Density Estimation in Infinite Dimensional Exponential Families

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Abstract

In this paper, we consider an infinite dimensional exponential family, \( \mathcal{P} \) of probability densities, which are parametrized by functions in a reproducing kernel Hilbert space, \( \mathcal{H} \) and show it to be quite rich in the sense that a broad class of densities on \( \mathbb{R}^d \) can be approximated arbitrarily well in Kullback-Leibler (KL) divergence by elements in \( \mathcal{P} \). The main goal of the paper is to estimate an unknown density, \( p_0 \) through an element in \( \mathcal{P} \). Standard techniques like maximum likelihood estimation (MLE) or pseudo MLE (based on the method of sieves), which are based on minimizing the KL divergence between \( p_0 \) and \( \mathcal{P} \), do not yield practically useful estimators because of their inability to efficiently handle the log-partition function. Instead, we propose an estimator, \( \hat{p}_n \) based on minimizing the Fisher divergence, \( J(p_0||p) \) between \( p_0 \) and \( p \in \mathcal{P} \), which involves solving a simple finite-dimensional linear system. When \( p_0 \in \mathcal{P} \), we show that the proposed estimator is consistent, and provide a convergence rate of \( n^{-\min\left\{ d, \frac{d+1}{\beta+1}\right\}} \) in Fisher divergence under the smoothness assumption that \( \log p_0 \in \mathcal{R}(C^\beta) \) for some \( \beta \geq 0 \), where \( C \) is a certain Hilbert-Schmidt operator on \( \mathcal{H} \) and \( \mathcal{R}(C^\beta) \) denotes the image of \( C^\beta \). We also investigate the misspecified case of \( p_0 \notin \mathcal{P} \) and show that \( J(p_0||\hat{p}_n) \to \inf_{p \in \mathcal{P}} J(p_0||p) \) as \( n \to \infty \), and provide a rate for this convergence under a similar smoothness condition as above. Through numerical simulations we demonstrate that the proposed estimator outperforms the non-parametric kernel density estimator, and that the advantage with the proposed estimator grows as \( d \) increases.

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1 Introduction

Exponential families are among the most important classes of parametric models studied in statistics. In its “natural form”, the family generated by a probability density \( q_0 \) (defined over \( \Omega \subseteq \mathbb{R}^d \)) is defined as

\[
\mathcal{P}_{\text{fin}} := \left\{ p_0(x) = q_0(x)e^{\theta^T T(x) - A(\theta)}, x \in \Omega : \theta \in \Theta \subseteq \mathbb{R}^m \right\}
\]

(1)

where \( A(\theta) := \log \int_{\Omega} e^{\theta^T T(x)} q_0(x) \, dx \) is the cumulant generating function (also called the log-partition function), \( \Theta \subset \{ \theta \in \mathbb{R}^m : A(\theta) < \infty \} \) is the natural parameter space, \( \theta \) is a finite-dimensional vector called the natural parameter, and \( T(x) \) is a finite-dimensional vector of statistics called the sufficient statistic.

In this paper, we consider the following infinite dimensional generalization \([7,14]\) of \([1]\) as

\[
\mathcal{P} = \left\{ p_f(x) = e^{f(x) - A(f)} q_0(x), x \in \Omega : f \in \mathcal{F} \right\}
\]

(2)

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where the function space $\mathcal{F}$ is defined as
\[
\mathcal{F} = \left\{ f \in \mathcal{H} : A(f) := \log \int_{\Omega} e^{f(x)} q_0(x) \, dx < \infty \right\},
\]

$A(f)$ is the cumulant generating function and $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ is a reproducing kernel Hilbert space (RKHS) with $k$ as its reproducing kernel (see Section 2 for definitions, and a more detailed introduction to the RKHS). While various generalizations are possible for different choices of $\mathcal{F}$ (e.g., Orlicz space as in [24]), the connection of $\mathcal{P}$ to the natural exponential family in [14] is particularly enlightening when $\mathcal{H}$ is an RKHS. This is due to the reproducing property of the kernel, $f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}}$, through which $k$ takes the role of the sufficient statistic. In fact, it can be shown (Section 3 and Example 1 for more details) that every $\mathcal{P}_{\text{fin}}$ is generated by $\mathcal{P}$ induced by a finite dimensional RKHS $\mathcal{H}$, and therefore the family $\mathcal{P}$ with $\mathcal{H}$ being an infinite dimensional RKHS is a natural infinite dimensional generalization to $\mathcal{P}_{\text{fin}}$. Furthermore, this generalization is interesting from the point of view of applications in statistics. For example, the first and second Fréchet derivatives of $A(f)$ yield a mean element and covariance operator in $\mathcal{H}$ (see Section 1.2.3 of [Fukumizu-09a]). The mean and covariance operators have found many applications in nonparametric hypothesis testing [20, 18] and dimensionality reduction [16, 17]. The family $\mathcal{P}$ has also found interest in Bayesian non-parametric density estimation where the densities in $\mathcal{P}$ are chosen as a prior distribution on a collection of probability densities (e.g., see [10]).

Having motivated the appropriateness of the infinite dimensional generalization, the goal of this paper is to perform statistical estimation in $\mathcal{P}$ when $\mathcal{H}$ is an infinite dimensional RKHS. Formally, given i.i.d. random samples $(X_i)_{i=1}^n$ drawn from an unknown density, $p_0$, the goal is to estimate $p_0$ through $\mathcal{P}$. Throughout the paper, we refer to case of $p_0 \in \mathcal{P}$ as well-specified in contrast to the misspecified case where $p_0 \notin \mathcal{P}$. The problem is interesting and useful because it can be shown that $\mathcal{P}$ is a rich class of densities (depending on the choice of $k$ and therefore $\mathcal{H}$) that can approximate a broad class of probability densities arbitrarily well (see Propositions 1, 13 and Corollary 2). This implies that instead of using non-parametric density estimation methods (e.g., kernel density estimation (KDE)) to estimate the class of densities mentioned in Propositions 1, 13 and Corollary 2 it is reasonable to estimate densities in $\mathcal{P}$. In the finite-dimensional case where $\theta \in \Theta \subset \mathbb{R}^m$, estimating $p_0$ through maximum likelihood (ML) leads to solving elegant likelihood equations ([3] Chapter 5). However, in the infinite dimensional case (assuming $p_0 \in \mathcal{P}$), as in many non-parametric estimation methods, a straightforward extension of maximum likelihood estimation (MLE) suffers from the problem of ill-posedness ([14] Section 1.3.1).

To address the above problem, [14] proposed a sieves method involving pseudo-MLE by restricting the infinite dimensional manifold $\mathcal{P}$ to a series of finite-dimensional submanifolds, which enlarge as the sample size increases, i.e., $p_{f(l)}$ is the density estimator with $\hat{f}(l) = \arg \max_{f \in \mathcal{F}(l)} \frac{1}{n} \sum_{i=1}^n f(X_i) - A(f)$ where $\mathcal{F}(l) = \{ f \in \mathcal{H}(l) : A(f) < \infty \}$ and $(\mathcal{H}(l))_{l=1}^{\infty}$ is a sequence of finite-dimensional subspaces of $\mathcal{H}$ such that $\mathcal{H}(l) \subset \mathcal{H}(l+1)$ for all $l \in \mathbb{N}$. While the consistency of $p_{f(l)}$ is proved in Kullback-Leibler (KL) divergence ([14] Theorem 6), the method suffers from many drawbacks that are both theoretical and computational in nature. On the theoretical front, the consistency in [14] Theorem 6] is established by assuming a decay rate on the eigenvalues of the covariance operator (see (A-2) and the discussion in Section 1.4 of [14] for details), which is usually difficult to check in practice. Moreover, it is not clear which classes of RKHS should be used to obtain a consistent estimator ([14] (A-1)]. In addition, the paper does not provide any discussion about the convergence rates. On the practical side, the estimator is not attractive as it can be quite difficult to construct the sequence $(\mathcal{H}(l))_{l=1}^{\infty}$ that satisfies the assumptions in [14] Theorem 6]. In fact, the impracticality of the estimator, $\hat{f}(l)$ is accentuated by the difficulty in efficiently handling $A(f)$ (though it can be approximated by numerical integration).

A related work was carried out by Barron and Sheu [2] (see also references therein) where the goal is to estimate a density, $p_0$ by approximating its logarithm as an expansion in terms of basis functions, such as polynomials, splines or trigonometric series. Similar to [14], Barron and Sheu proposed the ML estimator, $p_{f_m}$ where $f_m = \arg \max_{f \in \mathcal{F}_m} \frac{1}{n} \sum_{i=1}^n f(X_i) - A(f)$ and $\mathcal{F}_m$ is the linear space of dimension $m$ spanned by the chosen basis functions. Under the assumption that $\log p_0$ has $r$ square-integrable derivatives, they showed that $KL(p_0\|p_{f_m}) = O_p(n^{-2r/(2r+1)})$ with $m = n^{1/(2r+1)}$ for each of the approximating families, where $KL(p\|q) = \int p(x) \log(p(x)/q(x)) \, dx$ is the KL divergence between $p$ and $q$. Though these results are theoretically interesting, the estimator is obtained from a procedure similar to that in [14], and therefore suffers from the practical drawbacks discussed above.

The discussion so far shows that the ML approach to estimate $p_0 \in \mathcal{P}$ results in estimators that are of limited practical interest. To alleviate this, one can treat the problem of estimating $p_0 \in \mathcal{P}$ in a completely non-parametric
fashion (ignoring the parametrization of \( p_0 \)) by using KDE, which is well-studied \([38\text{ Chapter 1}]\) and easy to implement. This approach ignores the structure of \( \mathcal{P} \), however, and is known to perform poorly for moderate to large \( d \) \([42\text{ Section 6.5}]\) (see also Section 6 of this paper).

1.1 Score matching and Fisher divergence

To counter the disadvantages of KDE and pseudo-MLE, in this paper, we propose to use the score matching method introduced by Hyv"{a}rinen \([21, 22]\), which provides an efficient way to address the problem at hand. While MLE is based on minimizing the KL divergence, the score matching method involves minimizing the Fisher divergence (also called the Fisher information distance; see Definition 1.13 in \([23]\)) between two continuously differentiable densities, \( p \) and \( q \) on an open set \( \Omega \subset \mathbb{R}^d \), given as

\[
J(p||q) = \frac{1}{2} \int p(x) \left\| \frac{\partial \log p(x)}{\partial x} - \frac{\partial \log q(x)}{\partial x} \right\|^2_2 \, dx,
\]

where \( \frac{\partial \log p(x)}{\partial x} = \left( \frac{\partial \log p(x)}{\partial x_1}, \ldots, \frac{\partial \log p(x)}{\partial x_d} \right) \). Fisher divergence is closely related to the KL divergence through de Bruijn’s identity \([23\text{ Appendix C}]\) and it can be shown that \( KL(p||q) = \int_0^\infty J(p_t||q_t) \, dt \), where \( p_t = p \ast N(0, tI_d) \), \( q_t = q \ast N(0, tI_d) \), \( \ast \) denotes the convolution and \( N(0, tI_d) \) denotes a normal distribution on \( \mathbb{R}^d \) with mean zero and diagonal covariance with \( t > 0 \) (see Proposition 8.1 in Section 8.1 for a precise statement; also see \([26\text{ Theorem 1}]\)). Moreover, convergence in Fisher divergence is a stronger form of convergence than that in KL, total variation and Hellinger distances \([23\text{ Lemmas E.2 & E.3}, 25\text{ Corollary 5.1}]\).

To understand the advantages associated with the score matching method, let us consider the problem of density estimation where the data generating distribution (say \( p \)) is unknown (as a function of \( \theta \)), see Theorem 1 Hyvarinen-05 under the condition that \( p \) is differentiable (w.r.t. \( x \)) and \( \int p_0(x)\left\| \frac{\partial \log p_0(x)}{\partial x} \right\|^2_2 \, dx < \infty \), \( \forall \theta \in \Theta \), \( J(p_0||p_0) =: J(\theta) \) in \((3)\) reduces to

\[
J(\theta) = \sum_{i=1}^d \int p_0(x) \left( \frac{1}{2} \left( \frac{\partial \log p_0(x)}{\partial x_i} \right)^2 + \frac{\partial^2 \log p_0(x)}{\partial x_i^2} \right) \, dx + J(p_0||1),
\]

through partial integration \([?, \text{ see[Theorem 1]Hyvarinen-05}]\) under the condition that \( p_0(x)\frac{\partial \log p_0(x)}{\partial x_i} \to 0 \) as \( x_i \to \pm \infty \), \( \forall i = 1, \ldots, d \). The main advantage of the objective in \((3)\) (and also \((4)\)) is that when it is applied to the situation discussed above where \( p_\theta(x) = \frac{r_\theta(x)}{A(\theta)} \), \( J(\theta) \) is independent of \( A(\theta) \) and an estimate of \( \theta_0 \) can be obtained by simply minimizing the empirical counterpart of \( J(\theta) \), given by

\[
J_n(\theta) := \frac{1}{n} \sum_{a=1}^n \sum_{t=1}^d \left( \frac{1}{2} \left( \frac{\partial \log p_\theta(X_{a,t})}{\partial x_i} \right)^2 + \frac{\partial^2 \log p_\theta(X_{a,t})}{\partial x_i^2} \right) + J(p_0||1).
\]

Since \( J_n(\theta) \) is also independent of \( A(\theta) \), \( \hat{\theta}_n = \arg \min_{\theta \in \Theta} J_n(\theta) \) may be easily computable, unlike the MLE. We would like to highlight that while the score matching approach may have computational advantages over MLE, it only estimates \( p_0 \) up to the scaling factor \( A(\theta) \), and therefore requires the approximation or computation of \( A(\theta) \) through numerical integration to estimate \( p_0 \) (note that this issue exists even with MLE but not with KDE).

1.2 Contributions

(i) The main results of this paper regarding the estimation of \( p_0 \in \mathcal{P} \) (well-studied case) through the minimization of Fisher divergence are presented in Section 3. First, we show that estimating \( p_0 := p_{f_0} \) using the score matching method
reduces to estimating \( f_0 \) by solving a simple finite-dimensional linear system (Theorems 3, 4). Hyvärinen [22] obtained a similar result for \( \mathcal{F}_n \) where the estimator is obtained by solving a linear system, which in the case of Gaussian family matches the MLE [21]. The estimator obtained in the infinite dimensional case is not a simple extension of its finite-dimensional counterpart, however, as the former requires an appropriate regularizer (we use \( \| \cdot \|_p^2 \) to make the problem well-posed. Moreover, it is not straightforward to show that the estimator in the infinite dimensional setting can be obtained by solving a finite-dimensional linear system (see Theorem 4).

(ii) In contrast to [22] where no guarantees on consistency or convergence rates are provided for the density estimator in \( \mathcal{F}_n \), we establish in Theorem 3 the consistency and rates of convergence for the proposed estimator of \( f_0 \), and use these to prove consistency and rates of convergence for the corresponding plug-in estimator of \( p_0 \) (Theorems 6, 7), even when \( \mathcal{H} \) is infinite dimensional. An interesting aspect of these results is that while the estimator of \( f_0 \) (and therefore \( p_0 \)) is obtained by minimizing the Fisher divergence, the resultant density estimator is shown to be consistent in KL divergence (and therefore in Hellinger and total-variation distances) and we provide convergence rates in all these distances.

Formally, we show that if \( f_0 \in \mathcal{R}(C^\beta) \) for some \( \beta > 0 \), then \( \| f_0 - \hat{f}_n \|_{2\mathcal{H}} = O_p(n^{-\alpha}), \ KL(p_0\|p_{\hat{f}_n}) = O_p(n^{-2\alpha}) \) and \( J(p_0\|p_{\hat{f}_n}) = O_p\left(n^{-\min\left\{\frac{d}{2},\frac{2\beta+1}{2\beta+2}\right\}}\right) \), where \( \alpha = \min\{\frac{1}{4},\frac{\beta}{2\beta+2}\} \), \( \hat{f}_n \) is the proposed estimator, \( \mathcal{R}(A) \) denotes the range or image of an operator, \( A, C : = \sum_{i=1}^d \int \frac{\partial^k i(x)}{\partial x_i} \otimes \frac{\partial^k i(x)}{\partial x_i} p_0(x) \, dx \) is a Hilbert-Schmidt operator on \( \mathcal{H} \) (see Theorem 5), with \( k \) being the r.k. and \( \otimes \) denotes the tensor product. When \( \mathcal{H} \) is a finite-dimensional RKHS, we show that the estimator enjoys parametric rates of convergence, i.e., \( \| f_0 - \hat{f}_n \|_{2\mathcal{H}} = O_p(n^{-1/2}), \ KL(p_0\|p_{\hat{f}_n}) = O_p(n^{-1}) \) and \( J(p_0\|p_{\hat{f}_n}) = O_p(n^{-1}) \). Note that the convergence rates are obtained under a non-classical smoothness assumption on \( f_0 \), namely that it lies in the image of certain fractional power of \( C \), which reduces to a more classical assumption if we choose \( k \) to be a Matérn kernel (see Section 2 for its definition) as it induces a Sobolev space. In Section 1.2 we discuss in detail the smoothness assumption on \( f_0 \) for the choice of Gaussian (Example 2) and Matérn (Example 3) kernels. Another interesting point to observe is that unlike in the classical function estimation methods (e.g., kernel density estimation and regression), the rates presented above for the proposed estimator tend to saturate for \( \beta > 1 \) (\( \beta > 1 \) w.r.t. \( J \)), with the best rate attained at \( \beta = 1 \) (\( \beta = 1 \) w.r.t. \( J \)), which means the smoothness of \( f_0 \) is not appropriately captured by the estimator. Such a saturation behavior is well-studied in the inverse problem literature [12] where it has been attributed to the choice of regularizer. In Section 4 we discuss alternative regularization strategies using ideas from [3], which covers non-parametric least squares regression: we show that for appropriately chosen regularizers, the above mentioned rates hold for any \( \beta > 0 \) and do not saturate for the aforementioned ranges of \( \beta \) (see Theorem 4).

(iii) In Section 3 we study the problem of density estimation in the misspecified setting, i.e., \( p_0 \notin \mathcal{P} \), which is not addressed in [22]. Using a more complicated analysis than in the well-specified case, we show in Theorem 12 that \( J(p_0\|p_{\hat{f}_n}) \to \inf_{p \in \mathcal{P}} J(p_0\|p) \) as \( n \to \infty \). Under an appropriate smoothness assumption on \( \log \hat{p}_{\hat{f}_n} \) (see the statement of Theorem 12 for details), we show that \( J(p_0\|p_{\hat{f}_n}) \to 0 \) as \( n \to \infty \) along with a rate for this convergence, even though \( p_0 \notin \mathcal{P} \). However, unlike the well-specified case where the consistency is obtained not only in \( J \) but also in other distances, we obtain convergence only in \( J \) for the misspecified case. Note that while [2] considered the estimation of \( p_0 \) in the misspecified setting, the results are restricted to the approximating families consisting of polynomials, splines or trigonometric series. Our results are more general, as they hold for abstract RKHSs.

(iv) In Section 5 we present numerical results comparing the proposed estimator with KDE in estimating a Gaussian and mixture of Gaussians, with the goal of empirically evaluating their performance as \( d \) gets large for a fixed sample size. In these two estimation problems, we show that the proposed estimator outperforms KDE, and the advantage with the proposed estimator grows as \( d \) gets large.

Various notations and definitions that were introduced throughout the paper are collected in Section 2. The proofs of the results are provided in Section 8 along with some supplementary results in an appendix.

