynomials with respect to the Gaussian distribution \( W \). The representation in (66) is motivated by the asymmetric structure of the marginal distribution of \( x \) (See Figure 3). With the estimate \( \hat{p}_{eq} \) of \( p_{eq} \), we define the corresponding kernel embedding linear response,

\[
\hat{k}_A(t) = -\mathbb{E}_{\hat{p}_{eq}} \left[ (x(t), v(t))^T \otimes \nabla \log(\hat{p}_{eq}(x(0), v(0))) \right],
\] (67)

Figure 2: The linear response operator \( k_A \) in (59) (blue solid) and the corresponding estimates \( \hat{k}_A \) in (61) (red dot-dash) via kernel embedding linear response. As two-point statistics, both \( k_A \) and \( \hat{k}_A \) are computed via Monte-Carlo. The diagonal entries of \( k_A \) and \( \hat{k}_A \) are normalized so that they share the same initial value 1.
as the estimates of $k_A(t)$ in (65), which does not rely on the independence of $x$ and $v$ at the equilibrium.

![Marginal distribution of $x$: Laguerre](image1)

![Marginal distribution of $v$: Hermite](image2)

Figure 3: The marginal distribution of $x$ (left) and $v$ (right) of the Langevin dynamics (63) at equilibrium. The blue solid curves are determined based on the explicit form of the $p_{eq}$ in (64), and the red dot-dash curves are the marginal distribution of the resulting kernel embedding estimates based on a total of $1 \times 10^7$ samples.

In the numerical test, we set $\gamma = 0.5, k_B T = 1.0, \epsilon = 0.2, a = 10, \text{ and } x_0 = 0$. The data, in the form of a time series, are generated from the model (63) using an operator-splitting method (10) with step size $h = 1 \times 10^{-3}$, followed by a 1/10-subsample. Figure 3 presents the marginals of the kernel embedding estimates $\hat{p}_{eq}$ in (65) with $M_1 = 100$ and $M_2 = 4$. Notice that the domain of the Laguerre polynomials $\ell_m^{(1)}$ in (66) is $[0, \infty)$. In the computation of the coefficients $\hat{p}_{mn}$ in (66) via Monte-Carlo, we have shifted the observations of $x$ so that they are all positive. For the variable $v$, we use very few bases, since the marginal distribution is already Gaussian. Figure 4 compares the linear response operator $k_A$ in (65) with its estimates $\hat{k}_A$ in (67) based on the kernel embedding linear response. In our Langevin dynamics, the damping coefficient $\gamma = 0.5$ in (63) is used, which is in the under-damping regime (37) in the sense that we have a relatively strong memory effect and the two-point statistics $k_A(t)$ in (65) exhibits a more complicated behavior. The numerical result suggests that our kernel embedding linear response is able to capture such behavior.

6 Summary and discussion

In this paper, we considered nonparametric estimation of the equilibrium density from non-i.i.d time series of unperturbed dynamics to estimate linear response statistics. In particular, we employed a nonparametric density estimator formulated by the kernel embedding of distribution. We chose the corresponding hypothesis space (model) as an RKHS so that the properties of the kernel can be carried to the functions in the RKHS. To avoid the computational expense arises using radial type kernels, we considered the “Mercer-type” kernels constructed based on the classical orthogonal bases defined on non-compact domains, e.g., $\mathbb{R}^d$. Here, the orthogonality corresponds to a weighted-$L^2$ space, which naturally provides the integral definition of the coefficients in the estimates. In practice, the number of bases involved, thanks to the orthogonality, are much fewer than the sample size. For example, in the test models, the sample size is of order $10^7$, while the number of bases is of order $10^2$.

We used the orthogonal polynomials, assigned with a specific power of the corresponding weight, to build the “Mercer-type” kernel of our RKHS. To overcome the difficulty caused by the non-compact domain, we showed the boundedness of the kernel either based on the asymptotic behavior of a class of orthogonal polynomials (e.g., Hermite polynomials) or existing identities (e.g., Laguerre polynomials). By studying the orthogonal polynomial approximation in the RKHS setting, we established the uniform convergence of the estimator, which justifies the use of the estimator for interpolation. With this choice of basis representation, we arrived at the well-known polynomial chaos approximation. However, the convergence is valid in both $L^2$-norm sense and uniform-norm sense.