2 Definitions and notation

We introduce the notation used throughout the paper. Define \( [d] := \{1, \ldots, d\} \). For \( a := (a_1, \ldots, a_d) \in \mathbb{R}^d \), \( \|a\|_2 := \sqrt{\sum_{i=1}^d a_i^2} \). For a topological space \( X \), \( C(X) \) (resp. \( C_b(X) \)) denotes the space of all continuous (resp. bounded continuous) functions on \( X \). For a locally compact Hausdorff space \( X \), \( f \in C(X) \) is said to vanish at infinity if for
every $\epsilon > 0$ the set \( \{ x : |f(x)| \geq \epsilon \} \) is compact. The class of all continuous $f$ on $\mathcal{X}$ which vanish at infinity is denoted as $C_0(\mathcal{X})$. For open $\mathcal{X} \subset \mathbb{R}^d$, $C^1(\mathcal{X})$ denotes the space of continuously differentiable functions on $\mathcal{X}$. For $f \in C_0(\mathcal{X})$, $\|f\|_\infty := \sup_{x \in \mathcal{X}} |f(x)|$ denotes the supremum norm of $f$. $M_1(\mathcal{X})$ denotes the set of all finite Borel measures on $\mathcal{X}$. For $\mu \in M_1(\mathcal{X})$, $L^r(\mathcal{X},\mu)$ denotes the Banach space of $r$-power ($r \geq 1$) $\mu$-integrable functions. For $\mathcal{X} \subset \mathbb{R}^d$, we will use $L^r(\mathcal{X})$ for $L^r(\mathcal{X},\mu)$ if $\mu$ is a Lebesgue measure on $\mathcal{X}$. For $f \in L^p(\mathcal{X},\mu), \|f\|_{L^p(\mathcal{X},\mu)} := \left( \int_{\mathcal{X}} |f|^r \, d\mu \right)^{1/r}$ denotes the $L^r$-norm of $f$ for $1 \leq r < \infty$ and we denote it as $\|f\|_{L^r(\mathcal{X})}$ if $\mathcal{X} \subset \mathbb{R}^d$ and $\mu$ is the Lebesgue measure. The convolution $f * g$ of two measurable functions $f$ and $g$ on $\mathbb{R}^d$ is defined as $(f * g)(x) := \int_{\mathbb{R}^d} f(y)g(x-y) \, dy$, provided the integral exists for all $x \in \mathbb{R}^d$. For $f \in L_1(\mathbb{R}^d)$, the Fourier transform is defined as $\hat{f}(y) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} f(x)e^{-iy}\cdot x \, dx$ where $i$ denotes the imaginary unit $\sqrt{-1}$. For $x \in H_1$ and $y \in H_2, x \otimes y$ denotes the tensor product of $x$ and $y$, and can be seen as an operator from $H_2$ to $H_1$ as $(x \otimes y)z = x(y,z)_{H_2}$ for any $z \in H_2$, where $H_1$ and $H_2$ are Hilbert spaces. For an operator $A : H_1 \rightarrow H_2, R(A)$ denotes the range space (or image) of $A$. For a bounded linear operator $A$, $\|A\|$ and $\|A\|_{HS}$ denote the operator and Hilbert-Schmidt norms of $A$, respectively.

A real-valued symmetric function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is called a positive definite (pd) kernel if, for all $n \in \mathbb{N}$, $\alpha_1, \ldots, \alpha_n \in \mathbb{R}$ and all $x_1, \ldots, x_n \in \mathcal{X}$, we have $\sum_{i,j=1}^n \alpha_i \alpha_j k(x_i, x_j) \geq 0$. A function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, $(x,y) \mapsto k(x,y)$ is a reproducing kernel of the Hilbert space $(H_k, \langle \cdot, \cdot \rangle_{H_k})$ of functions if and only if (i) $\forall y \in \mathcal{X}, k(\cdot,y) \in H_k$ and (ii) $\forall y \in \mathcal{X}, \forall f \in H_k, \langle f, k(\cdot,y) \rangle_{H_k} = f(y)$ holds. If such a $k$ exists, then $H_k$ is called a reproducing kernel Hilbert space. Since $(k(\cdot,x), k(\cdot,y))_{H_k} = k(x,y), \forall x,y \in \mathcal{X}$, it is easy to show that every reproducing kernel (r.k.), $k$ is symmetric and positive definite. It can be shown that $H_k = \text{span}\{k(\cdot,x) : x \in \mathcal{X}\}$ where the closure is taken w.r.t. the RKHS norm (see [3] Chapter 1, Theorem 3), which means the kernel function, $k$ generates the RKHS. Examples of $k$ include the Gaussian kernel, $k(x,y) = \exp(-\sigma \|x-y\|^2_2), x,y \in \mathbb{R}^d, \sigma > 0$ that induces the following Gaussian RKHS,

$$H_k = H_\sigma := \left\{ f \in L^2(\mathbb{R}^d) \cap C(\mathbb{R}^d) : \int |\hat{f}(\omega)|^2 e^{\|\omega\|^2_2/4\sigma} \, d\omega < \infty \right\},$$

the inverse multiquadratic kernel, $k(x,y) = (1 + \|x-y\|_2^{-2})^{-\beta}, x,y \in \mathbb{R}^d, \beta > 0, c \in (0,\infty)$ and the Matérn kernel, $k(x,y) = \frac{1}{\Gamma(\beta)} \|x-y\|_2^{-\beta} \mathbb{I}_{\beta/2}(\|x-y\|_2), x,y \in \mathbb{R}^d, \beta > d/2$ that induces the Sobolev space, $H^2_2$,

$$H_k = H^2_2 := \left\{ f \in L^2(\mathbb{R}^d) \cap C(\mathbb{R}^d) : \int (1 + \|\omega\|^2_2)^{-\beta} |\hat{f}(\omega)|^2 \, d\omega < \infty \right\},$$

where $\Gamma$ is the Gamma function, and $\mathbb{I}_{\beta}$ is the modified Bessel function of the third kind of order $v$ ($v$ controls the smoothness of $k$).

Given two probability densities, $p$ and $q$ on $\Omega \subset \mathbb{R}^d$, the Kullback-Leibler divergence (KL) and Hellinger distance ($h$) are defined as $KL[p,q] = \int p(x) \log \frac{p(x)}{q(x)} \, dx$ and $h(p,q) = \|\sqrt{p} - \sqrt{q}\|_{L^2(\Omega)}$ respectively. We refer to $\|p-q\|_{L^1(\Omega)}$ as the total variation (TV) distance between $p$ and $q$.

### 3 Approximation of densities by $\mathcal{P}$

In this section, we first show that every finite dimensional exponential family is generated by the family $\mathcal{P}$ induced by a finite dimensional RKHS, which naturally leads to the infinite dimensional generalization of $\mathcal{P}_\infty$ when $\mathcal{H}$ is an infinite dimensional RKHS. Next, we investigate the approximation properties of $\mathcal{P}$ in Proposition[4] and Corollary[5] when $\mathcal{H}$ is an infinite dimensional RKHS.

Let us consider a $r$-dimensional exponential family, $\mathcal{P}_\infty$ with sufficient statistic $r' \supset T(x) := (T_1(x), \ldots, T_r(x))$ and construct a finite dimensional Hilbert space, $\mathcal{H} = \text{span}\{T_1(x), \ldots, T_r(x)\}$. It is easy to verify that $\mathcal{P}$ induced by $\mathcal{H}$ is exactly the same as $\mathcal{P}_\infty$ since any $x \in \mathcal{H}$ can be written as $x = \sum_{i=1}^{r'} \theta_i T_i(x)$ for some $(\theta_i)_{i=1}^{r'} \subset \mathbb{R}$. In fact, by defining the inner product between $f \in \mathcal{H}$ can be written as $f(x) = \sum_{i=1}^{r'} \theta_i T_i(x)$ for some $(\theta_i)_{i=1}^{r'} \subset \mathbb{R}$. In fact, by defining the inner product between $f = \sum_{i=1}^{r'} \theta_i T_i$ and $g = \sum_{i=1}^{r'} \gamma_i T_i$ as $(f, g)_{\mathcal{H}} := \sum_{i=1}^{r'} \theta_i \gamma_i$, it follows that $\mathcal{H}$ is an RKHS with the r.k. $k(x,y) = \langle T(x), T(y) \rangle_{r'd}$ since $(k, k(\cdot,x))_{\mathcal{H}} = \sum_{i=1}^{r'} \theta_i \gamma_i$ follows. Based on this equivalence between $\mathcal{P}_\infty$ and $\mathcal{P}$ induced by a finite dimensional RKHS, it is therefore clear that $\mathcal{P}$ induced by a infinite dimensional RKHS is a strict generalization to $\mathcal{P}_\infty$ with $(k, x)$ playing the role of a sufficient statistic.

**Example 1.** The following are some popular examples of probability distributions that belong to $\mathcal{P}_\infty$. Here we show the corresponding $(\mathcal{H}, k)$ that generates it. In some of these examples, we choose $q_0(x) = 1$ and ignore the fact that $q_0$ is a probability distribution as assumed in the definition of $\mathcal{P}$.
Exponential: $\Omega = \mathbb{R}_+ := \mathbb{R}^+ \setminus \{0\}$, $k(x, y) = xy$.

Normal: $\Omega = \mathbb{R}$, $k(x, y) = xy + x^2y^2$.

Beta: $\Omega = (0, 1)$, $k(x, y) = \log x \log y + \log(1 - x) \log(1 - y)$.

Gamma: $\Omega = \mathbb{R}_+^d$, $k(x, y) = \log x \log y + xy$. $k(x, y) = xy + \frac{1}{xy}$.

Poisson: $\Omega = \mathbb{N} \cup \{0\}$, $k(x, y) = xy$, $q_0(x) = (x!)^{-1}$.

Geometric: $\Omega = \mathbb{N} \cup \{0\}$, $k(x, y) = xy$, $q_0(x) = 1$.

Binomial: $\Omega = \{0, \ldots, m\}$, $k(x, y) = xy$, $q_0(x) = 2^{-m}(m)$.

While Example 1 shows that all popular probability distributions are contained in $\mathcal{P}$ for an appropriate choice of finite-dimensional $\mathcal{H}$, it is of interest to understand the richness of $\mathcal{P}$ (i.e., what class of distributions can be approximated arbitrarily well by $\mathcal{P}$?) when $\mathcal{H}$ is an infinite dimensional RKHS. This is addressed by the following result, which is proved in Section 8.3.

**Proposition 1.** Define $\mathcal{P}_0 := \left\{ \pi_f(x) = \frac{e^{f(x)q_0(x)}}{\sum_{x \in \Omega} e^{f(x)q_0(x)}}, x \in \Omega : f \in C_0(\Omega) \right\}$ where $\Omega \subset \mathbb{R}^d$ is a non-empty set. Suppose $k(\cdot, x) \in C_0(\Omega)$, $\forall x \in \Omega$ and

$$
\int \int k(x, y) d\mu(x) d\mu(y) > 0, \forall \mu \in M_0(\Omega) \setminus \{0\}.
$$

Then $\mathcal{P}$ is dense in $\mathcal{P}_0$ w.r.t. Kullback-Leibler divergence, total variation ($L^1$ norm) and Hellinger distances. In addition, if $q_0 \in L^1(\Omega) \cap L^r(\Omega)$ for some $1 < r \leq \infty$, then $\mathcal{P}$ is dense in $\mathcal{P}_0$ w.r.t. $L^r$ norm.

If $k(x, y) = \psi(x - y), x, y \in \Omega = \mathbb{R}^d$ where $\psi \in C_b(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$, then $[\ref{prop1}]$ can be shown to be equivalent to $\text{supp}(\psi^\wedge) = \mathbb{R}^d$ (see $[\ref{prop5}]$ Proposition 5). Examples of kernels that satisfy the conditions in Proposition 1 include the Gaussian, Matérn and inverse multiquadrics. In fact, any compactly supported non-zero $\psi \in C_b(\mathbb{R}^d)$ satisfies the assumptions in Proposition 1 as $\text{supp}(\psi^\wedge) = \mathbb{R}^d$ ($[\ref{prop5}]$ Corollary 10). Though $\mathcal{P}_0$ is still a parametric family of densities indexed by a Banach space (here $C_0(\Omega)$), the following corollary (proved in Section 8.3 to Proposition 1) shows that a broad class of continuous densities are included in $\mathcal{P}_0$ and therefore can be approximated arbitrarily well in $L^r$ norm ($1 \leq r \leq \infty$), Hellinger distance and KL divergence by $\mathcal{P}$.

**Corollary 2.** Let $q_0 \in C_0(\Omega)$ be a probability density such that $q_0(x) > 0$ for all $x \in \Omega$, where $\Omega$ is a non-empty subset of $\mathbb{R}^d$. Define

$$
\mathcal{P}_c := \left\{ p \in C_0(\Omega) : \int_{\Omega} p(x) dx = 1, p(x) \geq 0, \forall x \in \Omega \text{ and } \left\| p \right\|_{q_0} < \infty \right\}.
$$

Suppose $k(\cdot, x) \in C_0(\Omega)$, $\forall x \in \Omega$ and $[\ref{prop2}]$ holds. Then $\mathcal{P}$ is dense in $\mathcal{P}_c$ w.r.t. KL divergence, TV and Hellinger distances. Moreover, if $q_0 \in L^1(\Omega) \cap L^r(\Omega)$ for some $1 < r \leq \infty$, then $\mathcal{P}$ is dense in $\mathcal{P}_c$ w.r.t. $L^r$ norm.

By choosing $\Omega$ to be compact and $q_0$ to be a uniform distribution on $\Omega$, Corollary 2 reduces to an easily interpretable result that any continuous density $p_0$ on $\Omega$ can be approximated arbitrarily well by densities in $\mathcal{P}$ in KL, Hellinger and $L^r$ ($1 \leq r \leq \infty$) distances.

Similar to the results so far, an approximation result for $\mathcal{P}$ can also be obtained w.r.t. Fisher divergence (see Proposition 1). Since this result is heavily based on the notions and results developed in Section 5, we defer its presentation until that section. Briefly, this result states that if $\mathcal{H}$ is sufficiently rich (i.e., dense in an appropriate class of functions), then any $p \in C^1(\mathbb{R}^d)$ with $J(p\|q_0) < \infty$ can be approximated arbitrarily well by elements in $\mathcal{P}$ w.r.t. Fisher divergence, where $q_0 \in C^1(\mathbb{R}^d)$.

## 4 Density estimation in $\mathcal{P}$: Well-specified case

In this section, using the score matching approach, we present our estimator to estimate an unknown density $p_0 := p_{f_0} \in \mathcal{P}$ (well-specified case) from i.i.d. random samples $(X_i)_{i=1}^n$ drawn from it. This involves choosing the minimizer
of the (empirical) Fisher divergence between \( p_0 \) and \( p_f \in \mathcal{P} \) as the estimator, \( \hat{f} \) which we show in Theorem 4 to be obtained by solving a simple finite-dimensional linear system. In contrast, we would like to remind the reader that the MLE is practically infeasible due to the difficulty in handling \( A(\hat{f}) \). The consistency and convergence rates of \( \hat{f} \in \mathcal{F} \) and the plug-in estimator \( p_f \) are provided in Section 8.4 (see Theorems 5–7). Before we proceed, we list the assumptions on \( p_0 \), \( q_0 \) and \( \mathcal{H} \) that we need to make in our analysis.

(A) \( \Omega := \prod_{j=1}^d (a_j, b_j) \subset \mathbb{R}^d \) where \( a_j < b_j \) and \( a_j, b_j \in \mathbb{R} \cup \{\pm \infty\}, \forall j \in [d] \).

(B) \( k \) is twice continuously differentiable on \( \Omega \times \Omega \), i.e., \( \partial^{\alpha \cdot \beta} k : \Omega \times \Omega \to \mathbb{R} \) exists and is continuous for all multi-indexes \( \alpha := (\alpha_1, \ldots, \alpha_r) \in \mathbb{N}^d \) such that \( \sum_{i=1}^d \alpha_i \leq 2 \) where \( \partial^{\alpha \cdot \beta} := \partial_1^{\alpha_1} \cdots \partial_d^{\alpha_d} \partial_1^{\beta_1} \cdots \partial_d^{\beta_d} \) and \( \beta := \frac{\partial}{\partial \beta} \).

(C) For any fixed \( i \in \{1, \ldots, d\} \) and \( \tilde{x}_k \in (a_k, b_k) \) \( (k \neq i) \), let \( x = (\tilde{x}_1, \ldots, \tilde{x}_{i-1}, x_i, \tilde{x}_{i+1}, \ldots, \tilde{x}_d) \). Then

\[
\lim_{x_i \to a_i + \text{or } b_i -} \frac{\partial^2 k(x,y)}{\partial x_i \partial y_i} \bigg|_{y=x} p_0^2(x) = 0.
\]

(D) \( (\varepsilon\text{-Integrability}) \) For some \( \varepsilon \geq 1 \),

\[
\left\| \frac{\partial k(\cdot, x)}{\partial x_i} \right\|_{\mathcal{H}} \in L^{2\varepsilon}(\Omega, p_0), \quad \left\| \frac{\partial^2 k(\cdot, x)}{\partial x_i^2} \right\|_{\mathcal{H}} \in L^{\varepsilon}(\Omega, p_0) \quad \text{and} \quad \left\| \frac{\partial k(\cdot, x)}{\partial x_i} \right\|_{\mathcal{H}} \frac{\partial \log q_0(x)}{\partial x_i} \in L^{\varepsilon}(\Omega, p_0), \forall i \in [d],
\]

where \( q_0 \in C^1(\Omega) \).

Remark 1. (i) (A) along with \( k \) being continuous (as in (B)) ensures that \( \mathcal{H} \) is separable [35, Lemma 4.33]. (B) ensures that every \( f \in \mathcal{H} \) is twice continuously differentiable [35, Corollary 4.36]. (C) ensures that \( J \) in (B) is equivalent to the one in (4) through partial integration for densities in \( \mathcal{P} \).

(ii) When \( \varepsilon = 1 \), the first condition in (D) ensures that \( J(p_0\|p_f) < \infty \) for any \( p_f \in \mathcal{P} \). The other two conditions ensure the validity of alternate representation for \( J(p_0\|p_f) \) in (4) which will be useful in constructing estimators of \( p_0 \) (see Theorem 4). Examples of kernels that satisfy (D) are Gaussian, Matérn (with \( \beta > \max\{2, d/2\} \)) and inverse multiquadrics, for which it is easy to show that there exists \( q_0 \) that satisfies (D).

(iii) \( (\text{Identifiability}) \) The above list of assumptions do not include the identifiability condition that ensures \( p_{f_1} = p_{f_2} \) if and only if \( f_1 = f_2 \). It is clear that if constant functions are included in \( \mathcal{H} \), i.e., \( 1 \in \mathcal{H} \), then \( p_f = p_{f+e} \) for any \( e \in \mathbb{R} \). On the other hand, it can be shown that if \( 1 \notin \mathcal{H} \) and \( \text{supp}(q_0) = \Omega \), then \( p_{f_1} = p_{f_2} \Leftrightarrow f_1 = f_2 \). A sufficient condition for \( 1 \notin \mathcal{H} \) is \( k \in C_0(\Omega \times \Omega) \). We do not explicitly impose the identifiability condition as a part of our blanket assumptions because the assumptions under which consistency and rates are obtained in Theorem 4 automatically ensure identifiability.

Under these assumptions, the following result—proved in Section 8.4—shows that the problem of estimating \( p_0 \) through the minimization of Fisher divergence reduces to the problem of estimating \( f_0 \) through a weighted least squares minimization in \( \mathcal{H} \) (see parts (i) and (ii)). This motivates the minimization of the regularized empirical weighted least squares (see part (iv)) to obtain an estimator \( f_{\lambda,n} \) of \( f_0 \), which is then used to construct the plug-in estimate \( p_{f_{\lambda,n}} \) of \( p_0 \).

**Theorem 3.** Suppose (A)–(D) hold with \( \varepsilon = 1 \). Then \( J(p_0\|p_f) < \infty \) for all \( f \in \mathcal{F} \). In addition, the following hold.

(i) For all \( f \in \mathcal{F} \),

\[
J(f) := J(p_0\|p_f) = \frac{1}{2} \langle f - f_0, C(f - f_0) \rangle_{\mathcal{H}},
\]

where \( C : \mathcal{H} \to \mathcal{H}, C := \int p_0(x) \sum_{i=1}^d \frac{\partial k(\cdot, x)}{\partial x_i} \otimes \frac{\partial k(\cdot, x)}{\partial x_i} \, dx \) is a trace-class positive operator with

\[
Cf = \int p_0(x) \sum_{i=1}^d \frac{\partial k(\cdot, x)}{\partial x_i} \frac{\partial f(x)}{\partial x_i} \, dx
\]

for any \( f \in \mathcal{H} \).

(ii) Alternatively,

\[
J(f) = \frac{1}{2} \langle f, Cf \rangle_{\mathcal{H}} + \langle f, \xi \rangle_{\mathcal{H}} + J(p_0\|q_0)
\]
Then

Theorem 4

While this is not an issue when studying the convergence of by minimizing \( J \) respectively. However, there is no guarantee that \( \alpha \) in Theorem 3(iv) should in principle be computable. In practice, however, it is not easy to compute the expression for \( \alpha \).

\[ f_{\lambda,n} = -(C + \lambda I)^{-1} \xi, \]

where \( J(f) = \frac{1}{2} \langle f, \mathcal{C} f \rangle_{\mathcal{H}} + \langle f, \xi \rangle_{\mathcal{H}} + J(p_0) \| q_0 \|_{\mathcal{F}} \) and \( \mathcal{C} \) is obtained from \( J(f) \) as it is obtained from \( J(f) \).

(iv) (Estimator of \( f_0 \)) Given samples \((X_a)_{a=1}^{n}\) drawn i.i.d. from \( p \), for any \( \lambda > 0 \), the unique minimizer \( f_{\lambda,n} \) of \( \hat{J}(f) := J(f) + \frac{\lambda}{2} \| f \|_{\mathcal{H}}^2 \) over \( \mathcal{H} \) exists and is given by

\[ f_{\lambda,n} = -(C + \lambda I)^{-1} \xi, \]

where \( \hat{J}(f) := \frac{1}{2} \langle f, \mathcal{C} f \rangle_{\mathcal{H}} + \langle f, \xi \rangle_{\mathcal{H}} + J(p_0) \| q_0 \|_{\mathcal{F}} \) and \( \mathcal{C} \) is obtained from \( J(f) \) as it is obtained from \( J(f) \).

An important remark we would like to make about Theorem 3 is that though \( J(f) \) in (ii) over (iii) is that it provides a simple way to obtain an empirical estimate of \( J(f) \)—by replacing \( C \) and \( \xi \) by their empirical estimators, \( \hat{C} \) and \( \hat{\xi} \) respectively—from finite samples drawn i.i.d. from \( p_0 \), which is then used to obtain an estimator of \( f_0 \). Note that the empirical estimate of \( J(f) \), i.e., \( J(f) \) depends only on \( C \) and \( \xi \) which in turn depend on the known quantities, \( k \) and \( q_0 \), and therefore \( f_{\lambda,n} \) in Theorem 3(iv) should in principle be computable. In practice, however, it is not easy to compute the expression for \( f_{\lambda,n} \).

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We further discuss the choice of regularizer in Section 4.3.2 using ideas from the inverse problem literature.
We would like to highlight that though \( f_{\lambda,n} \) requires solving a simple linear system in \( \mathbb{S} \), it can still be computationally intensive when \( d \) and \( n \) are large as \( H \) is a \( (nd+1) \times (nd+1) \) matrix. This is still a better scenario than that of MLE, however, since computationally efficient methods exist to solve large linear systems such as \( \mathbb{S} \), whereas MLE can be intractable due to the difficulty in handling the log-partition function (though it can be approximated). On the other hand, MLE is statistically well-understood, with consistency and convergence rates established in general for the problem of density estimation \cite{39} and in particular for the problem at hand \cite{14}. In order to ensure that \( f_{\lambda,n} \) and \( p_{f_{\lambda,n}} \) are statistically useful, in the following section, we investigate their consistency and convergence rates under some smoothness conditions on \( f_0 \).

### 4.1 Consistency and rate of convergence

In this section, we prove the consistency of \( f_{\lambda,n} \) (see Theorem\ref{5} (ii)) and \( p_{f_{\lambda,n}} \) (see Theorems\ref{5} (iii)\ref{7}). Under the smoothness assumption that \( f_0 \in \mathcal{R}(C^\beta) \) for some \( \beta > 0 \), we present convergence rates for \( f_{\lambda,n} \) and \( p_{f_{\lambda,n}} \) in Theorems\ref{5} (ii), \ref{6} and \ref{7}. In reference to the following results, for simplicity we suppress the dependence of \( \lambda \) on \( n \) by defining \( \lambda := \lambda_n \) where \( (\lambda_n)_n \in \mathbb{N} \subset (0, \infty) \).

**Theorem 5** (Consistency and convergence rates for \( f_{\lambda,n} \)). Suppose \( (A)-(D) \) with \( \varepsilon = 2 \) hold.

(i) If \( f_0 \in \mathcal{R}(C) \), then \( \| f_{\lambda,n} - f_0 \|_{\mathcal{H}} = O_p(\varepsilon) \) as \( \lambda \to 0 \), \( \lambda \sqrt{n} \to \infty \) and \( n \to \infty \).

(ii) If \( f_0 \in \mathcal{R}(C^\beta) \) for some \( \beta > 0 \), then

\[
\| f_{\lambda,n} - f_0 \|_{\mathcal{H}} = O_p(n^{-1/2})
\]

with \( \lambda = n^{-\frac{\beta}{2}} \) as \( n \to \infty \).

(iii) Suppose \( E_1 := \sup_{x \in \Omega \times \Omega} \left\| \frac{\partial^k (\cdot)}{\partial x^i} \right\|_{\mathcal{H}} < \infty \) and \( \| C^{-1} \| < \infty \). Then

\[
\| f_{\lambda,n} - f_0 \|_{\mathcal{H}} = O_p(n^{-1/2})
\]

with \( \lambda = n^{-\frac{\beta}{2}} \) as \( n \to \infty \).

**Remark 2.**

(i) While Theorem\ref{5} (proved in Section \ref{6}) provides an asymptotic behavior for \( \| f_{\lambda,n} - f_0 \|_{\mathcal{H}} \) under conditions that depend on \( p_0 \) (and are therefore not easy to check in practice), a non-asymptotic bound on \( \| f_{\lambda,n} - f_0 \|_{\mathcal{H}} \) that holds for all \( n \geq 1 \) can be obtained under stronger assumptions through an application of Bernstein’s inequality in separable Hilbert spaces. See Proposition \ref{3} in Section \ref{7} for details.

(ii) The proof of Theorem\ref{5} (i) involves decomposing \( \| f_{\lambda,n} - f_0 \|_{\mathcal{H}} \) into an estimation error part, \( E(\lambda, n) := \| f_{\lambda,n} - f_\|_{\mathcal{H}} \), and an approximation error part, \( A_0(\lambda) := \| f_\lambda - f_0 \|_{\mathcal{H}} \), where \( f_\lambda = (C + \lambda I)^{-1}Cf_0 \). While \( E(\lambda, n) \to 0 \) as \( \lambda \to 0 \), \( \lambda \sqrt{n} \to \infty \) and \( n \to \infty \) without any assumptions on \( f_0 \) (see the proof in Section \ref{6} for details), it is not reasonable to expect \( A_0(\lambda) \to 0 \) as \( \lambda \to 0 \) without assuming \( f_0 \in \mathcal{R}(C) \). This is because, if \( f_0 \) lies in the null space of \( C \), then \( f_\) is zero irrespective of \( \lambda \) and therefore cannot approximate \( f_0 \).

(iii) The condition \( f_0 \in \mathcal{R}(C) \) is difficult to check in practice as it depends on \( p_0 \) (which in turn depends on \( f_0 \)). However, since the null space of \( C \) is just constant functions if the kernel is bounded and supp \( p_0 \) = \( \Omega \) (see Lemma \ref{14} in Section \ref{8} for details), assuming \( 1 \notin \mathcal{H} \) yields that \( \mathcal{R}(C) = \mathcal{H} \) and therefore consistency can be attained under conditions that are easy to impose in practice. As mentioned in Remark \ref{11} (iii), the condition \( 1 \notin \mathcal{H} \) ensures identifiability and a sufficient condition for it to hold is \( k \in C_0(\Omega \times \Omega) \), which is satisfied by Gaussian, Matérn and inverse multiquadric kernels.

(iv) It is well known that convergence rates are possible only if the quantity of interest (here \( f_0 \)) satisfies some additional conditions. In function estimation, this additional condition is classically imposed by assuming \( f_0 \) to be sufficiently smooth, e.g., \( f_0 \) lies in a Sobolev space of certain smoothness. By contrast, the smoothness condition in Theorem\ref{5} (ii) is imposed in an indirect manner by assuming \( f_0 \in \mathcal{R}(C^\beta) \) for some \( \beta > 0 \)—so that the results hold for abstract RKHSs and not just Sobolev spaces—which then provides a rate, with the best rate being \( n^{-1/4} \) that is attained when \( \beta \geq 1 \). While such a condition has already been used in various works \cite{5} \cite{22} \cite{19} in the context of non-parametric least squares regression, we explore it in more detail in Proposition\ref{8} and Examples\ref{2} and \ref{3}. Note that this condition is common in the inverse problem theory (see \cite{12}), and it naturally arises here through the connection of \( f_{\lambda,n} \) being...
a Tikhonov regularized solution to the ill-posed linear system $\hat{\mathcal{C}} f = -\hat{\mathcal{C}}$. An interesting observation about the rate is that it does not improve with increasing $\beta$ (for $\beta > 1$), in contrast to the classical results in function estimation (e.g., kernel density estimation and kernel regression) where the rate improves with increasing smoothness. This issue is discussed in detail in Section 4.3.

(v) Since $\|C^{-1}\| < \infty$ only if $\mathcal{H}$ is finite-dimensional, we recover the parametric rate of $n^{-1/2}$ in a finite-dimensional situation with an automatic choice for $\lambda$ as $n^{-1/2}$. ■

While Theorem 3 provides statistical guarantees for parameter convergence, the question of primary interest is the convergence of $p_{f_{\lambda,n}}$ to $p_0$. This is guaranteed by the following result, which is proved in Section 5.8.

Theorem 6 (Consistency and rates for $p_{f_{\lambda,n}}$). Suppose (A)–(D) with $\varepsilon = 2$ hold and $\|k\|_\infty := \sup_{x \in \Omega} k(x,x) < \infty$.

(i) Assume $\text{supp}(q_0) = \Omega$. Then for any $1 < r \leq \infty$ with $q_0 \in L^1(\Omega) \cap L^r(\Omega)$,

\[ \|p_{f_{\lambda,n}} - p_0\|_{L^r(\Omega)} \to 0, h(p_{f_{\lambda,n}}, p_0) \to 0, KL(p_0\|p_{f_{\lambda,n}}) \to 0 \] as $\lambda \sqrt{n} \to \infty$, $\lambda \to 0$ and $n \to \infty$.

In addition, if $f_0 \in \mathcal{R}(C^\beta)$ for some $\beta > 0$, then

\[ \|p_{f_{\lambda,n}} - p_0\|_{L^r(\Omega)} = O_\bar{p_0}(\theta_n), h(p_0, p_{f_{\lambda,n}}) = O_\bar{p_0}(\theta_n), KL(p_0\|p_{f_{\lambda,n}}) = O_\bar{p_0}(\theta_n^2) \]

where $\theta_n := n^{-\min\left\{ \frac{1}{2}, \frac{\beta}{2(\beta + 1)} \right\}}$ with $\lambda = n^{-\max\left\{ \frac{1}{2}, \frac{1}{2(\beta + 1)} \right\}}$.

(ii) If $E := \sup_{x \in \Omega, i \in [d]} \left\| \frac{\partial k(x,\cdot)}{\partial x_i} \right\|_{\mathcal{H}} < \infty$, then

\[ J(p_0\|p_{f_{\lambda,n}}) \to 0 \] as $\lambda n \to \infty$, $\lambda \to 0$ and $n \to \infty$.

In addition, if $f_0 \in \mathcal{R}(C^\beta)$ for some $\beta \geq 0$, then

\[ J(p_0\|p_{f_{\lambda,n}}) = O_\bar{p_0} \left( n^{-\min\left\{ \frac{1}{2}, \frac{\beta}{2(\beta + 1)} \right\}} \right) \]

with $\lambda = n^{-\max\left\{ \frac{1}{2}, \frac{1}{2(\beta + 1)} \right\}}$.

(iii) If $\|C^{-1}\| < \infty$ and $E < \infty$, then $\theta_n = n^{-\frac{1}{2}}$ and $J(p_0\|p_{f_{\lambda,n}}) = O_\bar{p_0}(n^{-1})$ with $\lambda = n^{-\frac{1}{2}}$.

Remark 3. (i) Comparing the results of Theorem 3(i) and Theorem 6(i) (for $L^r$, Hellinger and KL divergence), we would like to highlight that while the conditions on $\lambda$ and $n$ match in both the cases, the latter does not require $f_0 \in \mathcal{R}(C^\beta)$ to ensure consistency. While a similar condition can be imposed in Theorem 6 to attain consistency, we replaced this condition with $\text{supp}(q_0) = \Omega$—a simple and easy condition to work with—which along with the boundedness of the kernel ensures that for any $f_0 \in \mathcal{H}$, there exists $\hat{f}_0 \in \mathcal{R}(C^\beta)$ such that $p_{\hat{f}_0} = p_0$ (see Lemma 14).

(ii) In contrast to the results in $L^r$, Hellinger and KL divergence, consistency in $J$ can be obtained with $\lambda$ converging to zero at a rate faster than in these results. Another interesting aspect of convergence in $J$ is that it does not even require $\text{supp}(q_0) = \Omega$ to hold, unlike for convergence in other distances. This is due to the fact that the convergence in these other distances is based on the convergence of $\|f_{\lambda,n} - f_0\|_{\mathcal{H}}$, which in turn involves convergence of $A_\lambda(\lambda) := \|\sqrt{C}(f_{\lambda} - f_0)\|_{\mathcal{H}}$ to zero and therefore requires $f_0 \in \mathcal{R}(C^\beta)$ or $\text{supp}(q_0) = \Omega$ to hold. On the other hand, convergence in $J$ is controlled by $A_{\lambda/2}(\lambda) := \|\sqrt{C}(f_{\lambda} - f_0)\|_{\mathcal{H}}$ which can be shown to behave as $O(\sqrt{\lambda})$ as $\lambda \to 0$, without requiring any assumptions on $f_0$ (see Proposition 12.1). For this reason, one can obtain rates in $J$ with $\beta = 0$, i.e., no smoothness assumption on $f_0$, while no rates are possible in other distances (the latter might also be an artifact of the proof technique, as these results are obtained through an application of Theorem 3(ii) in Lemma 14). Indeed, as a further consequence, the rate of convergence in $J$ is faster than in other distances.

(iii) An interesting aspect in Theorem 6 is that $p_{f_{\lambda,n}}$ is consistent in various distances such as $L^r$, Hellinger and KL, despite being obtained by minimizing a different loss function, i.e., $J$. However, we will see in Section 5 that such nice results are difficult to obtain in the misspecified case, where consistency and rates are provided only in $J$. ■

While Theorem 6 addresses the case of bounded kernels, the case of unbounded kernels requires a small modification which we discuss below. The reason for this modification, as alluded to in the discussion following Theorem 3, is due to the fact that $f_{\lambda,n}$ may not be in $\mathcal{F}$ when $k$ is unbounded, and therefore the corresponding density estimator, $p_{f_{\lambda,n}}$.
may not be well-defined. To handle this, in the following, we assume that there exists a positive constant \( M \) such that \( \| f_0 \|_{\mathcal{H}} \leq M \), so that an estimator of \( f_0 \) can be constructed as

\[
\hat{f}_{\lambda,n} = \arg \inf_{\hat{f} \in \mathcal{F}} \hat{J}_\lambda(f) \quad \text{subject to} \quad \| f \|_{\mathcal{H}} \leq M,
\]

where \( \hat{J}_\lambda \) is defined in Theorem B(iv). This modification yields a valid estimator \( p_{\hat{f}_{\lambda,n}} \) as long as \( k \) satisfies

\[
\int \exp(M \sqrt{k(x,x)}) q_0(x) \, dx < \infty,
\]

since this implies \( \hat{f}_{\lambda,n} \in \mathcal{F} \). The construction of \( \hat{f}_{\lambda,n} \) requires the knowledge of \( M \), however, which we assume is known \textit{a priori}. Using the ideas in the proof of Theorem 6 it can be shown (see Section 8.4) that

\[
\hat{f}_{\lambda,n} = \alpha \hat{\xi} + \sum_{b=1}^{d} \sum_{j=1}^{\beta_{b,j}} \frac{\partial k(\cdot, X_k)}{\partial x_j}
\]

where \( \alpha \) and \( (\beta_{b,j}) \) are obtained by solving the following quadratically constrained quadratic program (QCQP),

\[
\begin{aligned}
(\alpha) & : \hat{\Theta} = \arg \min_{\Theta \in \mathbb{R}^{n+1}} \frac{1}{2} \Theta^T H \Theta + \Theta^T \Delta \quad \text{subject to} \quad \Theta^T B \Theta \leq M^2, \\
\end{aligned}
\]

with \( \Delta := (||\hat{\xi}||_2^2, h_b^2) \), \( \Theta := (\alpha, \beta_{b,j}) \) and \( B := (||\hat{\xi}||_2^2, h_b^2, G_{ab}) \), where \( ||\hat{\xi}||_2^2, h_b^2 \) and \( G_{ab} \) are defined in Theorem 4 with \( H \) being the matrix in the linear system \( H \Theta = -\Delta \) in (8). The following result investigates the consistency and convergence rates for \( p_{\hat{f}_{\lambda,n}} \), which is proved in Section 8.10.

**Theorem 7** (Consistency and rates for \( p_{\hat{f}_{\lambda,n}} \)). Let \( M \geq \| f_0 \|_{\mathcal{H}} \) be a fixed constant, and \( \hat{f}_{n,\lambda} \) be a clipped estimator given by (4). Suppose (A) - (D) with \( \varepsilon = 2 \) hold. Let \( \text{supp}(q_0) = \Omega \) and \( \int e^{M \sqrt{k(x,x)}} q_0(x) \, dx < \infty \). Define \( \eta(x) = \sqrt{k(x,x)} e^{M \sqrt{k(x,x)}} \). Then, as \( \lambda \sqrt{n} \to \infty \), \( \lambda \to 0 \) and \( n \to \infty \),

(i) \( \| p_{\hat{f}_{\lambda,n}} - p_0 \|_{L^r(\Omega)} \to 0 \) if \( \eta \in L^1(\Omega, q_0) \);

(ii) \( \| p_{\hat{f}_{\lambda,n}} - p_0 \|_{L^r(\Omega)} \to 0 \) if \( \eta q_0 \in L^1(\Omega) \cap L^r(\Omega) \) and \( e^{M \sqrt{k(x,x)}} q_0 \in L^r(\Omega) \);

(iii) \( h(p_{\hat{f}_{\lambda,n}}, p_0) \to 0 \) if \( \sqrt{k(x,x)} \eta \in L^1(\Omega, q_0) \);

(iv) \( J(p_0, p_{\hat{f}_{\lambda,n}}) \to 0 \).

In addition, if \( f_0 \in \mathcal{R}(C^\beta) \) for some \( \beta > 0 \), then

\[
\| p_{\hat{f}_{\lambda,n}} - p_0 \|_{L^r(\Omega)} = O_\lambda(\theta_n), \quad h(p_0, p_{\hat{f}_{\lambda,n}}) = O_\lambda(\theta_n), \quad KL(p_0, p_{\hat{f}_{\lambda,n}}) = O_\lambda(\theta_n) \quad \text{and} \quad J(p_0, p_{\hat{f}_{\lambda,n}}) = O_\lambda(\theta_n^2)
\]

where \( \theta_n := n \min\left\{ \frac{1}{\lambda}, \frac{\rho}{\sqrt{\lambda} \sigma \gamma_{(\varepsilon)}} \right\} \) with \( \lambda = n \max\left\{ \frac{1}{\lambda}, \frac{\rho}{\sqrt{\lambda} \sigma \gamma_{(\varepsilon)}} \right\} \) assuming the respective conditions in (i)-(iii) above hold.

**Remark 4.** The following observations can be made while comparing the scenarios of using bounded vs. unbounded kernels in the problem of estimating \( p_0 \) through Theorems 6 and 7. First, the consistency results in \( L^r \), Hellinger and KL distances are the same but for additional integrability conditions on \( k \) and \( q_0 \). The additional integrability conditions are not too difficult to hold in practice as they involve \( k \) and \( q_0 \) which can be chosen appropriately. However, the unbounded situation in Theorem 7 requires the knowledge of \( M \) which is usually not known. On the other hand, the consistency result in J in Theorem 6 is slightly weaker than in Theorem 7. This may be an artifact of our analysis as we are not able to adapt the bounding technique used in the proof of Theorem 7 to bound \( J(p_0, p_{\hat{f}_{\lambda,n}}) \) as it critically depends on the boundedness of \( k \). Therefore, we used a trivial bound of \( J(p_0, p_{\hat{f}_{\lambda,n}}) = \frac{1}{2} \| \sqrt{C} (\hat{f}_{\lambda,n} - f_0) \|_{\mathcal{H}}^2 \) as it may not be well-defined. To handle this, in the following, we assume that there exists a positive constant \( M \) such that \( \| f_0 \|_{\mathcal{H}} \leq M \), so that an estimator of \( f_0 \) can be constructed as

\[
\hat{f}_{\lambda,n} = \arg \inf_{\hat{f} \in \mathcal{F}} \hat{J}_\lambda(f) \quad \text{subject to} \quad \| f \|_{\mathcal{H}} \leq M,
\]
4.2 Range space assumption

While Theorems 5 and 8 are satisfactory from the point of view of consistency, it is not clear whether the obtained rates are minimax optimal. The minimax optimality is closely tied to the smoothness assumptions on $f_0$, which in our case is the range space assumption, i.e., $f_0 \in \mathcal{R}(C^\beta)$ for some $\beta > 0$, and which is quite different from the classical smoothness conditions that appear in non-parametric function estimation. While the range space assumption has been made in various earlier works (e.g., [8, 22, 19] in the context of non-parametric least square regression), in the following, we investigate the implicit smoothness assumptions that it makes on $f_0$ in our context. To this end, first it is easy to show (see the proof of Proposition 5.3 in Section 8.14) that

$$\mathcal{R}(C^\beta) = \left\{ \sum_{i \in I} c_i \phi_i : \sum_{i \in I} c_i^2 \alpha_i^{2\beta} < \infty \right\},$$

where $(\alpha_i)_{i \in I}$ are the positive eigenvalues of $C$, $(\phi_i)_{i \in I}$ are the corresponding eigenvectors that form an orthonormal basis for $\mathcal{R}(C)$, and $I$ is an index set which is either finite (if $\mathcal{H}$ is finite-dimensional) or $I = \mathbb{N}$ with $\lim_{i \to \infty} \alpha_i = 0$ (if $\mathcal{H}$ is infinite dimensional). From (10) it is clear that larger the value of $\beta$, the faster is the decay of the Fourier coefficients $(c_i)_{i \in I}$, which in turn implies that the functions in $\mathcal{R}(C^\beta)$ are smoother. Using (10), an interpretation can be provided for $\mathcal{R}(C^\beta)$ ($\beta > 0$ and $\beta \notin \mathbb{N}$) as interpolation spaces (see Section 8.11 for the definition of interpolation spaces) between $\mathcal{R}(C^{\beta_1})$ and $\mathcal{R}(C^{\beta_2})$ where $\mathcal{R}(C^\beta) : = \mathcal{H}$ (see Proposition 8.3 in Section 8.11 for details). While it is not completely straightforward to obtain a sufficient condition for $f_0 \in \mathcal{R}(C^\beta)$, Proposition 8.12 provides a necessary condition for $f_0 \in \mathcal{R}(C^\beta)$ and therefore a necessary condition for $f_0 \in \mathcal{R}(C^\beta)$, $\forall \beta > 1$ for translation invariant kernels on $\Omega = \mathbb{R}^d$, whose proof is presented in Section 8.12.