Another critical issue we addressed is the “richness” of the resulting RKHS, that is, whether we can find a good approximation of the target density function which is not in the hypothesis space. Since the decaying property of the target density function is quantifiable based on the available data, we generalized the theory of $c_0$-universality so that one can construct the appropriate hypothesis space, as an RKHS, that can estimate the target function with the corresponding decaying property.
In terms of linear response estimation, we defined the kernel embedding linear response based on the kernel embedding estimates of the equilibrium density. Our study provides practical conditions for the well-posedness of not only the estimator but also the well-posedness of the underlying response statistics. Given a well-posed estimator, supported by the theory of RKHS, we provided a theoretical guarantee for the convergence of the estimator to the underlying actual linear response statistics. Finally, since we approximate the coefficients in the estimates using Monte-Carlo average, we derived a statistical error bound for the density estimation that accounts for the Monte-Carlo averaging over non-i.i.d time series with $\alpha$-mixing property and biases due to finite basis truncation. This error bound provides a mean to understand the feasibility as well as limitation of the kernel embedding with the “Mercer-type” kernel.

Numerically, we validated the kernel embedding linear response estimator on two stochastic dynamics with known but non-trivial equilibrium densities. In the triple-well model, we explored the effectiveness of the kernel embedding estimates in a two-dimensional target density with Gaussian decay. In the Langevin model, since the marginal distribution of the displacement, due to the Morse potential, is asymmetric, that is, the decaying properties are different on two sides, we considered a hypothesis space (RKHS) based on a tensor product of Hermite (for the velocity) and Laguerre (for the displacement) polynomials in constructing the kernel.

Overall, our kernel embedding linear response provides a systematic and data-driven approach in computing the linear response statistics without knowing the explicit form of the underlying density function. However, we are still subject to the curse of dimensionality due to the usage of the tensor product, which is the major limitation of our method.
A Proof of Proposition 3.4

In this Appendix, we discuss the proof of Proposition 3.4 which specifies the RKHS $\mathcal{H}_\beta$ constructed using Mercer kernel in [19].

i. To begin with, notice that $\forall n \geq 0$, and $\forall x \in \mathbb{R}^d$,

$$\left| f_n(x) \right| \leq \sum_{n_1 \leq n} \left| \hat{f}_m \psi_{\beta, m} (x) \right| \leq \left( \sum_{n_0 \geq 0} \frac{\hat{f}_2^2}{\lambda_m} \right)^{\frac{1}{2}} \left( \sum_{n_0 \geq 0} \frac{\lambda_m \psi_{\beta, m}(x)^2}{\lambda_m} \right)^{\frac{1}{2}} = \left( \sum_{n_0 \geq 0} \frac{\hat{f}_2^2}{\lambda_m} \right)^{\frac{1}{2}} k_{\beta}^*(x, x), \quad (68)$$

and together with the decay rate [20], we have, by Eq. [24], $\{ f_n \} \subset C_0(\mathbb{R}^d)$. Following the same idea, for positive integers $n_2 > n_1$, and $\forall x \in \mathbb{R}^d$,

$$\left| f_{n_2}(x) - f_{n_1}(x) \right| \leq \sum_{n_1 < n_2 \leq n_2} \left| \hat{f}_m \psi_{\beta, m} (x) \right| \leq \left( \sum_{n_1 < n_2} \sum_{n_1 \leq n_2} \frac{\hat{f}_2^2}{\lambda_m} \right)^{\frac{1}{2}} k_{\beta}^*(x, x) \leq C_3 \left( \sum_{n_1 < \| n \|_1} \frac{\hat{f}_2^2}{\lambda_m} \right)^{\frac{1}{2}},$$

which, as a result of Eq. [24], implies that $\{ f_n \}$ is a Cauchy sequence in $C_0(\mathbb{R}^d)$, and $f_n$ uniformly converges to a function $f^* \in C_0(\mathbb{R}^d)$ satisfying

$$f^*(x) = \sum_{m \geq 0} \hat{f}_m \psi_{\beta, m}(x), \quad \forall x \in \mathbb{R}^d.$$

In particular,

$$\int_{\mathbb{R}^d} (f^*(x))^2 W^{1-2\beta}(x) \ dx = \sum_{m \geq 0} \hat{f}_m^2 < \infty,$$

that is, $f^* \in L^2(\mathbb{R}^d, W^{1-2\beta}) \subset C_0(\mathbb{R}^d)$.

ii. From the first result, we have learned that $\mathcal{H}_\beta$ [25] is a well-defined subspace of $L^2(\mathbb{R}^d, W^{1-2\beta}) \cap C_0(\mathbb{R}^d)$. With the positivity of $(\lambda_n)$, it is straightforward to show that $(\cdot, \cdot)$ defines an inner product on $\mathcal{H}_\beta$. We now prove $\mathcal{H}_\beta$ is closed with respect to the topology induced by the inner product $(\cdot, \cdot)$.

Take a Cauchy sequence $\{ f^{(n)} \} \subset \mathcal{H}_\beta$ with

$$f^{(n)} = \sum_{m \geq 0} \hat{f}^{(n)}_m \psi_{\beta, m}, \quad n = 1, 2, \ldots,$$

that is, $\forall \epsilon > 0$, there exists $N > 0$ such that $\forall n_1, n_2 > N$, we have $\| f^{(n_1)} - f^{(n_2)} \|_{\mathcal{H}_\beta} < \epsilon$. Here, $\| \cdot \|_{\mathcal{H}_\beta}$ denotes the norm induced by the inner product $(\cdot, \cdot)$. Since $\lambda_n \to 0$ as $n \to \infty$, we are able to show that $\{ f^{(n)} \}$ is also Cauchy in $L^2(\mathbb{R}^d, W^{1-2\beta})$. In particular, let $f^{(n)} \to f^*$ in $L^2(\mathbb{R}^d, W^{1-2\beta})$ with

$$f^* = \sum_{m \geq 0} \hat{f}^*_m \psi_{\beta, m}, \quad \lim_{n \to \infty} \hat{f}^{(n)}_m = \hat{f}^*_m, \quad \forall m \geq 0,$$

(69)

By Fatou’s Lemma, we have

$$\sum_{m \geq 0} \left( \frac{\hat{f}^*_m}{\lambda_m} \right)^2 \leq \liminf_{n \to \infty} \sum_{m \geq 0} \left( \frac{\hat{f}^{(n)}_m}{\lambda_m} \right)^2 = \liminf_{n \to \infty} \| f^{(n)} \|^2_{\mathcal{H}_\beta} < \infty,$$

which means $f^* \in \mathcal{H}_\beta$ with

$$f^*(x) = \sum_{m \geq 0} \hat{f}^*_m \psi_{\beta, m}(x), \quad \forall x \in \mathbb{R}^d,$$

is a bounded continuous function as a representative of $f^* \in L^2(\mathbb{R}^d, W^{1-2\beta})$.

Finally, we need to show that $f^{(n)} \to f^*$ in $\mathcal{H}_\beta$. We first claim that $\forall \epsilon > 0$, there exist positive integers $N_0$ and $M_0$ such that

$$\sum_{\| m \|_1 > M_0} \frac{\hat{f}^{(n)}_m^2}{\lambda_m} \leq \frac{\epsilon}{8}, \quad \forall n > N_0.$$