**Proposition 8** (Necessary condition). Suppose $\psi, \phi \in C_b(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$ are positive definite functions on $\mathbb{R}^d$ with Fourier transforms $\psi^\wedge$ and $\phi^\wedge$ respectively. Let $\mathcal{H}$ and $\mathcal{G}$ be the RKHSs associated with $k(x, y) = \psi(x - y)$ and $l(x, y) = \phi(x - y)$, $x, y \in \mathbb{R}^d$ respectively. For $1 \leq r \leq 2$, suppose the following hold:

(i) $\int \|\omega\|^2 \psi^\wedge(\omega) d\omega < \infty$;

(ii) $\|\phi^\wedge\|_r < \infty$;

(iii) $\frac{\|k(\cdot, \cdot)\|^2}{\|l(\cdot, \cdot)\|} \in L^{\frac{r}{2}}(\mathbb{R}^d)$;

(iv) $\|q_0\|_{L^r(\mathbb{R}^d)} < \infty$.

Then $f_0 \in \mathcal{R}(C)$ implies $f_0 \in \mathcal{G} \subset \mathcal{H}$.

In the following, we apply the above result in two examples involving Gaussian and Matérn kernels to get insights into the range space assumption.

**Example 2** (Gaussian kernel). Let $\psi(x) = e^{-\sigma \|x\|^2}$ with $\mathcal{H}_\sigma$ as its corresponding RKHS (see Section 2 for its definition). By Proposition 8 it is easy to verify that $f_0 \in \mathcal{R}(C)$ implies $f_0 \in \mathcal{H}_\alpha \subset \mathcal{H}_\sigma$ for $\frac{d}{2} \leq \alpha \leq \sigma$. Since $\mathcal{H}_\beta \subset \mathcal{H}_\alpha$ for $\beta < \gamma$ (i.e., Gaussian RKHSs are nested), $f_0 \in \mathcal{R}(C)$ ensures that $f_0$ at least lies in $\mathcal{H}_{\frac{d}{2} + \epsilon}$ for arbitrary small $\epsilon > 0$.

**Example 3** (Matérn kernel). Let $\psi(x) = \frac{\Gamma(s + \frac{d}{2})}{\Gamma(s - \frac{d}{2}) \Gamma(d/2)} \|x\|^{s - \frac{d}{2}} r_{d/2 - s}(\|x\|)$, $x \in \mathbb{R}^d$ with $H^s_2(\mathbb{R}^d)$ as its corresponding RKHS (see Section 2 for its definition) where $s > \frac{d}{2}$. By Proposition 8 we have that if $g_0 \in L^r(\mathbb{R}^d)$ for some $1 \leq r \leq 2$ and $f_0 \in \mathcal{R}(C)$, then $f_0 \in H^s_2(\mathbb{R}^d) \subset H^s_2(\mathbb{R}^d)$ for $1 + \frac{d}{2} - s \leq \alpha < 2s - 1 - \frac{(2s - 1)}{2r}$. Since $H^s_2(\mathbb{R}^d) \subset H^s_2(\mathbb{R}^d)$ for $\gamma < \beta$ (i.e., Sobolev spaces are nested), this means $f_0$ should at least lie in $H^s_2(\mathbb{R}^d) - \epsilon(\mathbb{R}^d)$ for arbitrarily small $\epsilon > 0$, i.e., $f_0$ has at least $2s - 1 - \frac{(d - 1)}{2r}$ weak-derivatives. By the minimax theory [28, Chapter 2], it is well known that for any $\alpha > \beta \geq 0$,

$$\inf_{f_0 \in H^s_2(\mathbb{R}^d)} \sup_{f_n} \|f_n - f_0\|_{H^s_2(\mathbb{R}^d)} \asymp n^{-\frac{\alpha - \beta}{s + 1}}$$

where the infimum is taken over all possible estimators and $\asymp$ means “proportional up to constants.” Suppose $f_0 \notin H^s_2(\mathbb{R}^d)$ for $\alpha = 2s - 1 - \frac{(d - 1)}{2r}$, which means $f_0 \in H^s_2(\mathbb{R}^d)$ for arbitrarily small $\epsilon > 0$. This implies that
the rate of $n^{-1/4}$ obtained in Theorem 2 is minimax optimal if $\mathcal{H}$ is chosen to be $H_2^{1+\frac{d}{p}+r}(\mathbb{R}^d)$. This example also explains away the dimension independence of the rate provided by Theorem 3 by showing that the dimension effect is captured in the relative smoothness of $f_0$ w.r.t. $\mathcal{H}$.

While Example 3 provides some understanding about the minimax optimality of $f_{\lambda,n}$ under additional assumptions on $f_0$, the problem is not completely resolved. A sufficient condition for the range space assumption should provide a complete picture about the optimality of $f_{\lambda,n}$, although this remains an open question. In the following section, however, we show that the rate in Theorems 3 is not optimal for $\beta > 1$, and that improved rates can be obtained by choosing the regularizer appropriately.

### 4.3 Choice of regularizer

We understand from the characterization of $\mathcal{R}(C^\beta)$ in (10) that larger $\beta$ values yield smoother functions in $\mathcal{R}(C^\beta)$. However, the smoothness of $f_0 \in \mathcal{R}(C^\beta)$ for $\beta > 1$ is not captured in the rates in Theorem 3(ii), where the rate saturates at $\beta = 1$ providing the best possible rate of $n^{-1/4}$ (irrespective of the size of $\beta$). This is unsatisfactory on the part of the estimator, as it does not effectively capture the smoothness of $f_0$. We remind the reader that the estimator $f_{\lambda,n}$ is obtained by minimizing the regularized empirical Fisher divergence (see Theorem 3(iv)) yielding $f_{\lambda,n} = -\langle \hat{C} + \lambda I \rangle^{-1}\hat{\xi}$, which can be seen as a heuristic to solve the (non-linear) inverse problem $Cf_0 = -\xi$ (see Theorem 3(ii)) from finite samples, by replacing $C$ and $\xi$ with their empirical counterparts. This heuristic, which ensures that the finite sample inverse problem is well-posed, is popular in inverse problem literature under the name of Tikhonov regularization [12, Chapter 5]. Note that Tikhonov regularization helps to make the ill-posed inverse problem well-defined by approximating a well-posed one by approximating $\alpha$ with their empirical counterparts. This heuristic, which can be infinite dimensional, is not invertible and therefore the regularized estimator is constructed as $f_{\lambda,n} = -g_\lambda(C)\hat{\xi}$ where $g_\lambda(C)$ is defined through functional calculus (see [12 Section 2.3]) as

$$g_\lambda(C) = \sum_{i \in I} g_\lambda(\hat{\alpha}_i)\langle \hat{\phi}_i \rangle_C \hat{\phi}_i$$

with $g_\lambda : \mathbb{R}_+ \to \mathbb{R}$ and $g_\lambda(\alpha) := (\alpha + \lambda)^{-\gamma}$. Since the Tikhonov regularization is well-known to saturate (as explained above) — see [12 Sections 4.2 and 5.1] for details — better approximations to $\alpha^{-1}$ have been used in the inverse problems literature to improve the rates by using $g_\lambda$ other than $(\alpha + \lambda)^{-\gamma}$ where $g_\lambda(\alpha) \to \alpha^{-1}$ as $\lambda \to 0$. In the statistical context, [29, 3] have used the ideas from [12] in non-parametric regression for learning a square integrable function from finite samples through regularization in RKHS. In the following, we use these ideas to construct an alternate estimator for $f_0$ (and therefore for $p_0$) that appropriately captures the smoothness of $f_0$ by providing a better convergence rate when $\beta > 1$. To this end, we need the following assumption — quoted from [12 Theorems 4.1–4.3 and Corollary 4.4] and [3] Definition 1— that is standard in the theory of inverse problems.

(E) There exists finite positive constants $A_g$, $B_g$, $C_g$, $\eta_0$ and $(\gamma_\eta)_{\eta \in (0, \eta_0]}$ (all independent of $\lambda > 0$) such that $g_\lambda : [0, dE^2_{\lambda}] \to \mathbb{R}$ satisfies:

$$(a) \sup_{\alpha \in D} |\alpha g_\lambda(\alpha)| \leq A_g, \quad (b) \sup_{\alpha \in D} |g_\lambda(\alpha)| \leq \frac{B_g}{\lambda}, \quad (c) \sup_{\alpha \in D} |1 - \alpha g_\lambda(\alpha)| \leq C_g \text{ and } (d) \sup_{\alpha \in D} |1 - \alpha g_\lambda(\alpha)| \eta^\gamma \leq \gamma_\eta \lambda^\gamma, \quad \forall \eta \in (0, \eta_0] \text{ where } D := [0, dE^2_{\lambda}].$$

The constant $\eta_0$ is called the qualification of $g_\lambda$ which is what determines the point of saturation of $g_\lambda$. We show in Theorem 3 that if $g_\lambda$ has a finite qualification, then the resultant estimator cannot fully exploit the smoothness of $f_0$ and therefore the rate of convergence will suffer for $\beta > \eta_0$. Given $g_\lambda$ that satisfies (E), we construct our estimator of $f_0$ as

$$f_{g,\lambda,n} = -g_\lambda(C)\hat{\xi}.$$  

Note that the above estimator can be obtained by using the data dependent regularizer, $\frac{1}{2}\langle f, (g_\lambda(C))^{-1} - \hat{C} \rangle f|_{C}$ in the minimization of $\tilde{J}(f)$ defined in Theorem 3(iv), i.e.,

$$f_{g,\lambda,n} = \arg \inf_{f_{C}} \tilde{J}(f) + \frac{1}{2} \langle f, (g_\lambda(C))^{-1} - \hat{C} \rangle f|_{C}.$$
However, unlike $f_{\lambda,n}$ for which a simple form is available in Theorem 4 by solving a linear system, we are not able to obtain such a nice expression for $f_{g,\lambda,n}$. The following result (proved in Section 8.13) presents an analog of Theorems 5 and 6 for the new estimators, $f_{g,\lambda,n}$ and $p_{f_{g,\lambda,n}}$.

**Theorem 9** (Consistency and convergence rates for $f_{g,\lambda,n}$ and $p_{f_{g,\lambda,n}}$). Suppose (A)–(E) hold with $\varepsilon = 2$.

(i) If $f_0 \in \mathcal{R}(C^3)$ for some $\beta > 0$, then for any $\lambda \geq n^{-1/2}$,

$$
\|f_{g,\lambda,n} - f_0\|_{\mathcal{C}} = O_p(\theta_n),
$$

where $\theta_n := n^{-\min\{\frac{\beta}{2(\beta+1)}, \frac{\eta_0}{2(\lambda+1)}\}}$ with $\lambda = n^{-\max\{\frac{1}{2(\beta+1)}, \frac{1}{2(\lambda+1)}\}}$. In addition, if $\|k\|_{\infty} < \infty$, then for any $1 < r \leq \infty$ with $q_0 \in L^1(\Omega) \cap L^r(\Omega)$,

$$
\|p_{f_{g,\lambda,n}} - p_0\|_{L^r(\Omega)} = O_p(\theta_n), \ h(p_0, p_{f_{g,\lambda,n}}) = O_p(\theta_n) \text{ and } KL(p_0\|p_{f_{g,\lambda,n}}) = O_p(\theta_n^2).
$$

(ii) If $f_0 \in \mathcal{R}(C^3)$ for some $\beta \geq 0$, then for any $\lambda \geq n^{-1/2}$,

$$
J(p_0\|p_{f_{g,\lambda,n}}) = O_p\left(n^{-\min\{\frac{\beta}{2(\beta+1)}, \frac{\eta_0}{2(\lambda+1)}\}}\right)
$$

with $\lambda = n^{-\min\{\frac{1}{2}, \frac{\eta_0}{2(\lambda+1)}\}}$.

(iii) If $\|C^{-1}\| < \infty$, then for any $\lambda \geq n^{-1/2}$,

$$
\|f_{g,\lambda,n} - f_0\|_{\mathcal{C}} = O_p(\theta_n) \text{ and } J(p_0\|p_{f_{g,\lambda,n}}) = O_p(\theta_n^2)
$$

with $\theta_n = n^{-\frac{1}{4}}$ and $\lambda = n^{-\min\{\frac{1}{2}, \frac{\eta_0}{\lambda}\}}$.

Theorem 9 shows that if $g_\lambda$ has infinite qualification, then smoothness of $f_0$ is fully captured in the rates and as $\beta \to \infty$, we attain $O_p(n^{-1/2})$ rate for $\|f_{g,\lambda,n} - f_0\|_{\mathcal{C}}$ in contrast to $n^{-1/4}$ (similar improved rates are also obtained for $p_{f_{g,\lambda,n}}$ in various distances) in Theorem 6. In the following example, we present two choices of $g_\lambda$ that improve on Tikhonov regularization. We refer the reader to [29, Section 3.1] for more examples of $g_\lambda$.

**Example 4** (Choices of $g_\lambda$). (i) **Tikhonov regularization** involves $g_\lambda(\alpha) = (\alpha + \lambda)^{-1}$ for which it is easy to verify that $\eta_0 = 1$ and therefore the rates saturate at $\beta = 1$, leading to the results in Theorems 6 and 7.

(ii) **Showalter’s method and spectral cut-off** use

$$
g_\lambda(\alpha) = \frac{1 - e^{-\alpha/\lambda}}{\alpha} \quad \text{and} \quad g_\lambda(\alpha) = \begin{cases} 
\frac{1}{\alpha}, & \alpha \geq \lambda \\
0, & \alpha < \lambda
\end{cases}
$$

respectively for which it is easy to verify that $\eta_0 = +\infty$ (see [12, Examples 4.7 & 4.8] for details) and therefore improved rates are obtained for $\beta > 1$ in Theorem 4 compared to that of Tikhonov regularization.

## 5 Density estimation in $\mathcal{P}$: Misspecified case

In this section, we analyze the misspecified case where $p_0 \notin \mathcal{P}$, which is a more reasonable case than the well-specified one, as in practice it is not easy to check whether $p_0 \in \mathcal{P}$. To this end, we consider the same estimator $p_{f_{g,\lambda,n}}$ as considered in the well-specified case where $f_{\lambda,n}$ is obtained from Theorem 4. The following result shows that $J(p_0\|p_{f_{g,\lambda,n}}) \rightarrow \inf_{p \in \mathcal{P}} J(p_0\|p)$ as $\lambda \rightarrow 0$, $\lambda n \rightarrow \infty$ and $n \rightarrow \infty$ under the assumption that there exists $f^* \in \mathcal{F}$ such that $J(p_0\|p_{f^*}) = \inf_{p \in \mathcal{P}} J(p_0\|p)$. We present the result for bounded kernels although it can be easily extended to unbounded kernels as in Theorem 7. Also, the presented result for Tikhonov regularization extends easily to $p_{f_{g,\lambda,n}}$ using the ideas in the proof of Theorem 9. Note that unlike in the well-specified case where convergence in other distances can be shown even though the estimator is constructed from $J$, it is difficult to show such a result in the misspecified case.
Theorem 10. Let \( p_0, q_0 \in C^1(\Omega) \) be probability densities such that \( J(p_0\|q_0) < \infty \) where \( \Omega \) satisfies (A). Assume that (B), (C) and (D) with \( \varepsilon = 2 \) hold. Suppose \( \|k\|_{\infty} < \infty \), \( E_1 := \sup_{x \in \Omega, t \in [a]} \left\| \frac{\partial k(x)}{\partial x_t} \right\|_{\infty} < \infty \) and there exists \( f^* \in \mathcal{F} \) such that \( J(p_0\|p_{f^*}) = \inf_{p \in \mathcal{P}} J(p_0\|p) \). Then for an estimator \( p_{f_{\lambda,n}} \) constructed from random samples \( (X_i)_{i=1}^n \) drawn i.i.d. from \( p_0 \), where \( f_{\lambda,n} \) is defined in \( \mathcal{F} \)—also see Theorem 3(iv)—with \( \lambda > 0 \), we have

\[
J(p_0\|p_{f_{\lambda,n}}) \rightarrow \inf_{p \in \mathcal{P}} J(p_0\|p) \quad \text{as} \quad \lambda \to 0, \ \lambda n \to \infty \quad \text{and} \quad n \to \infty.
\]

In addition, if \( f^* \in \mathcal{R}(C^\beta) \) for some \( \beta \geq 0 \), then

\[
\sqrt{J(p_0\|p_{f_{\lambda,n}})} \leq \sqrt{\inf_{p \in \mathcal{P}} J(p_0\|p)} + O_{p_0}\left(n^{-\min\left\{\frac{\beta+1}{2\beta+1}, 1\right\}}\right)
\]

with \( \lambda = n^{-\max\left\{\frac{1}{2\beta+1}, 1\right\}} \). If \( \|C^{-1}\| < \infty \), then

\[
\sqrt{J(p_0\|p_{f_{\lambda,n}})} \leq \sqrt{\inf_{p \in \mathcal{P}} J(p_0\|p)} + O_{p_0}\left(\frac{1}{n^{\frac{1}{\beta}}}\right)
\]

with \( \lambda = n^{-\frac{1}{\beta}} \).

While the above result is useful and interesting, the assumption about the existence of \( f^* \) is quite restrictive. This is because if \( p_0 \) (which is not in \( \mathcal{P} \)) belongs to a family \( \mathcal{Q} \) where \( \mathcal{P} \) is dense in \( \mathcal{Q} \) w.r.t. \( J \), then there is no \( f \in \mathcal{H} \) that attains the infimum, i.e., \( f^* \) does not exist and therefore the proof technique employed in Theorem 10 will fail. In the following, we present a result (Theorem 12) that does not require the existence of \( f^* \) but attains the same result as in Theorem 10 but requiring a more complicated proof. Before we present Theorem 12, we need to introduce some notation.