(70)
Simply notice that
\[
\sum_{\|\hat{m}\| > M_0} \left( \frac{\hat{f}^{(n)}_m}{\hat{\lambda}_m} \right)^2 = \sum_{\|\hat{m}\| > M_0} \left( \frac{\hat{f}^{(n)}_m - \hat{f}^{(N_0)}_m}{\hat{\lambda}_m} + \frac{\hat{f}^{(N_0)}_m}{\hat{\lambda}_m} \right)^2 \leq 2 \left\| f^{(n)} - f^{(N_0)} \right\|_{\mathcal{H}_\beta}^2 + 2 \sum_{\|\hat{m}\| > M_0} \left( \frac{\hat{f}^{(N_0)}_m}{\hat{\lambda}_m} \right)^2,
\]
and, by the fact that \( \{f^{(n)}\} \) is Cauchy in \( \mathcal{H}_\beta \), we first pick \( N_0 \) large enough such that
\[
2 \left\| f^{(n)} - f^{(N_0)} \right\|_{\mathcal{H}_\beta}^2 \leq \frac{\epsilon}{16}, \quad \forall n > N_0.
\]
Then, from \( f^{(N_0)} \in \mathcal{H}_\beta \), we pick \( M_0 \) large enough such that
\[
2 \sum_{\|\hat{m}\| > M_0} \left( \frac{\hat{f}^{(N_0)}_m}{\hat{\lambda}_m} \right)^2 \leq \frac{\epsilon}{16}.
\]
Meanwhile, since \( f^1 \in \mathcal{H}_\beta \), there exists a positive integer \( M_1 \) such that
\[
\sum_{\|\hat{m}\| > M_1} \left( \frac{\hat{f}^{(n)}_m}{\hat{\lambda}_m} \right)^2 \leq \frac{\epsilon}{8}. \tag{71}
\]
Fix \( M = \max\{M_0, M_1\} \), we decompose \( \left\| f^1 - f^{(n)} \right\|_{\mathcal{H}_\beta}^2 \) as follows,
\[
\left\| f^1 - f^{(n)} \right\|_{\mathcal{H}_\beta}^2 = \sum_{\|\hat{m}\| \leq M} \left( \frac{\hat{f}^1_m - \hat{f}^{(n)}_m}{\hat{\lambda}_m} \right)^2 + \sum_{\|\hat{m}\| > M} \left( \frac{\hat{f}^1_m - \hat{f}^{(n)}_m}{\hat{\lambda}_m} \right)^2,
\]
and, by the convergence of \( \hat{f}^{(n)}_m \), there exists a positive integer \( N_1 \) such that
\[
\sum_{\|\hat{m}\| \leq M} \left( \frac{\hat{f}^1_m - \hat{f}^{(n)}_m}{\hat{\lambda}_m} \right)^2 < \frac{\epsilon}{2}, \quad \forall n > N_1. \tag{72}
\]
Finally, take \( N = \max\{N_0, N_1\} \), combining (70), (71), and (72), and \( \forall n > N \) we have
\[
\left\| f^1 - f^{(n)} \right\|_{\mathcal{H}_\beta}^2 < \frac{\epsilon}{2} + \sum_{\|\hat{m}\| > M} \left( \frac{\hat{f}^1_m - \hat{f}^{(n)}_m}{\hat{\lambda}_m} \right)^2 \leq \frac{\epsilon}{2} + 2 \sum_{\|\hat{m}\| > M} \left( \frac{\hat{f}^{(n)}_m}{\hat{\lambda}_m} \right)^2 + 2 \sum_{\|\hat{m}\| > M} \left( \frac{\hat{f}^1_m}{\hat{\lambda}_m} \right)^2 < \epsilon,
\]
that is, \( f^{(n)} \to f^1 \) in \( \mathcal{H}_\beta \).

iii With all the preparation work we have done so far, the reproducing property (10) of \( \mathcal{H}_\beta \) becomes almost trivial. For any fixed \( x_0 \in \mathbb{R}^d \), \( k_\beta(\cdot, x_0) \in \mathcal{H}_\beta \). From (21),
\[
\langle k_\beta(\cdot, x_0), k_\beta(\cdot, x_0) \rangle = \sum_{\hat{m} \in \mathbb{Z}^d} \hat{\lambda}_m \Psi_{\hat{\omega}_\beta, \hat{m}}^2 (x_0) = k_\beta(x_0, x_0) < \infty,
\]
which means, \( \forall f \in \mathcal{H}_\beta \), the inner product \( \langle f, k_\beta(\cdot, x_0) \rangle \) is well-defined \( \forall x_0 \in \mathbb{R}^d \). In particular, we have
\[
\langle f, k_\beta(\cdot, x_0) \rangle = \sum_{\hat{m} \in \mathbb{Z}^d} \hat{f}_{\hat{m}} \Psi_{\hat{\omega}_\beta, \hat{m}} (x_0) = f(x_0),
\]
which leads to the reproducing property.

### B Proof of Lemma 3.6

In this Appendix we discuss the proof of Lemma 3.6 which provides a class of bounded kernel based on Laguerre polynomials. As prerequisites, we need the notions of the Bessel and modified Bessel functions.

We focus on the (first kind) Bessel functions of integer order [31][32], which can be defined as
\[
J_\theta(z) = \sum_{m=0}^{\infty} \frac{(-1)^m (z/2)^{\theta+2m}}{m! (m + \theta + 1)}, \quad \theta = 0, 1, \ldots, \quad z \in \mathbb{C},
\]
where \( \Gamma(\cdot) \) denotes the Gamma function. For \( \arg z \in \left( -\frac{\pi}{2}, \frac{3\pi}{2} \right) \), we have the following asymptotic expansion (Eq. (1.71.9) of [32])
\[
i^\theta J_\theta(-i z) = (2 \pi z)^{-\frac{1}{2}} \left[ e^{i z} - (-1)^\theta i e^{-z} \right] \left( 1 + O(|z|^{-1}) \right), \quad |z| \to \infty,
\]
which plays a critical role in proving the boundedness of the kernel. The modified Bessel functions (of the first kind) [31] satisfies,
\[
I_\theta(z) = i^{-\theta} J_\theta(i z), \quad \theta = 0, 1, \ldots
\]
To prove Lemma 3.6, we first introduce Hille-Hardy formula [30], for \( \rho \in (0, 1), \)
\[
\sum_{m=0}^{\infty} \rho^m \ell_m^{(\theta)}(x) \ell_m^{(\theta)}(y) G^{(2)}(x; \theta) G^{(2)}(y; \theta) = \frac{\rho^{\frac{1}{2} \theta}}{1 - \rho} \exp \left[ -\frac{1}{2} (x + y) \frac{1 + \rho}{1 - \rho} \right] I_\theta \left( \frac{2 \sqrt{x y \rho}}{1 - \rho} \right), \quad \theta = 0, 1, \ldots,
\]
where \( \{\ell_m^{(\theta)}\} \) denote the normalized Laguerre polynomials with respect to the Gamma distribution \( G(x; \theta) \propto x^\theta e^{-x} \). A mordern proof of the Hille-Hardy formula can be found in [31]. For general \( d \)-dimensional case, by Eq. (75), the Mercer-type kernel defined by [36] satisfies
\[
k_{\rho, \theta}(x, y) = \prod_{i=1}^{d} \sum_{m=0}^{\infty} \rho^m \ell_m^{(\theta)}(x_i) \ell_m^{(\theta)}(y_i) G^{(\beta)}(x_i; \theta_i) G^{(\beta)}(y_i; \theta_i)
\]
\[
= \prod_{i=1}^{d} \rho^{\frac{1}{2} \theta_i} \exp \left[ -\frac{1}{2} (x_i + y_i) \frac{1 + \rho}{1 - \rho} \right] \left( \frac{2 \sqrt{x_i y_i \rho}}{1 - \rho} \right), \quad \theta = 0, 1, \ldots,
\]
To prove the boundedness of the kernel \( k_{\rho, \theta}(x, y) \) in [36], it is enough to show that the one-dimensional kernel \( k_{\rho, \theta}(x, y) \) is bounded \( \forall \rho \in (0, 1) \) and \( \forall \theta \in (0, 1, \ldots) \). Notice that by Eq. (75), (73), and (74), we have
\[
\left| k_{\rho, \theta}(x, x) \right| \propto \exp \left[ -x \frac{1 + \rho}{1 - \rho} \left( \frac{2 \sqrt{x \rho}}{1 - \rho} \right) \right] = \exp \left[ -x \frac{1 + \rho}{1 - \rho} \right] \left( \frac{2 \sqrt{x \rho}}{1 - \rho} \right),
\]
where \( z = \frac{2 \sqrt{\rho}}{1 - \rho} > 0 \). Thus, for \( x \) large, \( \left| k_{\rho, \theta}(x, x) \right| \) yields the following asymptotic expansion,
\[
\left| k_{\rho, \theta}(x, x) \right| \propto \exp \left[ -x \frac{1 + \rho}{1 - \rho} \right] \exp \left[ \frac{2 \sqrt{x \rho}}{1 - \rho} \left( O \left( x^{\frac{1}{2}} \right) + O \left( x^{-\frac{1}{2}} \right) \right) \right],
\]
\[
= \exp \left[ -x \frac{1 - \sqrt{\rho}}{1 + \sqrt{\rho}} \right] \left( O \left( x^{\frac{1}{2}} \right) + O \left( x^{-\frac{1}{2}} \right) \right) \to 0,
\]
as \( x \to +\infty \) since \( \frac{1 - \sqrt{\rho}}{1 + \sqrt{\rho}} > 0 \). Thus, the kernel \( k_{\rho, \theta}(x, y) \) in [36] is bounded \( \forall \rho \in (0, 1), \beta \geq \frac{1}{2}, \) and \( \theta \in (0, 1, 2, \ldots) \). In particular, notice that \( \frac{1 - \sqrt{\rho}}{1 + \sqrt{\rho}} \to 0 \) as \( \rho \to 1^{-} \), the expansion (76) suggests that \( \frac{1}{2} \) is indeed the lower bound for \( \beta \) to ensure the boundedness \( \forall \rho \in (0, 1) \). On the other hand, for a fix \( \rho \in (0, 1) \), the kernel \( k_{\rho, \theta}(x, y) \) is bounded for \( \beta \geq \frac{1}{2} \). Figure 5 evaluates the kernel \( k_{\rho, \theta}(x, y) \) under \( \rho = 0.64, \theta = 1 \), and three different values of \( \beta \). The graph does support the asymptotic expansion (76).