To this end, let us return to the objective function under consideration,

\[
J(p_0\|p_f) = \frac{1}{2} \int p_0(x) \left\| \frac{\partial}{\partial x} \log \frac{p_0}{p_f} \right\|_2^2 dx = \frac{1}{2} \int p_0(x) \sum_{i=1}^d \left( \frac{\partial f_i}{\partial x_i} - \frac{\partial f}{\partial x_i} \right)^2 dx,
\]

where \( f_* = \log \frac{p_0}{q_0} \) and \( p_0 \notin \mathcal{P} \). Define

\[
\mathcal{W}_2(p_0) := \{ f \in C^1(\Omega) : \partial^\alpha f \in L^2(\Omega, p_0), \ \forall |\alpha| = 1 \}.
\]

This is a reasonable class of functions to consider as under the condition \( J(p_0\|q_0) < \infty \), it is clear that \( f_* \in \mathcal{W}_2(p_0) \). Endowed with a semi-norm,

\[
\|f\|_{\mathcal{W}_2}^2 := \sum_{|\alpha| = 1} \|\partial^\alpha f\|_{L^2(\Omega, p_0)}^2,
\]

\( \mathcal{W}_2(p_0) \) is a vector space of functions, from which a normed space can be constructed as follows. Let us define \( f, f' \in \mathcal{W}_2(p_0) \) to be equivalent, i.e., \( f \sim f' \), if \( \|f - f'\|_{\mathcal{W}_2} = 0 \). In other words, \( f \sim f' \) if and only if \( f \) and \( f' \) differ by a constant \( p_0 \)-almost everywhere. Now define the quotient space \( \mathcal{W}_2^\sim(p_0) := \{ [f] : f \in \mathcal{W}_2(p_0) \} \) where \( [f] := \{ f' \in \mathcal{W}_2(p_0) : f \sim f' \} \) denotes the equivalence class of \( f \). Defining \( \|f\|_{\mathcal{W}_2^\sim} := \|f\|_{\mathcal{W}_2} \), it is easy to verify that \( \| \cdot \|_{\mathcal{W}_2^\sim} \) defines a norm on \( \mathcal{W}_2^\sim(p_0) \). In addition, endowing the following bilinear form on \( \mathcal{W}_2^\sim(p_0) \)

\[
\langle [f], [g] \rangle_{\mathcal{W}_2^\sim} := \int p_0(x) \sum_{|\alpha| = 1} (\partial^\alpha f)(x)(\partial^\alpha g)(x) dx
\]

makes it a pre-Hilbert space. Let \( \mathcal{W}_2(p_0) \) be the Hilbert space obtained by completion of \( \mathcal{W}_2^\sim(p_0) \). As shown in Proposition 11 below, under some assumptions, a continuous mapping \( I_k : \mathcal{H} \to \mathcal{W}_2(p_0), f \mapsto [f] \), can be defined, which is injective modulo constant functions. Since addition of a constant does not contribute to \( p_f \), the space \( \mathcal{W}_2(p_0) \) can be regarded as a parameter space extended from \( \mathcal{H} \). In addition to \( I_k \), Proposition 11 (proved in Section 8.13) describes the adjoint of \( I_k \) and relevant self-adjoint operators, which will be useful in analyzing \( p_{f_{\lambda,n}} \) in Theorem 12.
**Proposition 11.** Let supp($q_0$) = $\Omega$ where $\Omega \subset \mathbb{R}^d$ is non-empty and open. Suppose $k$ satisfies (B) and $\left\| \frac{\partial k(-,x)}{\partial x_i} \right\|_{\mathcal{H}} \in L^2(p_0)$ for all $i \in [d]$. Then $I_k : \mathcal{H} \rightarrow W_2(p_0)$, $f \mapsto [f]_\sim$ defines a continuous mapping with the null space $\mathcal{H} \cap \mathbb{R}$. The adjoint of $I_k$ is $S_k : W_2(p_0) \rightarrow \mathcal{H}$ whose restriction to $W_2^\sim(p_0)$ is given by

$$S_k[h]_\sim(y) = \int \sum_{i=1}^d \frac{\partial k(y,x)}{\partial x_i} \frac{\partial h(x)}{\partial x_i} p_0(x) \, dx, \quad [h]_\sim \in W_2^\sim(p_0), \ y \in \Omega.$$ 

In addition, $I_k$ and $S_k$ are Hilbert-Schmidt and therefore compact. Also, $E_k := S_k I_k$ and $T_k := I_k S_k$ are compact, positive and self-adjoint operators on $\mathcal{H}$ and $W_2(p_0)$ respectively where

$$E_k g(y) = \int \sum_{i=1}^d \frac{\partial k(y,x)}{\partial x_i} \frac{\partial g(x)}{\partial x_i} p_0(x) \, dx, \quad g \in \mathcal{H}, \ y \in \Omega$$

and the restriction of $T_k$ to $W_2^\sim(p_0)$ is given by

$$T_k[h]_\sim = \left[ \int \sum_{i=1}^d \frac{\partial k(y,x)}{\partial x_i} \frac{\partial h(x)}{\partial x_i} p_0(x) \, dx \right]_\sim, \quad [h]_\sim \in W_2^\sim(p_0).$$

Note that for $[h]_\sim \in W_2^\sim(p_0)$, the derivatives $\frac{\partial h}{\partial x}$ do not depend on the choice of a representative element almost surely w.r.t. $p_0$, and thus the above integrals are well defined. Having constructed $W_2(p_0)$, it is clear that $J(p_0\|p_f) = \frac{1}{2}\|f_*\|_{W_2}^2 - I_k f \|_{W_2}^2$, which means estimating $p_0$ is equivalent to estimating $f_*$ in $W_2(p_0)$ by $f \in \mathcal{F}$. With all these preparations, we are now ready to present a result (see Section 8.16 for a proof) on consistency and convergence rate for $p_{\lambda,n}$, without assuming the existence of $f^*$.

**Theorem 12.** Let $p_0$, $q_0 \in C^1(\Omega)$ be probability densities such that $J(p_0\|q_0) < \infty$. Assume that (A)-(D) hold with $\varepsilon = 2$. Let $\|C^{-1}\| < \infty$ and $E_1 := \sup_{x \in \Omega, i \in [d]} \left\| \frac{\partial k(-,x)}{\partial x_i} \right\|_{\mathcal{H}} < \infty$. Then the following hold.

(i) As $\lambda \rightarrow 0$, $\lambda n \rightarrow \infty$ and $n \rightarrow \infty$,

$$J(p_0\|p_{\lambda,n}) \rightarrow \inf_{p \in \mathcal{P}} J(p_0\|p).$$

(ii) Define $f_* := \log \frac{p_0}{q_0}$. If $[f_*]_\sim \in \mathcal{R}(T_k)$, then

$$J(p_0\|p_{\lambda,n}) \rightarrow 0 \text{ as } \lambda \rightarrow 0, \ \lambda n \rightarrow \infty \text{ and } n \rightarrow \infty.$$

In addition, if $[f_*]_\sim \in \mathcal{R}(T_k^{\beta})$ for some $\beta > 0$, then

$$J(p_0\|p_{\lambda,n}) = O_{p_0}\left(n^{-\min\left\{\frac{\beta}{2}, \frac{\beta}{2\beta + 1}\right\}}\right)$$

with $\lambda = n^{-\max\left\{\frac{1}{2\beta}, \frac{1}{3}\right\}}$.

(iii) If $\|E_k^{-1}\| < \infty$ and $\|T_k^{-1}\| < \infty$, then $J(p_0\|p_{\lambda,n}) = O_{p_0}(n^{-1})$ with $\lambda = n^{-\frac{1}{2}}$.

**Remark 5.** (i) The result in Theorem 12(ii) is particularly interesting as it shows that $[f_*]_\sim \in W_2(p_0) \setminus I_k(\mathcal{H})$ can be consistently estimated by $p_{\lambda,n} \in \mathcal{P}$, in which turn implies that certain $p_0 \in \mathcal{P}$ can be consistently estimated by $p_{\lambda,n} \in \mathcal{P}$. In particular, if $S_k$ is injective, then $I_k(\mathcal{H})$ is dense in $W_2(p_0)$ w.r.t. $\|\cdot\|_{W_2}$, which implies $\inf_{p \in \mathcal{P}} J(p_0\|p) = 0$ though there does not exist $f^* \in \mathcal{H}$ for which $J(p_0\|p_{f^*}) = 0$. While Theorem 10 cannot handle this situation, (i) and (ii) in Theorem 12 coincide showing that $p_0 \notin \mathcal{P}$ can be consistently estimated by $p_{\lambda,n} \in \mathcal{P}$. While the question of when $I_k(\mathcal{H})$ is dense in $W_2(p_0)$ is open, we refer the reader to Section 8.17 for a related discussion.

(ii) Replicating the proof of Theorem 4.6 in [30], it is easy to show that for all $0 < \gamma < 1$, $\mathcal{R}(T_k^{\frac{1}{\gamma}}) = \left[ W_2(p), I_k(\mathcal{H}) \right]_{\gamma, 2}$, where the r.h.s. is an interpolation space obtained through the real interpolation of $W_2(p_0)$ and $I_k(\mathcal{H})$ (see Section 8.11 for the notation and definition). Here $I_k(\mathcal{H})$ is endowed with the Hilbert space structure by $I_k(\mathcal{H}) \cong \mathcal{H} / \mathbb{R}$. This interpolation space interpretation means that, for $\beta \geq \frac{1}{2}$, $\mathcal{R}(T_k^{\beta}) \subset \mathcal{H}$ modulo constant functions. It is nice to note that the rates in Theorem 12(ii) for $\beta \geq \frac{1}{2}$ match with the rates in Theorem 8 (i.e., the well-specified case) w.r.t. $J$.
for $0 \leq \beta \leq \frac{1}{2}$. We highlight the fact that $\beta = 0$ corresponds to $\mathcal{H}$ in Theorem 5 whereas $\beta = \frac{1}{2}$ corresponds to $\mathcal{H}$ in Theorem 12 ii) and therefore the range of comparison is for $\beta \geq \frac{1}{2}$ in Theorem 12 ii) versus $0 \leq \beta \leq \frac{1}{2}$ in Theorem 6. In contrast, Theorem 14 is very limited as it only provides a rate for the convergence of $J(p_0||p_{j, n})$ to inf$_{p \in \mathcal{P}} J(p_0||p)$ assuming that $f_*$ is sufficiently smooth.

Based on the observation in Remark 5 i) that inf$_{p \in \mathcal{P}} J(p_0||p) = 0$ if $I_k(\mathcal{H})$ is dense in $W_2(p_0)$ w.r.t. $\|\cdot\|_{W_2}$, it is possible to obtain an approximation result for $\mathcal{P}$ (similar to those discussed in Section 3) w.r.t. Fisher divergence as shown below, whose proof is provided in Section 8.18.

**Proposition 13.** Suppose (A) holds. Let $q_0 \in C^1(\Omega)$ be a probability density and

$$\mathcal{P}_{FD} := \left\{ p \in C^1(\Omega) : \int_{\Omega} p(x) dx = 1, p(x) \geq 0, \forall x \in \Omega \text{ and } J(p||q_0) < \infty \right\}.$$  

For any $p \in \mathcal{P}_{FD}$, if $I_k(\mathcal{H})$ is dense in $W_2(p)$ w.r.t. $\|\cdot\|_{W_2}$, then for every $\epsilon > 0$, there exists $\tilde{p} \in \mathcal{P}$ such that $J(p||\tilde{p}) \leq \epsilon$.

### 6 Numerical simulations

We have proposed an estimator of $p_0$ that is obtained by minimizing the regularized empirical Fisher divergence and presented its consistency along with convergence rates. As discussed in Section 4 however one can simply ignore the structure of $\mathcal{P}$ and estimate $p_0$ in a completely non-parametric fashion, for example using the kernel density estimator (KDE). In fact, consistency and convergence rates of KDE are also well-studied [38, Chapter 1] and the kernel density estimator is very simple to compute—requiring only $O(n)$ computations—compared to the proposed estimator, which is obtained by solving a linear system of size $(nd+1) \times (nd+1)$. This raises questions about the applicability of the proposed estimator in practice, though it is very well known that KDE performs poorly for moderate to large $d$ [12, Section 6.5]. In this section, we numerically demonstrate that the proposed score matching estimator performs significantly better than the KDE, and in particular, that the advantage with the proposed estimator grows as $d$ gets large. Note further that the maximum likelihood approach of [2, 14] does not yield estimators that are practically feasible, and therefore to the best of our knowledge, the proposed estimator is the only viable estimator for estimating densities through $\mathcal{P}$.

We consider the problems of estimating a standard normal distribution on $\mathbb{R}^d$, $N(0, I_d)$ and mixture of Gaussians, through the score matching approach and KDE, and compare their estimation accuracies. Here $\phi_d(x; \mu, \Sigma)$ is the p.d.f. of $N(\mu, \Sigma I_d)$. By choosing the kernel, $k(x, y) = \exp(- \frac{\|x-y\|^2}{2\sigma^2}) + r(x^T y + c)^2$, which is a Gaussian plus polynomial of degree 2, it is easy to verify that Gaussian distributions lie in $\mathcal{P}$, and therefore the first problem considers the well-specified case while the second problem deals with the misspecified case. In our simulations, we chose $r = 0.1$, $c = 0.5$, $\alpha = 4$ and $\beta = -4$. The bandwidth parameter $\sigma$ and the regularization parameter $\lambda$ are chosen by cross-validation (CV) of the objective function $J_\lambda$ (see Theorem 5 iv)). For KDE, the Gaussian kernel is used for the smoothing kernel, and the bandwidth parameter is chosen by cross-validation, where for both the methods, 5-fold CV is applied. Since it is difficult to accurately estimate the normalization constant in the proposed method, we use two methods to evaluate the accuracy of estimation. One is the objective function for the score matching method,

$$\hat{J}(p) = \sum_{i=1}^d \int \left( \frac{1}{2} \left| \frac{\partial \log p(x)}{\partial x_i} \right|^2 + \frac{\partial^2 \log p(x)}{\partial x_i^2} \right) p_0(x) dx,$$

and the other is correlation of the estimator with the true density function,

$$\text{Cor}(p, p_0) := \frac{\mathbb{E}_R[p(X)p_0(X)]}{\sqrt{\mathbb{E}_R[p(X)^2]\mathbb{E}_R[p_0(X)^2]}}$$

where $R$ is a probability distribution. For $R$, we use the empirical distribution based on 10000 random samples drawn i.i.d. from $p_0(x)$. 

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Figure 1: Experimental comparisons with the score objective function: proposed method and kernel density estimator

Figures 1 and 2 show the score objective function ($\tilde{J}(p)$) and the correlation ($\text{Cor}(p, p_0)$) (along with their standard deviation as error bars) of the proposed estimator and KDE for the tasks of estimating a Gaussian and a mixture of Gaussians, for different sample sizes ($n$) and dimensions ($d$). From the figures, we see that the proposed estimator outperforms (i.e., lower function values) KDE in all the cases except the low dimensional cases (($n, d$) = (500, 2) for the Gaussian, and ($n, d$) = (300, 2), (300, 4) for the Gaussian mixture). In the case of the correlation measure, the score matching method yields better results (i.e., higher correlation) besides in the Gaussian mixture cases of $d = 2, 4, 6$.

The proposed method shows an increased advantage over KDE as the dimensionality increases, thereby demonstrating the advantage of the proposed estimator for high dimensional data.

7 Summary & discussion

We have considered an infinite dimensional generalization, $\mathcal{P}$, of the finite-dimensional exponential family, where the densities are indexed by functions in a reproducing kernel Hilbert space (RKHS), $\mathcal{H}$. We showed that $\mathcal{P}$ is a rich object that can approximate a large class of probability densities arbitrarily well in Kullback-Leibler divergence, and addressed the main question of estimating an unknown density, $p_0$ from finite samples drawn i.i.d. from it, in well-specified ($p_0 \in \mathcal{P}$) and misspecified ($p_0 \notin \mathcal{P}$) settings. We proposed a density estimator based on minimizing the regularized version of the empirical Fisher divergence, which results in solving a simple finite-dimensional linear system. Our estimator provides a computationally efficient alternative to maximum likelihood based estimators, which suffer from the computational intractability of the log-partition function. The proposed estimator is also shown to empirically outperform the classical kernel density estimator, with advantage increasing as the dimension of the space increases. In addition to these computational and empirical results, we have established the consistency and convergence rates under certain smoothness assumptions (e.g., $\log p_0 \in \mathcal{R}(C^\beta)$) for both well-specified and misspecified scenarios.

Two important questions still remain open in this work which we intend to address in our future work. First, the assumption $\log p_0 \in \mathcal{R}(C^\beta)$ is not well understood. Though we presented a necessary condition for this assumption (with $\beta = 1$) to hold for bounded continuous translation invariant kernels on $\mathbb{R}^d$, obtaining a sufficient condition can throw light on the minimax optimality of the proposed estimator. Another alternative is to directly study the minimax optimality of the rates for $0 < \beta \leq 1$ (for $\beta > 1$, we showed that the above mentioned rates can be improved by an
appropriate choice of the regularizer) by obtaining minimax lower bounds under the source condition \( \log p_0 \in \mathcal{R}(C^\beta) \), using the ideas in [10]. Second, the proposed estimator depends on the regularization parameter, which in turn depends on the smoothness scale \( \beta \). Since \( \beta \) is not known in practice, it is therefore of interest to construct estimators that are adaptive to unknown \( \beta \).

8 Proofs

We provide proofs of the results presented in Sections 1–5.

8.1 Relation between Fisher and Kullback-Leibler divergences

The following result provides a relationship between Fisher and Kullback-Leibler divergences.

**Proposition 8.1.** Let \( p \) and \( q \) be probability densities defined on \( \mathbb{R}^d \). Define \( p_t := p * N(0, tI_d) \) and \( q_t := q * N(0, tI_d) \) where \(*\) denotes the convolution and \( N(0, tI_d) \) denotes a normal distribution on \( \mathbb{R}^d \) with mean zero and diagonal covariance with \( t > 0 \). Suppose \( p_t \) and \( q_t \) satisfy

\[
\frac{\partial p_t}{\partial x_i} \log p_t(x) \to 0, \quad \frac{\partial p_t}{\partial x_i} \log q_t(x) \to 0, \quad \frac{\partial \log q_t}{\partial x_i} p_t(x) \to 0 \quad \text{as} \quad x_i \to \pm \infty, \forall i = 1, \ldots, d.
\]

Then

\[
KL(p\|q) = \int_0^\infty J(p_t\|q_t) \, dt,
\]

where \( J \) is defined in (5).

**Proof.** Under the conditions mentioned on \( p_t \) and \( q_t \), it can be shown that

\[
\frac{d}{dt} KL(p_t\|q_t) = -J(p_t\|q_t).
\]

\[
(11)
\]
See Theorem 1 in \cite{26} for a proof. The above identity is a simple generalization of de Bruijn’s identity that relates the Fisher information to the derivative of the Shannon entropy (see \cite{9} Theorem 16.6.2). Integrating w.r.t. $t$ on both sides of (12), we obtain $KL(p_\eta || q_\eta) \to 0$ as $t \to \infty$ and $KL(p_\eta || q) \to KL(p || q)$ as $t \to 0$.

\section{8.2 Proof of Proposition 1}

Proposition 5 shows that $H$ is dense in $C_0(\Omega)$ w.r.t. uniform norm if and only if $k$ satisfies (1). Therefore, the denseness in $L^1$, KL and Hellinger distances follow trivially from Lemma A.1. For $L^r$ norm ($r > 1$), the denseness follows by using the bound $\|p_f - p_g\|_{L^r(\Omega)} \leq 2e^{2\|f-g\|_{\infty}} e^{2\|f\|_{\infty}} \|q_0\|_{L^r(\Omega)}$ obtained from Lemma A.1(i) with $f \in C_0(\Omega)$ and $g \in H$.

\section{8.3 Proof of Corollary 2}

For any $p \in P$, define $p_0 := \frac{p + \delta}{p + q_0 \delta}$. Note that $p_0(x) > 0$ for all $x \in \Omega$ and $\|p - p_0\|_{L^1(\Omega)} = \frac{\delta \|p - q_0\|_{L^1(\Omega)}}{1 + \delta}$, implying that $\lim_{\delta \to 0} \|p - p_0\|_{L^1(\Omega)} = 0$ for any $1 \leq r \leq \infty$. This means, for any $\epsilon > 0$, $\exists \epsilon_\delta > 0$ such that for any $0 < \theta < \epsilon$, we have $\|p - p_0\|_{L^1(\Omega)} \leq \epsilon$, where $p_0(x) > 0$ for all $x \in \Omega$.

Define $f := \log \frac{p}{q_0}$. It is clear $f \in C_0(\Omega)$ since $p, q_0 \in C_0(\Omega)$ and $\|p/q_0\|_{\infty} < \infty$. Fix any $\eta > 0$ and define $A := \{ x : f(x) \geq \eta \}$. Then there exists $\lambda_\eta > 0$ such that $A \subset B := \{ x : q_0(x) \geq \lambda_\eta \}$ and therefore $A \subset C := \{ x : p(x) \geq \lambda_\eta (e^{\eta} - \frac{g}{1+\eta})(1 + \theta) \}$, i.e., $A \subset B \cap C$. Since $p, q_0 \in C_0(\Omega)$, $B$ and $C$ are compact and so $A$ is compact for any $\eta > 0$, i.e., $f \in C_0(\Omega)$, which implies $p_0 \in P_0$, where $P_0$ is defined in Proposition 1. Since $p_0 \in P_0$, by Proposition 1 for any $\epsilon > 0$, there exists $p_\epsilon \in P$ such that $\|p_\epsilon - p_0\|_{L^1(\Omega)} \leq \epsilon$ under the assumption that $q_0 \in L^1(\Omega) \cap L^r(\Omega)$. Therefore $\|p - p_\epsilon\|_{L^1(\Omega)} \leq 2\epsilon$ for any $1 \leq r \leq \infty$, which proves the denseness of $P$ in $\mathcal{H}$, w.r.t. $L^r$ norm for any $1 \leq r \leq \infty$. Since $\log \frac{p}{q_0} \leq \sqrt{\|p - q\|_{L^1(\Omega)}}$ for any probability densities $p, q$, the denseness in Hellinger distance follows.