C Proof of Proposition 4.3

Here we discuss the proof of Proposition 4.3 which provides an error bound for the empirical kernel embedding estimate \( f_{M,N} \) in [43]. To begin with, let’s briefly review the concept of \( \alpha \)-mixing process and the corresponding Davydov’s covariance inequality [18]. Given a stationary process \( \{X_n\}_{n=1}^{\infty} \), let \( \mathcal{F}_a^b \) (\( a < b \leq \infty \)) denote the \( \sigma \)-algebra generated by \( \{X_n, a \leq n \leq b\} \). We say \( \{X_n\} \) is \( \alpha \)-mixing if
\[
\alpha(k) := \sup_n \sup_{A \in \mathcal{F}_a^b, B \in \mathcal{F}_{a+k}} |\mathbb{P}(AB) - \mathbb{P}(A)\mathbb{P}(B)| \to 0, \quad k \to \infty,
\]
\[24\]
where $\alpha(k)$ is known as the $\alpha$-mixing coefficient. Such condition imposes restrictions on $X_n$ amounting to a weak interdependence of the beginning and the end of the process. Davydov’s covariance inequality states

$$|\text{cov}(h(X_1), h(X_{1+k}))| \leq 12\alpha(k)^{1/2} \left[ \mathbb{E} \left[ \left| h(X_1) \right|^{p/2} \right] \right]^{1/p} \left[ \mathbb{E} \left[ \left| h(X_1) \right|^{q/2} \right] \right]^{1/q},$$

where $1/r + 1/p + 1/q = 1$ given $\mathbb{E}[|h(X_1)|^p]$ and $\mathbb{E}[|h(X_1)|^q]$ exist.

To begin with, by the orthogonality of $\{\Psi_i, \phi_i\}$ over $L^2(\mathbb{R}^d, W^{1-\beta})$, we split the error $\|f - f_{M,N}\|_{L^2(W^{1-\beta})}^2$ into two parts,

$$\|f - f_{M,N}\|_{L^2(W^{1-\beta})}^2 = \sum_{|\vec{m}|1 \leq M} (\hat{f}_{\vec{m}} - f_{\vec{m},N})^2 + \sum_{|\vec{m}|1 > M} f_{\vec{m}}^2,$$

where the first term on the right-hand side can be interpreted as the “estimation error” introduced by approximating the coefficient $\hat{f}_{\vec{m}}$ using a Monte-Carlo sum (42); while the second term is the “approximation error” (or bias) caused by the truncation.

For the bias term, with $f \in \mathcal{H}_{\beta,\rho}$ and Eq. (31), we have

$$\sum_{|\vec{m}|1 \leq M} (\hat{f}_{\vec{m}} - f_{\vec{m},N})^2 \leq \rho^{M+1} \sum_{|\vec{m}|1 \geq M} \frac{f_{\vec{m}}^2}{\rho |\vec{m}|1} \leq \rho^{M+1} \|f\|_{\mathcal{H}_{\beta,\rho}}^2. \quad (78)$$

For the estimation error, notice that $\hat{f}_{\vec{m},N}$ in (42) is an unbiased estimator of $\hat{f}_{\vec{m}}$, and we have

$$\mathbb{E} \left[ \sum_{|\vec{m}|1 < M} (\hat{f}_{\vec{m}} - f_{\vec{m},N})^2 \right] = \sum_{|\vec{m}|1 < M} \mathbb{E} \left[ \frac{1}{N} \sum_{i=1}^N \psi_{\vec{m}}(X_i) W^{1-\beta}(X_i) - \frac{\hat{f}_{\vec{m}}}{N} \right]^2 \leq \frac{1}{N^2} \sum_{|\vec{m}|1 \leq M} \sum_{i, j=1}^N \text{cov} \left( \psi_{\vec{m}}(X_i) W^{1-\beta}(X_i), \psi_{\vec{m}}(X_j) W^{1-\beta}(X_j) \right).$$

Introduce $h_{\vec{m}} := \psi_{\vec{m}} W^{1-\beta}$. Since $\{X_n\}$ is stationary, the estimation error can be bounded by

$$\mathbb{E} \left[ \sum_{|\vec{m}|1 \leq M} (\hat{f}_{\vec{m}} - f_{\vec{m},N})^2 \right] \leq \frac{1}{N} \sum_{|\vec{m}|1 \leq M} \left[ \text{var} \left( h_{\vec{m}}(X_1) \right) + 2 \sum_{k=1}^{N-1} \text{cov} \left( h_{\vec{m}}(X_1), h_{\vec{m}}(X_1+k) \right) \right], \quad (79)$$

where the covariance terms represent the non-i.i.d. feature of $\{X_i\}$. To bound the variance term in (79), consider

$$\text{var} \left( h_{\vec{m}}(X_1) \right) \leq \int_{\mathbb{R}^d} h_{\vec{m}}^2(x) f(x) \, dx = \int_{\mathbb{R}^d} \psi_{\vec{m}}^2(x) W^{2-2\beta}(x) f(x) \, dx. \quad (80)$$

**Figure 5:** Graph of $k_{\beta,\rho,\theta}(x, x)$ in (36) for $\beta = 0.42$ (blue-solid), $\beta = 0.45$ (red-dot-dash), and $\beta = 0.48$ (yellow-dash). Notice that for $p = 0.64$, to ensure the boundedness, we need $\beta \geq \frac{0.8}{1+0.8} \approx 0.44$, which is consistent with the numerical results.
Moreover, by the decay rate of $f$ and the assumption $\beta \in \left[\frac{1}{2}, \frac{1}{\beta+1}\right]$, we have a new decay rate for $f \in H_{\beta+1}$,

$$
\left| f(x) \right| \leq (2\pi)^{\beta+1/2} \left( 1 - \rho^2 \right)^{-\beta/2} \left\| f \right\|_{H_{\beta+1}} W^{2\beta-1}(x).
$$

(81)

Let $C_f := (2\pi)^{\beta+1/2} \left( 1 - \rho^2 \right)^{-\beta/2} \left\| f \right\|_{H_{\beta+1}}$, and the variance in Eq. (80) can be further bounded by

$$
\text{var}(h_{\tilde{m}_1}(X_1)) \leq C_f \int \psi_{\tilde{m}_1}(x)^2 W(x) \, dx = C_f.
$$

To bound the covariance term in (79), we apply the Davydov’s covariance inequality for $h = h_{\tilde{m}_1}$, Set $p = q = 2 + \epsilon$ in (77) for $\epsilon \in (0, 2)$, we have

$$
|\text{cov}(h_{\tilde{m}_1}(X_1), h_{\tilde{m}_1}(X_{1+k}))| \leq 12\alpha(k) \frac{1}{\sqrt{2\pi}} \left( \text{E} \left[ \left| h_{\tilde{m}_1}(X_1)^2 \right| \right] \right)^{1/2} \leq 12\alpha(k) \frac{1}{\sqrt{2\pi}} \left( \text{E} \left[ h_{\tilde{m}_1}(X_1)^4 \right] \right)^{1/2},
$$

(82)

where we have used Jensen’s inequality in the last step.