We now prove the denseness in KL divergence by noting that

$$KL(p || p_\epsilon) = \int_{p > 0} p \log \frac{p}{p_\epsilon} dx \leq \int_{p > 0} p \left( \frac{p + \delta}{p + q_0 \delta} - 1 \right) dx \leq \delta \int_{p > 0} (p - q_0) \frac{p}{p + q_0 \delta} dx \leq \delta \|p - q_0\|_{L^1(\Omega)} \leq 2\delta,$$

which implies $\lim_{\delta \to 0} KL(p || p_\epsilon) = 0$. This implies, for any $\epsilon > 0$, $\exists \epsilon_\delta > 0$ such that for any $0 < \theta < \epsilon$, $KL(p || p_\epsilon) \leq \epsilon$. Arguing as above, we have $p_\theta \in P_0$, i.e., there exists $f \in C_0(\Omega)$ such that $p_\theta = \frac{e^{\theta f} q_0}{e^{\theta f} q_0 dx}$. Since $H$ is dense in $C_0(\Omega)$, for any $f \in C_0(\Omega)$ and any $\epsilon > 0$, there exists $g \in H$ such that $\|f - g\|_{\infty} \leq \epsilon$. For $p_\epsilon \in P$, since $\int p \log \frac{p}{p_\epsilon} dx \leq \|\log \frac{p}{p_\epsilon}\|_{\infty} \leq 2 \|f - g\|_{\infty} \leq 2\epsilon$, we have

$$KL(p || p_\epsilon) = \int p \log \frac{p}{p_\epsilon} dx = \int p \log \frac{p}{p_\theta} dx + \int p \log \frac{p_\theta}{p_\epsilon} dx \leq 3\epsilon,$$

and the result follows.

\section{8.4 Proof of Theorem 3}

(i) By the reproducing property of $H$, since $\frac{\partial k(x, \cdot)}{\partial x_i} = \left( f, \frac{\partial k(x, \cdot)}{\partial x_i} \right)_H$ for all $i \in [d]$, it is easy to verify that

$$J(f) = \frac{1}{2} \int p_\theta(x) \sum_{i=1}^d \left( f - f_0, \frac{\partial k(x, \cdot)}{\partial x_i} \right)_H \frac{\partial k(x, \cdot)}{\partial x_i} dx$$

$$= \frac{1}{2} \int p_\theta(x) \sum_{i=1}^d \left( f - f_0, \left( \frac{\partial k(x, \cdot)}{\partial x_i} \otimes \frac{\partial k(x, \cdot)}{\partial x_i} \right) (f - f_0) \right)_H dx$$

$$= \frac{1}{2} \int p_\theta(x) (f - f_0, C_z(f - f_0))_H dx,$$

(13)
where in the second line, we used \( \langle a, b \rangle_H^2 = \langle a, b \rangle_H \langle a, b \rangle_H = \langle a, (b \otimes b) a \rangle_H \) for \( a, b \in H \) with \( H \) being a Hilbert space and \( C_x := \sum_{i=1}^d \frac{\partial k(\cdot, x)}{\partial x_i} \otimes \frac{\partial k(\cdot, x)}{\partial x_i} \). Observe that for all \( x \in \Omega \), \( C_x \) is a Hilbert-Schmidt operator as \( \|C_x\|_{HS} \leq \sum_{i=1}^d \left\| \frac{\partial k(\cdot, x)}{\partial x_i} \right\|_p^2 < \infty \) and \( (f - f_0) \otimes (f - f_0) \) is also Hilbert-Schmidt as \( \|(f - f_0) \otimes (f - f_0)\|_H^2 = \|f - f_0\|_{\mathcal{H}}^2 < \infty \).

Therefore, (13) is equivalent to \( \int (f - f_0) \cdot (f - f_0) \, dx < \infty \), \( C_x \) is \( p_0 \)-integrable in the Bochner sense (see (11) Definition 1, Theorem 2)), and therefore it follows from (11) Theorem 6) that \( J(f) = \langle f - f_0 \rangle_{\mathcal{H}} (f - f_0), C_x \rangle_{HS}, \) where \( C := \int C_x p_0(x) \, dx \) is the Bochner integral of \( C_x \), thereby yielding (13).

We now show that \( C \) is trace-class. Let \( (e_i)_{i \in \mathbb{N}} \) be an orthonormal basis in \( \mathcal{H} \) (a countable ONB exists as \( \mathcal{H} \) is separable—see Remark (i)). Define \( B := \sum_i \langle C e_i, e_i \rangle_{\mathcal{H}} \) so that
\[
B = \sum_i \int \langle e_i, C x e_i \rangle_{\mathcal{H}} \, dx = \sum_i \int \left( \sum_i \left( e_i, \frac{\partial k(\cdot, x)}{\partial x_i} \right) \right)^2 \, dx
\]
\[
= \left( \sum_i \frac{\partial k(\cdot, x)}{\partial x_i} \right)^2 \, dx
\]
which means \( C \) is trace-class and therefore compact. Here, we used monotone convergence theorem in (13), Parseval’s identity in (13). Note that \( C \) is positive since \( \langle f, C f \rangle_{\mathcal{H}} = \int p_0(x) \left\| \frac{\partial f}{\partial x} \right\|_{L^2}^2 \, dx \geq 0, \forall f \in \mathcal{H}. \)

(ii) From (13), we have \( J(f) = \frac{1}{2} \langle f, C f \rangle_{\mathcal{H}} - (\langle f, C f_0 \rangle_{\mathcal{H}} + \frac{1}{2} \langle f_0, C f_0 \rangle_{\mathcal{H}}). \) Using \( \frac{\partial f_0(x)}{\partial x_i} = \frac{\partial log f_0(x)}{\partial x_i} - \frac{\partial log q_0(x)}{\partial x_i} \) for all \( i \in [d], \) we obtain that for any \( f \in \mathcal{H}, \)
\[
\langle f, C f_0 \rangle_{\mathcal{H}} = \int p_0(x) \sum_{i=1}^d \frac{\partial f(x)}{\partial x_i} \frac{\partial f_0(x)}{\partial x_i} \, dx
\]
\[
= \sum_{i=1}^d \frac{\partial f(x)}{\partial x_i} \frac{\partial p_0(x)}{\partial x_i} \, dx - \int p_0(x) \sum_{i=1}^d \frac{\partial f(x)}{\partial x_i} \frac{\partial log q_0(x)}{\partial x_i} \, dx \]
\[
= -\int p_0(x) \sum_{i=1}^d \frac{\partial^2 f(x)}{\partial x_i^2} \, dx - \int p_0(x) \sum_{i=1}^d \frac{\partial f(x)}{\partial x_i} \frac{\partial log q_0(x)}{\partial x_i} \, dx \]
\[
= -\int p_0(x) \sum_{i=1}^d \left( f, \frac{\partial^2 k(\cdot, x)}{\partial x_i^2} + \frac{\partial k(\cdot, x)}{\partial x_i} \frac{\partial log q_0(x)}{\partial x_i} \right) \, dx \]
\[
= \langle f, -\xi \rangle_{\mathcal{H}},
\]
where (b) follows from partial integration under (C) and the equality in (c) is valid as \( \sum_{i=1}^d \left( \frac{\partial^2 k(\cdot, x)}{\partial x_i^2} + \frac{\partial k(\cdot, x)}{\partial x_i} \frac{\partial log q_0(x)}{\partial x_i} \right) \) is Bochner \( p_0 \)-integrable under (D) with \( \varepsilon = 1 \). Therefore \( C f_0 = -\xi \). For the third term,
\[
\langle f_0, C f_0 \rangle_{\mathcal{H}} = \int p_0(x) \sum_{i=1}^d \left( \frac{\partial f_0(x)}{\partial x_i} \right)^2 \, dx
\]
and the result follows.

(iii) Define \( c_0 := J(p_0 \| q_0) \). For any \( \lambda > 0 \), it is easy to verify that
\[
J_\lambda(f) = \frac{1}{2} \| (C + \lambda I)^{-1/2} f \|_{\mathcal{H}}^2 - \frac{1}{2} \langle f, (C + \lambda I)^{-1/2} f \rangle_{\mathcal{H}} + c_0.
\]
Clearly, \( J_\lambda(f) \) is minimized if and only if \( (C + \lambda I)^{-1/2} f = -(C + \lambda I)^{-1/2} \xi \) and therefore \( f_\lambda = -(C + \lambda I)^{-1} \xi \) is the unique minimizer of \( J_\lambda(f) \).

(iv) Since (iv) is similar to (iii) with \( C \) replaced by \( \hat{C} \) and \( \xi \) replaced by \( \hat{\xi} \), we obtain \( f_{\lambda,n} = (\hat{C} + \lambda I)^{-1} \hat{\xi} \).
8.5 Proof of Theorem 4

From Theorem 3(iv), we have
\[ J_\lambda(f) = \frac{1}{2} \langle f, \hat{C} \rangle_\mathcal{H} + \langle f, \hat{\xi} \rangle_\mathcal{H} + \frac{\lambda}{2} \| f \|^2_\mathcal{H} \]
\[ = \frac{1}{2n} \sum_{i=1}^n \left( \frac{\partial k_i(X, \cdot)}{\partial x_i} \right) \hat{f}_i + \langle f, \hat{\xi} \rangle_\mathcal{H} + \frac{\lambda}{2} \| f \|^2_\mathcal{H}. \]

Define \( \mathcal{H}_\perp := \text{span}\left\{ \hat{\xi}, \frac{\partial k_i(X, \cdot)}{\partial x_i} \right\}_{b_j} \), which is a closed subset of \( \mathcal{H} \). Any \( f \in \mathcal{H} \) can be decomposed as \( f = f_\parallel + f_\perp \), where \( f_\parallel \in \mathcal{H}_\parallel \) and \( f_\perp \in \mathcal{H}_\perp := \{ g \in \mathcal{H} : \langle g, h \rangle_\mathcal{H} = 0, \forall h \in \mathcal{H}_\parallel \} \) so that \( \mathcal{H} = \mathcal{H}_\parallel \oplus \mathcal{H}_\perp \). This means \( \hat{J}_\lambda(f) \) is minimized when \( f_\perp = 0 \), i.e., the minimizer of \( \hat{J}_\lambda \) lies in \( \mathcal{H}_\parallel \), which means \( f_\lambda,n \) is of the form in \( \mathcal{H}_\parallel \). Using this in \( \hat{J}_\lambda \) and invoking the reproducing property of \( k \), we obtain a quadratic form with respect to \( \alpha, (\beta_{b,j}) \). In the following, we obtain explicit expressions.

For simplicity, denote \( \partial f := \frac{\partial k(X, \cdot)}{\partial x} \) and \( \partial f := \frac{\partial k(X, \cdot)}{\partial x} \). Noting \( \frac{\partial f}{\partial x} = \hat{\xi}, \frac{\partial f}{\partial x} = \hat{\xi}_j \), we have
\[ \frac{\partial \hat{J}_\lambda}{\partial \alpha} = \langle \hat{C} f, \hat{\xi} \rangle_\mathcal{H} + \langle \hat{\xi}, \hat{\xi} \rangle_\mathcal{H} + \lambda \langle \hat{\xi}, \hat{\xi} \rangle_\mathcal{H} \]
\[ = \alpha \langle \hat{C} \hat{\xi}, \hat{\xi} \rangle_\mathcal{H} + \sum_{b,j} \beta_{b,j} \langle \hat{C} \beta_{b,j}, \hat{\xi} \rangle_\mathcal{H} + \langle \hat{\xi}, \hat{\xi} \rangle_\mathcal{H} + \lambda \sum_{b,j} \beta_{b,j} \langle \hat{\xi}_j, \hat{\xi} \rangle_\mathcal{H} \]
\[ = \alpha (\hat{C} \hat{\xi}, \hat{\xi})_\mathcal{H} + \sum_{b,j} \beta_{b,j} (\hat{C} \beta_{b,j}, \hat{\xi}_j)_\mathcal{H} + \lambda \sum_{b,j} \beta_{b,j} \langle \hat{\xi}_j, \hat{\xi} \rangle_\mathcal{H} \]
(14)

and
\[ \frac{\partial \hat{J}_\lambda}{\partial \beta_{b,j}} = \langle \hat{C} \beta_{b,j}, \hat{\xi} \rangle_\mathcal{H} + \langle \hat{\xi}, \hat{\xi} \rangle_\mathcal{H} + \lambda \langle \hat{\xi}, \hat{\xi} \rangle_\mathcal{H} \]
\[ = \alpha (\hat{C} \hat{\xi}, \hat{\xi})_\mathcal{H} + \sum_{a,i} \beta_{a,i} (\hat{C} \beta_{a,i}, \hat{\xi}_j)_\mathcal{H} + \lambda \sum_{a,i} \beta_{a,i} \langle \hat{\xi}_j, \hat{\xi} \rangle_\mathcal{H} \]
(15)

This requires the computation of \( \langle \hat{C} \hat{\xi}, \hat{\xi} \rangle_\mathcal{H}, \langle \hat{C} \hat{\xi}, \hat{\xi}_j \rangle_\mathcal{H}, \langle \hat{\xi}, \hat{\xi} \rangle_\mathcal{H}, \langle \hat{\xi}_j, \hat{\xi} \rangle_\mathcal{H} \) and \( \langle \hat{\xi}_j, \hat{\xi}_j \rangle_\mathcal{H} \), which we do below.

First, by the reproducing property of derivatives, \( \langle \partial f, \partial f \rangle_\mathcal{H} = \frac{\partial^2 k(X, X)}{\partial x \partial y} \) and
\[ \langle \hat{C} \partial f, \partial f \rangle_\mathcal{H} = \frac{1}{n} \sum_i \frac{\partial^2 k(X, X)}{\partial x \partial y} \]
\[ = \frac{1}{n} \sum_i \frac{\partial^2 k(X, X, X)}{\partial x \partial y} \frac{\partial^2 k(X, X)}{\partial x \partial y}. \]

Next, define \( h^b_j := \langle \hat{\xi}, \hat{\xi}_j \rangle_\mathcal{H} \). Then, \( \hat{C} \hat{\xi} = \frac{1}{n} \sum_i h^b_i \frac{\partial k(X, \cdot)}{\partial x} \) and
\[ h^b_j = \langle \hat{\xi}, \hat{\xi}_j \rangle_\mathcal{H} = \frac{1}{n} \sum_i \frac{\partial^2 k(X, X, X)}{\partial x \partial y} \frac{\partial^2 k(X, X)}{\partial x \partial y}. \]

With this equation,
\[ \langle \hat{C} \hat{\xi}, \hat{\xi}_j \rangle_\mathcal{H} = \frac{1}{n} \sum_i h^b_i \frac{\partial^2 k(X, X, X)}{\partial x \partial y} \]
and \( \langle \hat{C} \hat{\xi}, \hat{\xi} \rangle_\mathcal{H} = \frac{1}{n} \sum_i (h^b_i)^2 \).

Finally,
\[ \| \hat{\xi} \|^2_\mathcal{H} = \frac{1}{n^2} \sum_i \sum_j \left( \frac{\partial^4 k(X, X, X)}{\partial x \partial y} + 2 \frac{\partial^2 k(X, X, X)}{\partial x \partial y} \frac{\partial^2 k(X, X, X)}{\partial x \partial y} \right) \]
\[ = \frac{1}{n^2} \sum_i \sum_j \left( \frac{\partial^4 k(X, X, X)}{\partial x \partial y} + 2 \frac{\partial^2 k(X, X, X)}{\partial x \partial y} \frac{\partial^2 k(X, X, X)}{\partial x \partial y} \right). \]
(16)

Using the above in (14) and (15), we have
\[ \frac{\partial \hat{J}_\lambda}{\partial \alpha} = \left( \frac{1}{n} \sum_{a,i} (h^b_i)^2 + \lambda \| \hat{\xi} \|^2_\mathcal{H} \right) \alpha + \sum_{b,j} \left( \frac{1}{n} \sum_{a,i} h^b_i \frac{\partial k(X, X, X)}{\partial x \partial y} \right) \beta_{b,j} + \| \hat{\xi} \|^2_\mathcal{H} \].
and
\[
\frac{\partial \hat{j}_k}{\partial \beta_{ij}} = \left( \frac{1}{n} \sum_{a,i} h^a_{ij} G^{ab}_{ij} + \lambda h^b_j \right) \alpha + \sum_{a,i} \left( \frac{1}{n} \sum_{c,m} G^{ac}_{im} G^{cb}_{mj} + \lambda G^{ab}_{ij} \right) \beta_{ai} + h^b_j.
\]
where \(G^{ab}_{ij} = \frac{\partial^2 k(x_i, x_j)}{\partial x_i \partial x_j} \). By equating the above two expressions to zero and solving for \(\alpha, (\beta_{ij})\) results in solving the linear system in (5).

\[\square\]

8.6 Proof of Theorem 5

(i) Consider
\[
f_{\lambda,n} - f_{\lambda} = -(\hat{C} + \lambda I)^{-1} \left( \hat{\xi} + (\hat{C} + \lambda I) f_{\lambda} \right)
\]
\[
\leq -(\hat{C} + \lambda I)^{-1} \left( \hat{\xi} + \hat{C} f_{\lambda} + C (f_0 - f_{\lambda}) \right)
\]
\[
= (\hat{C} + \lambda I)^{-1} (C - \hat{C})(f_{\lambda} - f_0) - (\hat{C} + \lambda I)^{-1} (\hat{\xi} + \hat{C} f_0)
\]
where we used \(\lambda f_{\lambda} = C (f_0 - f_{\lambda})\) in (*). Therefore,
\[
\|f_{\lambda,n} - f_{\lambda}\|_{2 \xi} \leq \|f_{\lambda,n} - f_{\lambda}\|_{2 \xi} + \|f_{\lambda} - f_0\|_{2 \xi}
\]
\[
\leq \|\|C + \lambda I\|^{-1}\| (\|C - \hat{C}\| (f_{\lambda} - f_0))\|_{2 \xi} + \|\hat{C} f_{\lambda} + \hat{\xi}\|_{2 \xi}) + A_0(\lambda),
\]
(17)
where \(A_0(\lambda) := \|f_{\lambda} - f_0\|_{2 \xi}\). It follows from \(\|(\hat{C} + \lambda I)^{-1}\| \leq 1/\lambda\) and \(\|\hat{C} - C\| \leq \|\hat{C} - C\|_{HS} = O_{p_0}(n^{-1/2})\) (where the ideas in the proof of Lemma 5 in [15] can be used to prove this claim under the assumption that the first term in (D) holds with \(\varepsilon = 2\) that the first term is of the order \(O_{p_0}\)). Since the second term is upper bounded by \(\|\hat{C} f_{\lambda} + \hat{\xi}\|_{2 \xi}/\lambda\), it suffices to prove \(\|\hat{C} f_{\lambda} + \hat{\xi}\|_{2 \xi} = O_{p_0}(n^{-1/2})\). To this end, after some algebra, it can be shown that
\[
E_{p_0} \|\hat{C} f_{\lambda} + \hat{\xi}\|_{2 \xi}^2 = \frac{n - 1}{n} \|\hat{C} f_{\lambda} + \hat{\xi}\|_{2 \xi}^2 + \frac{1}{n} \int \|C_{\hat{x}} f_{\lambda} + \hat{\xi}\|_{2 \xi}^2 p_0(x) dx,
\]
where \(\hat{\xi} := \sum_{i=1}^d \frac{\partial k(x_i)}{\partial x_i} \log q_0(x_i) + \frac{\partial^2 k(x_i)}{\partial x_i^2} \). The first term on the r.h.s. is zero since \(C f_0 + \xi = 0\) by Theorem 5. Since \(\|C_{\hat{x}} f_0 + \hat{\xi}\|_{2 \xi}^2 \leq 2\|C\|_{HS}^2 \|f_0\|_{2 \xi}^2 + 2\|\hat{\xi}\|_{2 \xi}^2\), it follows from (D) with \(\varepsilon = 2\) that the second term is finite and the proof is therefore completed by Chebyshev’s inequality. The result \(A_0(\lambda) \to 0\) as \(\lambda \to 0\) if \(f_0 \in \mathcal{R}(C)\) follows from Proposition A.2.

(ii) Since \(f_0 \in \mathcal{R}(C^\beta)\) for some \(\beta > 0\), Proposition A.2 yields that \(A_0(\lambda) \leq \max \{1, \|C\|^{\beta - 1} \lambda \|\xi\|^\beta \|C - \hat{C}\| f_0\|_{2 \xi}\} + \|\hat{C} f_0 + \hat{\xi}\|_{2 \xi}^{\beta - 1} \lambda \|\xi\|^\beta\), using which in (17), we obtain
\[
\|f_{\lambda,n} - f_{\lambda}\|_{2 \xi} \leq O_{p_0}(\lambda n^{-1/2}) + \max \{1, \|C\|^{\beta - 1} \lambda \|\xi\|^\beta \|C - \hat{C}\| f_0\|_{2 \xi}\}
\]
and therefore the result follows by choosing \(\lambda = n^{-\max\left\{\frac{1}{\beta}, \frac{1}{\beta - 1}\right\}}\).

(iii) Recall (17),
\[
\|f_{\lambda,n} - f_{\lambda}\|_{2 \xi} \leq \|(\hat{C} + \lambda I)^{-1}\| \|\|C - \hat{C}\| (f_{\lambda} - f_0)\|_{2 \xi} + \|\hat{C} f_{\lambda} + \hat{\xi}\|_{2 \xi}) + A_0(\lambda)
\]
\[
\leq \|C^{-1}\| \|\|C + \lambda I\|^{-1}\| \|\|C - \hat{C}\| (f_{\lambda} - f_0)\|_{2 \xi} + \|\hat{C} f_{\lambda} + \hat{\xi}\|_{2 \xi}) + \|\|C^{-1}\| \|\|C - \hat{C}\|\|f_{\lambda} - f_0\|_{2 \xi}.
\]
(18)
By Proposition A.2, we obtain \(\|\|C (f_{\lambda} - f_0)\|_{2 \xi} \leq \lambda \|f_0\|_{2 \xi}\). This implies \(\|\|C - \hat{C}\| (f_{\lambda} - f_0)\|_{2 \xi} \leq \|C - \hat{C}\| \|\|C - \hat{C}\|\|f_{\lambda} - f_0\|_{2 \xi} = O_{p_0}(\lambda n^{-1/2})\). Also it follows from (i) that \(\|\hat{C} f_{\lambda} + \hat{\xi}\|_{2 \xi} = O_{p_0}(n^{-1/2})\).

We now provide an estimate on \(\|\|C (f_{\lambda} - f_0)\|_{2 \xi}^{-1}\|\) using the idea used in the proof of Theorem 4 (see step 3.1) in [8]. Note that \(\|C (f_{\lambda} - f_0)\|_{2 \xi}^{-1} = \|C - \hat{C}\|^{-1} (I - (C - \hat{C})(C + \lambda I)^{-1})^{-1} = C (C + \lambda I)^{-1} \sum_{j=0}^\infty ((C - \hat{C})(C + \lambda I)^{-1})^j\), which implies
\[
\|C (f_{\lambda} - f_0)\|_{2 \xi}^{-1} \leq \|C (C + \lambda I)^{-1}\| \sum_{j=0}^\infty \left\|\left(\sum_{j=0}^\infty ((C - \hat{C})(C + \lambda I)^{-1})^j\right)^j\right\|^{-1}.
\]
where \((D) \leq \|(C - \hat{C})(C + \lambda I)^{-1}\|_{HS}\). Define \(\eta : \Omega \to HS(\mathcal{H}), \eta(x) = (C + \lambda I)^{-1}(C - C_x)\), where \(HS(\mathcal{H})\) is the space of Hilbert-Schmidt operators on \(\mathcal{H}\). Observe that \(E_{p_0} \sum_{i=1}^{n} \eta(X_i) = 0\). Also, for all \(i \in [n], \|\eta(X_i)\|_{HS} \leq \|(C + \lambda I)^{-1}\|_{HS} \leq \|C - C_x\|_{HS} \leq 2\sqrt{d} E_{p_0}^{2}\) and \(E_{p_0} \|\eta(X_i)\|^2_{HS} \leq \frac{4d^2 E_{p_0}^2}{\lambda}\). Therefore, by Bernstein’s inequality [35] Theorem 6.14, with probability at least \(1 - e^{-\tau}\) over the choice of \((X_i)\),

\[
\|(C - \hat{C})(C + \lambda I)^{-1}\|_{HS} \leq \frac{2(\sqrt{\tau} + 1)dE_{p_0}^2}{\lambda \sqrt{n}} + \frac{4\tau dE_{p_0}^2}{3\lambda n} \leq \frac{2(\sqrt{\tau} + 1)E_{p_0}^2}{\lambda \sqrt{n}}.
\]

For \(\lambda \geq \frac{4(\sqrt{\tau} + 1)^2 E_{p_0}^2}{\sqrt{n}}\) we obtain that \((D) \leq \|(C - \hat{C})(C + \lambda I)^{-1}\|_{HS} \leq \frac{1}{2}\) and therefore \(\|C(\hat{C} + \lambda I)^{-1}\| \leq 2\) where we used \(\|C(C + \lambda I)^{-1}\| \leq 1\). Using all these bounds in [20], we obtain that for \(\lambda \geq \frac{4(\sqrt{\tau} + 1)^2 E_{p_0}^2}{\sqrt{n}}\),

\[
\|f_{\lambda,n} - f_0\|_{\mathcal{H}} = O_{p_0}(n^{-1/2}) + O(\lambda)
\]

as \(\lambda \to 0, n \to \infty\) and the result follows.

\[\square\]

8.7 An exponential concentration inequality for \(\|f_{\lambda,n} - f_0\|_{\mathcal{H}}\)

Before presenting the result, we present a version of Bernstein’s inequality in Hilbert space—quoted from [35] Theorem 6.14—which will be used in its proof.

**Theorem 8.2.** Let \((\Omega, A, P)\) be a probability space, \(H\) be a separable Hilbert space, \(B > 0\), and \(\sigma > 0\). Furthermore, let \(\xi_1, \ldots, \xi_n : \Omega \to H\) be independent random variables satisfying \(E_P \xi_i = 0, \|\xi_i\|_H \leq B, \) and \(E_P \|\xi_i\|^2_H \leq \sigma^2\) for all \(i = 1, \ldots, n\). Then for all \(\tau > 0\), we have

\[
P \left( \left\| \frac{1}{n} \sum_{i=1}^{n} \xi_i \right\|_H \geq \sqrt{\frac{2\sigma^2 \tau}{n} + \frac{2\tau^2}{3n}} \right) \leq e^{-\tau}.
\]

**Proposition 8.3.** Suppose (A)–(C) hold and \(\eta_0 \in C^1(\Omega)\). Assume

\[
E_1 := \sup_{x \in \Omega, i \in [d]} \left\| \frac{\partial k(x, x)}{\partial x_i} \right\|_{\mathcal{H}} < \infty, E_2 := \sup_{x \in \Omega, i \in [d]} \left\| \frac{\partial^2 k(x, x)}{\partial x_i^2} \right\|_{\mathcal{H}} < \infty \text{ and } E_3 := \sup_{x \in \Omega, i \in [d]} \left\| \frac{\partial \log q_0(x)}{\partial x_i} \right\|_{\mathcal{H}} < \infty.
\]

Then for any \(\tau > 0\), there exists constants \((L_i)_{i=1}^3\) (that depend on \(d, \tau, (E_i)_{i=1}^3\) and \(\|f_0\|_{\mathcal{H}}\) but not on \(\lambda\) and \(n\)) such that with probability at least \(1 - 2e^{-\tau}\) over the choice of samples \((X_i)_{i=1}^n\) drawn from \(p_0\),

\[
\|f_{\lambda,n} - f_0\|_{\mathcal{H}} \leq \frac{L_1 A_0^2(\lambda)}{\lambda \sqrt{n}} + \frac{L_2 A_0(\lambda)}{\lambda n} + \frac{L_3}{\lambda \sqrt{n}} + A_0(\lambda)
\]

where \(A_0(\lambda)\) is defined in Proposition A.2. If \(f_0 \in \mathcal{R}(C)\), then

\[
\|f_{\lambda,n} - f_0\|_{\mathcal{H}} \xrightarrow{p_0} 0 \text{ as } \lambda \to 0, \lambda \sqrt{n} \to \infty \text{ and } n \to \infty.
\]

**Proof.** Recall [17],

\[
\|f_{\lambda,n} - f_0\|_{\mathcal{H}} \leq \left( \sqrt{\frac{\|\mathcal{H} + \lambda I\|^{-1}\|\mathcal{H} - \hat{\mathcal{H}}\|\|\mathcal{H} - \hat{\mathcal{H}}\|_{\mathcal{H}}} {\mathcal{H}}} + \sqrt{\frac{\|\mathcal{H} + \lambda I\|^{-1}\|\mathcal{H} - \hat{\mathcal{H}}\|\|\mathcal{H} - \hat{\mathcal{H}}\|_{\mathcal{H}}} {\mathcal{H}}} \right) + A_0(\lambda).
\]

By Remark [1],[1], since \(\mathcal{H}\) is a separable RKHS, in the following, we use Theorem 8.2 to bound (B) and (C). (A) can be bounded simply as \((A) := \|\mathcal{H} + \lambda I\|^{-1}\| \leq \lambda^{-1} - 1\).

**Bound on (B):** Define \(C_x := \sum_{i=1}^{d} \frac{\partial k_{i}(x, x)}{\partial x_i} \otimes \frac{\partial k_{i}(x, x)}{\partial x_i} \) and \(\eta : \Omega \to \mathcal{H}\) be such that \(\eta(x) = (C - C_x)(f_\lambda - f_0)\). It is easy to check that \(\frac{1}{n} \sum_{i=1}^{n} \eta(X_i) = (C - C_x)(f_{\lambda,n} - f_0)\) and \(E_{p_0} \|\eta(X_i)\| = 0, \forall i = 1, \ldots, n\). Define \(\|\eta\|_{\mathcal{H}} := \sup_{x \in \Omega} \|\mathcal{H}\|\). We now bound \(\|\eta(X_i)\|_{\mathcal{H}}\) and \(E_{p_0} \|\eta(X_i)\|^2_{\mathcal{H}}\) for all \(i \in [n]\). For all \(i \in [n]\),

\[
\|\eta(X_i)\|_{\mathcal{H}} \leq \|C(f_\lambda - f_0)\|_{\mathcal{H}} + \|C_{\eta}(f_\lambda - f_0)\|_{\mathcal{H}} \leq \sqrt{\|C\|_{\mathcal{H}} A_0^2(\lambda) + \|C_{\eta}\| A_0(\lambda)} \leq \sqrt{\|C\|_{\mathcal{H}} A_0^2(\lambda) + \|C\|_{\mathcal{H}} A_0(\lambda)}.
\]
and
\[ \mathbb{E}_{p_0} \| \eta(X_i) \|_2^2 \leq \mathbb{E}_{p_0} \| C_X(f_\lambda - f_0) \|_2^2 \leq \| C \| \mathbb{E}_{p_0} \sqrt{C_X(f_\lambda - f_0)} \|_2^2 \]
\[ = \| C \| \int (C_x(f_\lambda - f_0), (f_\lambda - f_0)) x \| dx = \| C \| \mathbb{A}^2_\lambda(\lambda). \]

Therefore, by Theorem 5.2 with probability at least \(1 - e^{-\tau}\) over the choice of \((X_i)\), \((B) \leq \left( \frac{\sqrt{2\tau + 1}}{\sqrt{n}} + \frac{2\tau}{3n} \right) \sqrt{\| C \| \mathbb{A}^2_\lambda(\lambda) + \frac{2\| C \|_{\infty} \mathbb{A}^0_\lambda(\lambda)}{3n}}.\) Using the fact that \(\| C \|_{\infty} = \sup_{x \in \mathcal{X}} \| C_x \| \leq \sup_{x \in \mathcal{X}} \| C_x \|_{HS} \leq \sup_{x \in \mathcal{X}} \sum_{i=1}^d \| \frac{\partial k_{(i,x)}}{\partial x_i} \|_2^2 \leq dE_1^2\), we obtain
\[ (B) \leq \frac{\sqrt{d(\sqrt{\tau} + 1)^2 E_1 \mathbb{A}^2_\lambda(\lambda)}}{\sqrt{n}} + \frac{2\tau dE_1^2 \mathbb{A}^0_\lambda(\lambda)}{3n}. \] (21)

**Bound on \((C)\):** Define \(\xi_x := \sum_{i=1}^d \left( \frac{\partial k_{(i,x)}}{\partial x_i} \frac{\partial \log g_0(x)}{\partial x_i} + \frac{\partial^2 k_{(i,x)}}{\partial x_i^2} \right) \) and let \(\psi : \mathcal{X} \rightarrow \mathcal{H}\) be such that \(\psi(x) := C_x f_0 + \xi_x\). It is clear that \(\hat{C} f_0 + \hat{\xi} = \frac{1}{\sum_{i=1}^n} \psi(X_i)\) and \(C f_0 + \xi = \int \psi(x) p_0(x) dx = 0\). Also, for all \(i \in [n]\), \(\| \psi(X_i) \|_{2\mathcal{H}} \leq \| C_x f_0 \|_{2\mathcal{H}} + \| \xi_x \|_{2\mathcal{H}} \leq \| C \|_{\infty} \| f_0 \|_{2\mathcal{H}} + d(E_2 + E_3) \leq \Theta\) and \(\mathbb{E}_{p_0} \| \psi(X_i) \|_{2\mathcal{H}} \leq \Theta^2\) where \(\Theta := d(E_1^2 \| f_0 \|_{2\mathcal{H}} + E_2 + E_3)\).

Therefore, by Theorem 5.2 with probability at least \(1 - e^{-\tau}\) over the choice of \((X_i)\),
\[ (C) \leq \frac{(\sqrt{2\tau + 1}) \Theta}{\sqrt{n}} + \frac{2\tau \Theta}{3n} \leq \frac{(\sqrt{\tau} + 1)^2 \Theta}{\sqrt{n}}. \] (22)

Using (21) and (22) in (20), we obtain the required concentration inequality.

Now, we will investigate the behavior of \(\mathbb{A}_0(\lambda)\) and \(\mathbb{A}_\lambda(\mathcal{X})\). From Proposition A.2 we have \(\mathbb{A}_\lambda(\mathcal{X}) \to 0\) as \(\lambda \to 0\) and if \(f_0 \in \overline{\mathcal{R}(C)}\), then \(\mathbb{A}_0(\lambda) \to 0\) as \(\lambda \to 0\). Note that \(\mathbb{A}_\lambda(\mathcal{X}) \mathbb{A}_0(\lambda) = o\left(\frac{1}{\sqrt{n}}\right)\) and \(\mathbb{A}_0(\lambda) = o\left(\frac{1}{\sqrt{n}}\right)\).

Therefore, \(\| f_{\lambda,n} - f_0 \|_{2\mathcal{H}} \to 0\) as \(\lambda \sqrt{n} \to \infty\), \(\lambda \to 0\) and \(n \to \infty\), resulting in \(f_{\lambda,n}\) as a consistent estimator of \(f_0\). \(\square\)

### 8.8 Proof of Theorem 6

Before we prove the result, we present a lemma.

**Lemma 14.** Suppose \(\sup_{x \in \mathcal{X}} k(x, x) < \infty\) and \(\text{supp}(p_0) = \mathcal{X}\). Then for any \(f_0 \in \mathcal{H}\) there exists \(\hat{f}_0 \in \overline{\mathcal{R}(C)}\) such that \(\hat{f}_0 = p_{f_0} = p_0\).

**Proof.** Under the assumptions on \(k\) and \(p_0\), it is easy to verify that \(\text{supp}(p_0) = \mathcal{X}\), which implies
\[ \mathcal{N}(C) = \left\{ f \in \mathcal{H} : \int \left\| \frac{\partial f}{\partial x} \right\|_2^2 p_0(x) dx = 0 \right\} \]
is either \(\mathbb{R}\) or \(\{0\}\), where \(\mathcal{N}(C)\) denotes the null space of \(C\). Let \(\hat{f}_0\) be the orthogonal projection of \(f_0\) onto \(\overline{\mathcal{R}(C)} = \mathcal{N}(C)\). Then \(\hat{f}_0 - f_0 \in \mathbb{R}\) and therefore \(p_{\hat{f}_0} = p_{f_0} = p_0\). \(\square\)

**Proof of Theorem 6.** From Theorem 3.3(iii), \(f_\lambda = (C + \lambda I)^{-1}C f_0 = (C + \lambda I)^{-1}C \hat{f}_0\) where the second equality follows from the proof of Lemma 14. Now, carrying out the decomposition as in the proof of Theorem 5(i), we obtain \(f_{\lambda,n} - f_\lambda = (\hat{C} + \lambda I)^{-1}(C - \hat{C})(f_\lambda - \hat{f}_0) - (C + \lambda I)^{-1}(\hat{\xi} + \hat{C} \hat{f}_0)\) and therefore,
\[ \| f_{\lambda,n} - f_\lambda \|_{2\mathcal{H}} \leq \| (\hat{C} + \lambda I)^{-1} \| \| (C - \hat{C})(f_\lambda - \hat{f}_0) \|_{2\mathcal{H}} + \| (C + \lambda I)^{-1}(\hat{\xi} + \hat{C} \hat{f}_0) \|_{2\mathcal{H}} + \| \hat{A}_0(\lambda) \|_{2\mathcal{H}}, \]
where \(\hat{A}_0(\lambda) = \| f_\lambda - \hat{f}_0 \|_{2\mathcal{H}}\). The bounds on these quantities follow those in the proof of Theorem 5(i) verbatim and so the consistency result in Theorem 5(i) holds for \(\| f_{\lambda,n} - f_\lambda \|_{2\mathcal{H}}\). By Lemma 14 since \(p_{f_0} = p_{\hat{f}_0}\), it is sufficient to consider the convergence of \(p_{f_{\lambda,n}}\) to \(p_{\hat{f}_0}\). Therefore, the convergence (along with rates) in \(L^r\) (for any \(1 \leq r \leq \infty\), Hellinger and KL distances follow from using the bound \(\| f_{\lambda,n} - f_0 \|_{\infty} \leq \sqrt{\| \hat{D} \|_{\infty} \| f_{\lambda,n} - \hat{f}_0 \|_{2\mathcal{H}}\})\) (obtained through the reproducing property of \(k\)) in Lemma A.1 and invoking Theorem 6.
In the following, we obtain a bound on $J(p_0∥p_{f_{\lambda,n}}) = \frac{1}{2}∥\sqrt{C}(f_{\lambda,n} - f_0)∥^2_{C}$, while one can trivially use the bound $∥\sqrt{C}(f_{\lambda,n} - f_0)∥_2 ≤ ∥\sqrt{C}∥^2∥f_{\lambda,n} - f_0∥_2$ to obtain a rate on $J(p_0∥p_{f_{\lambda,n}})$ through the result in Theorem ii, a better rate can be obtained by carefully bounding $∥\sqrt{C}(f_{\lambda,n} - f_0)∥^2_{C}$ as shown below. Consider

$$
\|\sqrt{C}(f_{\lambda,n} - f_0)\|_{2\epsilon} \leq \|\sqrt{C}(f_{\lambda,n} - f_0)\|_{2\epsilon} + A_{\|}(\lambda)
$$

where $A_{\|}(\lambda) := \|\sqrt{C}(f_{\lambda,n} - f_0)\|_{2\epsilon}$ and the first term in turn bounded as

$$\begin{align*}
(\text{A}) & \quad \|\sqrt{C}(f_{\lambda,n} - f_0)\|_{2\epsilon} \leq \left\|\sqrt{C}(\hat{C} + \lambda I)^{-1}\right\| \left\|\left(C - \hat{C}\right)(f_{\lambda,n} - f_0)\right\|_{2\epsilon} + \|\hat{C}f_0\|_{2\epsilon}.
\end{align*}
$$

In the following, we bound (A) using exactly the same idea that is used to bound $\|C(\hat{C} + \lambda I)^{-1}\|_{\epsilon}$ in the proof of Theorem iii, thereby yielding $\|A_{\|}(\lambda)\|_{\epsilon} \leq \frac{2}{\sqrt{\lambda}}$ if $\lambda \geq \frac{\kappa^2 f\epsilon d}{\sqrt{\alpha}}$. From Theorem i, we have $\|B\| = O(p_0(\lambda)n^{-1/2})$ and $\|C\| = O(p_0(n^{-1/2}))$, where $A_{\|}(\lambda) = \|f_{\lambda,n} - f_0\|_{2\epsilon}$, and therefore, $\|\sqrt{C}(f_{\lambda,n} - f_0)\|_{2\epsilon} = O(p_0(\lambda^{-1/2}n^{-1/2})$, using which in (23) along with $A_{\|}(\lambda) = O(\sqrt{\lambda})$ as $\lambda \to 0$ (from Proposition A.2) provides the consistency result. If $f_0 \in \mathcal{R}(C^\beta)$ for some $\beta \geq 0$, then Proposition A.2 yields $\|A_{\|}(\lambda)\|_{\epsilon} \leq \max\{1, \|C\|^{\beta-\frac{d}{2}}\lambda^{\min\{1,\beta+\frac{d}{2}\}}\|C^{-\beta}f_0\|_{2\epsilon}\}$ which when used in (23) with $\lambda = n^{-\max\{1,\beta+\frac{d}{2}\}}$ yields the result. If $\|C^{-1}\| < \infty$, then the result follows by noting $\|\sqrt{C}(f_{\lambda,n} - f_0)\|_{2\epsilon} \leq \|\sqrt{C}\|\|f_{\lambda,n} - f_0\|_{2\epsilon}$ and invoking the bound in (19).