To bound the fourth moment involved in (82), we introduce the following expansion formula for normalized Hermite polynomials.

$$
\psi_{\tilde{m}_1} = \sum_{r=0}^{m_1} 2^{-r} \binom{m_1}{r} \sqrt{(2m_1-2r)!} (m-r)! \psi_{2m-2r}.
$$

Then, together with the decay rate of $f$ in (81), the fourth moment in (82) can be bounded by

$$
\text{E} \left[ h_{\tilde{m}_1}(X_1)^4 \right] = \int \psi_{\tilde{m}_1}(x)^4 W^{4-4\beta}(x) \, dx \leq C_f \int \psi_{\tilde{m}_1}(x)^4 W^{3-2\beta}(x) \, dx \leq C_f \int \psi_{\tilde{m}_1}(x) W(x) \, dx = C_f.
$$

(83)

To simplify the upper bound in (83), recall the Stirling’s approximation of the factorials

$$
\sqrt{2\pi n^{n+1/2}} e^{-n} \leq n! \leq n^{n+1/2} e^{-n},
$$

which leads to

$$
\frac{\sqrt{(2\ell)!}}{\ell!} \leq \sqrt{\frac{e}{2\pi}} \left( \frac{2\ell}{e} \right)^{\ell+1/2} < 2^\ell.
$$

As a result, the summation in eq. (83) can be controlled by

$$
\sum_{r=0}^{m_1/2} 2^{-2r} \binom{m_1}{r} \frac{(2m_1-2r)!}{((m_1-r)!)^2} \leq \sum_{r=0}^{m_1/2} \binom{m_1}{r} 2^{2m_1-4r} < 2^{2m_1} \left( \sum_{r=0}^{m_1/2} \binom{m_1}{r} \left( \frac{1}{4} \right)^r \right)^2 = \left( \frac{5}{2} \right)^{2m_1}.
$$

(84)

Combine (82), (83) and (84) together, and we have

$$
|\text{cov}(h_{\tilde{m}_1}(X_1), h_{\tilde{m}_1}(X_{1+k}))| \leq 12\alpha(k) \frac{1}{\sqrt{2\pi}} C_f \left( \frac{5}{2} \right)^{\|\tilde{m}_1\|_1}.
$$

Finally notice that for a positive integer $j$ the total number of different $d$-dimensional multi-indices such that $\|\tilde{m}_1\|_1 = j$ is \binom{j+d-1}{d-1} and

$$
\frac{j + d - 1}{d - 1} = \left( \frac{j + 1}{d - 1} \right) \cdots \left( \frac{j + d - 1}{d - 1} \right) < \left( \frac{j + d - 1}{d - 1} \right)^{d-1} = \left( \frac{5}{2} \right)^{d-3},
$$

then the estimation error in (79) can be bounded by

$$
\text{E} \left[ \sum_{\|\tilde{m}_1\|_1 \leq M} \left( \hat{f}_{\tilde{m}_1} - \tilde{f}_{\tilde{m}_1} \right)^2 \right] \leq \frac{1}{N} \left[ (M+1)^d C_f + 24 C_f \left( \sum_{k=1}^{N-1} \alpha(k) \frac{1}{\sqrt{2\pi}} \left( \text{E} \left[ \left| h_{\tilde{m}_1}(X_1)^2 \right| \right] \right)^{1/2} \right) \right],
$$

(85)

where we have used the assumption (54). With $d \leq \frac{5}{2} M + 1$, the summation in (85) can be bounded by

$$
\sum_{j=0}^{M} \left( \frac{5}{2} \right)^{j-d+3} < (M + d - 1)^{d-1} M \sum_{j=0}^{M} \left( \frac{5}{2} \right)^{j-d+3} \leq M^{d-1} \sum_{j=0}^{M} \left( \frac{5}{2} \right)^{j+2} < M^{d-1} \left( \frac{5}{2} \right)^{M+3},
$$

which leads to

$$
\text{E} \left[ \sum_{\|\tilde{m}_1\|_1 \leq M} \left( \hat{f}_{\tilde{m}_1} - \tilde{f}_{\tilde{m}_1} \right)^2 \right] < \frac{1}{N} \left[ (M+1)^d C_f + 24 C_f \left( \frac{5}{2} \right)^{M+3} \right],
$$

(86)

and, together with (79), we obtain the error bound in (55).
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