### 8.9 Derivation of $\tilde{f}_{\lambda,n}$

As carried out in the proof of Theorem 4, any $f \in \mathcal{H}$ can be decomposed as $f = f_{\|} + f_{\perp}$ where

$$f_{\|} \in \text{span}\left\{\hat{e}_i, \left(\frac{\partial k(\cdot, X_0)}{\partial x_i}\right)_{b,j}\right\} =: \mathcal{H}_{\|},$$

which is a closed subset of $\mathcal{H}$ and $f_{\perp} \in \mathcal{H}_{\perp} := \{g \in \mathcal{H} : (g, h)_{2\epsilon} = 0, \forall h \in \mathcal{H}_{\|}\}$ so that $\mathcal{H} = \mathcal{H}_{\|} \Theta \mathcal{H}_{\perp}$. Since the objective function in (17) matches with the one in Theorem 4, using the above decomposition in (9), it is easy to verify that $\hat{J}$ depends only on $f_{\|} \in \mathcal{H}_{\|}$ so that (19) reduces to

$$(\hat{f}_{\lambda,n}, \tilde{f}_{\lambda,n}) = \arg\inf_{f_{\|} \in \mathcal{H}_{\|}, f_{\perp} \in \mathcal{H}_{\perp}} \left\|\hat{J}_{\lambda}(f_{\|}) + \frac{\lambda}{2}\|f_{\|}\|_{2\epsilon}^2 + \frac{\lambda}{2}\|f_{\perp}\|_{2\epsilon}^2\right\|_2,$$  

and $\tilde{f}_{\lambda,n} = \hat{f}_{\lambda,n} + \tilde{f}_{\lambda,n}$. Since $f_{\|}$ is of the form in (17), using it in (24), it is easy to show that $\hat{J}_{\lambda}(f_{\|}) + \frac{\lambda}{2}\|f_{\|}\|_{2\epsilon}^2 = \frac{1}{2}\Theta^T H\Theta + \Theta^T \Delta$. Similarly, it can be shown that (by simply following the derivation in the proof of Theorem 4) $\|f_{\perp}\|_{2\epsilon}^2 = \Theta^T B\Theta$. Since $f_{\perp}$ appears in (24) only through $\|f_{\perp}\|_{2\epsilon}^2$, (24) reduces to

$$(\Theta_{\|}, c_{\perp}) \overset{\text{argmin}}{\Theta_{\perp} \in \mathbb{R}^{n \times 1}, c_{\perp} \in \mathbb{R}^{n \times 1}} \left\{\frac{1}{2}\Theta^T H\Theta + \Theta^T \Delta + \frac{\lambda}{2}\|c_{\perp}\|_{2\epsilon}^2\right\},$$

where $\|\hat{f}_{\lambda,n}\|_{2\epsilon}$ is constructed as in (17) using $\Theta_{\|}$ and $\tilde{f}_{\lambda,n}$ is such that $\|\tilde{f}_{\lambda,n}\|_{2\epsilon} = c_{\perp}$. The necessary and sufficient conditions for the optimality of $(\Theta_{\|}, c_{\perp})$ is given by the following Karush-Kuhn-Tucker conditions,

$$\begin{align*}
(\text{Stationarity})
(H + 2\tau B)\Theta_{\|} + \Delta & = 0, & \frac{\lambda}{2} + \eta - \tau & = 0, \\
(\text{Primal feasibility})
\Theta_{\|}^T B\Theta_{\|} + c_{\perp} & \leq M^2, & c_{\perp} & \geq 0, \\
(\text{Dual feasibility})
\eta & \geq 0, & \tau & \geq 0, \\
(\text{Complementary slackness})
\tau c_{\perp} & = 0, & \eta (\Theta_{\|}^T B\Theta_{\|} + c_{\perp} - M^2) & = 0.
\end{align*}$$

Combining the dual feasibility and stationary conditions, we have $\eta = \tau - \frac{\lambda}{2} \geq 0$, i.e., $\tau \geq \frac{\lambda}{2}$. Using this in the complementary slackness involving $\tau$ and $c_{\perp}$, it follows that $c_{\perp} = 0$. Since $\|\tilde{f}_{\lambda,n}\|_{2\epsilon}^2 = c_{\perp}$, we have $\tilde{f}_{\lambda,n} = 0$, i.e., $\tilde{f}_{\lambda,n}$ is completely determined by $\hat{f}_{\lambda,n}$. Therefore $\|\hat{f}_{\lambda,n}\|^2 = c_{\perp}$ and the proof follows by noting $\|\sqrt{C}(f_{\lambda,n} - f_0)\|_{2\epsilon} \leq \|\sqrt{C}\|\|f_{\lambda,n} - f_0\|_{2\epsilon}$ and invoking the bound in (19).
8.10 Proof of Theorem 7

For any \( x \in \Omega \), since \( |f_0(x)| \leq \|f_0\|_\mathcal{H} \sqrt{k(x, x)} \leq M \sqrt{k(x, x)} \) and \( |\tilde{f}_{\lambda, n}(x)| \leq M \sqrt{k(x, x)} \), we have

\[
|e^{\tilde{f}_{\lambda, n}(x)} - e^{f_0(x)}| \leq e^{M \sqrt{k(x, x)}} |\tilde{f}_{\lambda, n}(x) - f_0(x)| \leq \eta(x) \|\tilde{f}_{\lambda, n} - f_0\|_\mathcal{H},
\]

where we used the fact that \( |e^z - e^y| \leq e^y |x - y| \) for \( x, y \in [-a, a] \) and \( \eta(x) := \sqrt{k(x, x)} e^{M \sqrt{k(x, x)}} \). In the following, we obtain bounds for \( \|p_{\tilde{f}_{\lambda, n}} - p_0\|_{L^r(\Omega)} \) for any \( 1 \leq r \leq \infty \), \( h(p_{\tilde{f}_{\lambda, n}}, p_0) \) and \( KL(p_0\|p_{\tilde{f}_{\lambda, n}}) \) in terms of \( \|\tilde{f}_{\lambda, n} - f_0\|_\mathcal{H} \).

Define \( A(f) := \int_\Omega e^f \, q_0 \, dx \). Since \( k \) satisfies \( \int e^{M \sqrt{k(x,x)}} q_0(x) \, dx < \infty \), then it is clear that \( \tilde{f}_{\lambda, n} \in \mathcal{F} \) as

\[
\int e^{\tilde{f}_{\lambda, n}(x)} q_0(x) \, dx \leq \int e^{\|\tilde{f}_{\lambda, n}\|_\mathcal{H} \sqrt{k(x,x)}} q_0(x) \, dx \leq \int e^{M \sqrt{k(x,x)}} q_0(x) \, dx < \infty
\]

and therefore \( A(\tilde{f}_{\lambda, n}) < \infty \). Similarly, it can be shown that \( A(f_0) < \infty \).

(i) Recalling (A.1), we have

\[
\|p_{\tilde{f}_{\lambda, n}} - p_0\|_{L^r(\Omega)} \leq \frac{|A(\tilde{f}_{\lambda, n}) - A(f_0)|}{A(\tilde{f}_{\lambda, n}) A(f_0)} + \frac{\|(e^{f_0} - e^{\tilde{f}_{\lambda, n}})q_0\|_{L^r(\Omega)}}{A(\tilde{f}_{\lambda, n})}.
\]

If \( r = 1 \), we obtain

\[
\|p_{\tilde{f}_{\lambda, n}} - p_0\|_{L^1(\Omega)} \leq \frac{|A(\tilde{f}_{\lambda, n}) - A(f_0)|}{A(\tilde{f}_{\lambda, n})} + \frac{\|(e^{f_0} - e^{\tilde{f}_{\lambda, n}})q_0\|_{L^1(\Omega)}}{A(\tilde{f}_{\lambda, n})}.
\]

Using (26), we bound \( |A(\tilde{f}_{\lambda, n}) - A(f_0)| \) as

\[
|A(\tilde{f}_{\lambda, n}) - A(f_0)| \leq \int |e^{\tilde{f}_{\lambda, n}(x)} - e^{f_0(x)}| q_0(x) \, dx \leq \|\eta\|_{L^1(\Omega,q_0)} \|\tilde{f}_{\lambda, n} - f_0\|_\mathcal{H}.
\]

Also for any \( f \in \mathcal{H} \) with \( \|f\|_\mathcal{H} \leq M \), we have \( A(f) \geq \int e^{-M \sqrt{k(x,x)}} q_0(x) \, dx =: \theta \), where \( \theta > 0 \). Again using (26), we have

\[
\|(e^{f_0} - e^{\tilde{f}_{\lambda, n}})q_0\|_{L^r(\Omega)} \leq \|\eta q_0\|_{L^r(\Omega)} \|\tilde{f}_{\lambda, n} - f_0\|_\mathcal{H}
\]

and \( \|e^{f_0}q_0\|_{L^r(\Omega)} \leq \|e^{M \sqrt{k(x,x)}} q_0\|_{L^r(\Omega)} \). Therefore,

\[
\|p_{\tilde{f}_{\lambda, n}} - p_0\|_{L^r(\Omega)} \leq \frac{\|\eta\|_{L^1(\Omega,q_0)} e^{M \sqrt{k(x,x)}} q_0}{\theta^2} \|\|\tilde{f}_{\lambda, n} - f_0\|_\mathcal{H} + \|\eta q_0\|_{L^r(\Omega)} \|\tilde{f}_{\lambda, n} - f_0\|_\mathcal{H}
\]

and for \( r = 1 \),

\[
\|p_{\tilde{f}_{\lambda, n}} - p_0\|_{L^1(\Omega)} \leq \frac{2 \|\eta\|_{L^1(\Omega,q_0)} \|\tilde{f}_{\lambda, n} - f_0\|_\mathcal{H}}{\theta}.
\]

(ii) Also

\[
KL(p_0\|p_{\tilde{f}_{\lambda, n}}) = \int p_0 \log \frac{p_0}{p_{\tilde{f}_{\lambda, n}}} \, dx = \int \log \left( \frac{e^{f_0} - \tilde{f}_{\lambda, n} A(\tilde{f}_{\lambda, n})}{A(f_0)} \right) p_0(x) \, dx
\]

\[
= \int \left( f_0 - \tilde{f}_{\lambda, n} + \log \frac{A(\tilde{f}_{\lambda, n})}{A(f_0)} \right) p_0(x) \, dx
\]

\[
\leq \frac{|A(\tilde{f}_{\lambda, n}) - A(f_0)|}{A(f_0)} + \int |\tilde{f}_{\lambda, n} - f_0| p_0(x) \, dx \leq \frac{2 \|\eta q_0\|_{L^1(\Omega)} \|\tilde{f}_{\lambda, n} - f_0\|_\mathcal{H}}{\theta}.
\]

(iii) It is easy to verify that

\[
\frac{e^{f_0/2}}{\|e^{f_0/2}\|_{L^2(\Omega,q_0)}} - \frac{e^{\tilde{f}_{\lambda, n}/2}}{\|e^{\tilde{f}_{\lambda, n}/2}\|_{L^2(\Omega,q_0)}} \leq \frac{2 \|e^{f_0/2} - e^{\tilde{f}_{\lambda, n}/2}\|_{L^2(\Omega,q_0)}}{\|e^{f_0/2}\|_{L^2(\Omega,q_0)}}
\]

(29)
where the above inequality is obtained by carrying out and simplifying the decomposition as in \(\text{A.1}\). Using \(\text{20}\), we therefore have
\[
h(p f_{\lambda,n}, p_0) \leq \sqrt{\int k(x, x)e^{\frac{M}{\theta}} \sqrt{C} f_{\lambda,n} \, dx} \|f_{\lambda,n} - f_0\|_\infty.
\]
(iv) As \(f_0, f_{\lambda,n} \in \mathcal{F}\), by Theorem \(\text{3}\) we obtain
\[
J(p_0 \|p f_{\lambda,n}) = \frac{1}{2} \sqrt{C} (\| f_{\lambda,n} - f_0 \|_2^2) \leq \frac{1}{2} \sqrt{C} (\| f_{\lambda,n} - f_0 \|_2^2).
\]
Note that we have bounded the various distances between \(p f_{\lambda,n}\) and \(p_0\) in terms of \(\| f_{\lambda,n} - f_0 \|_\infty\). Since \(\tilde{f}_{\lambda,n} = f_{\lambda,n}\) with probability converging to 1, the assertions on consistency are proved by Theorem \(\text{3} (i)\) in combination with Lemma \(\text{14}\) as we did not explicitly assume \(f_0 \in \mathcal{R}(C)\)—and the rates follow from Theorem \(\text{3} (iii)\).

\[
\square
\]

8.11 \(\mathcal{R}(C^\beta)\) and interpolation spaces

In this section, we present a result (see Proposition \(\text{8.3}\)) which provides an interpretation for \(\mathcal{R}(C^\beta)\) \((\beta > 0\) and \(\beta \not\in \mathbb{N}\)) as interpolation spaces between \(\mathcal{R}(C^{\beta_1})\) and \(\mathcal{R}(C^{\beta_2})\) where \(\mathcal{R}(C^0) := \mathcal{H}\). Before we the result, we need to briefly recall the definition of interpolation spaces of the real method. To this end, let \(E_0\) and \(E_1\) be two arbitrary Banach spaces that are continuously embedded in some topological (Hausdorff) vector space \(E\). Then, for \(x \in E_0 + E_1 := \{x_0 + x_1 : x_0 \in E_0, x_1 \in E_1\}\) and \(t > 0\), the \(K\)-functional of the real interpolation method, see \([4\text{, Definition 1.1, p. 293}]\), is defined by
\[
K(x, t, E_0 + E_1) := \inf\{\|x_0\|_{E_0} + t\|x_1\|_{E_1} : x_0 \in E_0, x_1 \in E_1, x = x_0 + x_1\}.
\]
Suppose \(E\) and \(F\) are two Banach spaces that satisfy \(F \hookrightarrow E\) (i.e., \(F \subset E\) and the inclusion operator \(\text{id} : F \to E\) is continuous), then the \(K\)-functional reduces to
\[
K(x, t, E, F) = \inf_{y \in F} \|x - y\|_E + t\|y\|_F.
\]
The \(K\)-functional can be used to define interpolation norms, for \(0 < \theta < 1\), \(1 \leq s \leq \infty\) and \(x \in E_0 + E_1\), as
\[
\|x\|_{\theta, s} := \left\{\begin{array}{ll}
(\int t^{-\theta} K(x, t)^s \, dt)^{1/s}, & 1 \leq s < \infty, \\
\sup_{t > 0} t^{-\theta} K(x, t), & s = \infty.
\end{array}\right.
\]
Moreover, the corresponding interpolation spaces, \([4\text{, Definition 1.7, p. 299}]\), are defined as
\[
[E_0, E_1]_{\theta, s} := \{x \in E_0 + E_1 : \|x\|_{\theta, s} < \infty\}.
\]
In addition to these preparations, we need an additional result which we quote from \([36\text{, Lemma 6.3}]\) (also see \([37\text{, Lemma 23.1}]\)) that interpolates \(L^2\)-spaces whose underlying measures are absolutely continuous with respect to a measure \(\nu\).

\[
\text{Lemma 8.4. Let } \nu \text{ be a measure on a measurable space } \Theta \text{ and } w_0 : \Theta \to [0, \infty) \text{ and } w_1 : \Theta \to [0, \infty) \text{ be measurable functions. For } 0 < \beta < 1, \text{ define } w_\beta := w_0^{1-\beta} w_1^\beta. \text{ Then we have }
\]
\[
[L^2(w_0 \, d\nu), L^2(w_1 \, d\nu)]_{\beta, 2} = L^2(w_\beta \, d\nu)
\]
and the norms on these two spaces are equivalent. Moreover, this result still holds for weights \(w_0 : \Theta \to (0, \infty)\) and \(w_1 : \Theta \to [0, \infty]\), if one uses the convention \(0 \cdot \infty := 0\) in the definition of the weighted spaces.

With these preparations, we now present a result that describes the image of the fractional power \(C^\beta\) by a suitable interpolation space. An inspection of its proof shows that the following result holds for any self-adjoint, bounded, compact operator defined on a separable Hilbert space.

\[
\text{Proposition 8.5. Suppose (B) and (D) hold with } \varepsilon = 1. \text{ Then for all } \beta > 0 \text{ and } \beta \not\in \mathbb{N}
\]
\[
\mathcal{R}(C^\beta) = \left[\mathcal{R}(C^{\beta_1}), \mathcal{R}(C^{\beta_2})\right]_{\beta - [\beta], 2}
\]
where \(\mathcal{R}(C^0) := \mathcal{H}\), and the spaces \(\mathcal{R}(C^\beta)\) and \([\mathcal{R}(C^{\beta_1}), \mathcal{R}(C^{\beta_2})]_{\beta - [\beta], 2}\) have equivalent norms.
Proof. The following proof is based on the ideas used in the proof of Theorem 4.6 in [36]. Recall that by the Hilbert-Schmidt theorem, \( C \) has the following representation,

\[
C = \sum_{i \in I} \alpha_i \langle \phi_i, \cdot \rangle_{\mathcal{H}}
\]

where \((\alpha_i)_{i \in I}\) are the positive eigenvalues of \( C \), \((\phi_i)_{i \in I}\) are the corresponding unit eigenvectors that form an ONB for \( \mathcal{R}(C) \) and \( I \) is an index set which is either finite (if \( \mathcal{H} \) is finite-dimensional) or \( I = \mathbb{N} \) with \( \lim_{i \to \infty} \alpha_i = 0 \) (if \( \mathcal{H} \) is infinite dimensional). Let \((\psi_i)_{i \in J}\) be an ONB for \( \mathcal{N}(C) \) where \( J \) is some index set so that any \( f \in \mathcal{H} \) can be written as

\[
f = \sum_{i \in I} \langle f, \phi_i \rangle_{\mathcal{H}} \phi_i + \sum_{i \in J} \langle f, \psi_i \rangle_{\mathcal{H}} \psi_i =: \sum_{i \in I \cup J} a_i \theta_i
\]

where \( \theta_i := \phi_i \) if \( i \in I \) and \( \theta_i := \psi_i \) if \( i \in J \) with \( a_i := \langle f, \theta_i \rangle_{\mathcal{H}} \). Let \( \beta > 0 \). By definition, \( g \in \mathcal{R}(C^\beta) \) is equivalent to \( \exists h \in \mathcal{H} \) such that \( g = C^\beta h \), i.e.,

\[
g = \sum_{i \in I} \alpha_i^\beta \langle h, \phi_i \rangle_{\mathcal{H}} \phi_i =: \sum_{i \in I} b_i \alpha_i^\beta \phi_i
\]

where \( b_i := \langle h, \phi_i \rangle_{\mathcal{H}} \). Clearly \( \sum_{i \in I} b_i^2 = \sum_{i \in I} \langle h, \phi_i \rangle^2_{\mathcal{H}} \leq \| h \|_{2\mathcal{H}}^2 < \infty \), i.e., \((b_i) \in \ell_2(I)\). Therefore

\[
\mathcal{R}(C^\beta) = \left\{ \sum_{i \in I} b_i \alpha_i^\beta \phi_i : (b_i) \in \ell_2(I) \right\} = \left\{ \sum_{i \in I} c_i \phi_i : (c_i) \in \ell_2(I, \alpha^{-2\beta}) \right\}
\]

where \( \alpha := (\alpha_i)_{i \in I} \). Let us equip this space with the bilinear form

\[
\left\langle \sum_{i \in I} c_i \phi_i, \sum_{i \in I} d_i \phi_i \right\rangle_{\mathcal{R}(C^\beta)} := \left\langle (c_i), (d_i) \right\rangle_{\ell_2(I, \alpha^{-2\beta})}
\]

so that it induces the norm

\[
\left\| \sum_{i \in I} c_i \phi_i \right\|_{\mathcal{R}(C^\beta)} := \left\| (c_i) \right\|_{\ell_2(I, \alpha^{-2\beta})}.
\]

It is easy to verify that \((\alpha_i^\beta \phi_i)_{i \in I}\) is an ONB of \( \mathcal{R}(C^\beta) \). Also since \( \mathcal{R}(C^{\beta_1}) \subset \mathcal{R}(C^{\beta_2}) \) for \( 0 < \beta_2 < \beta_1 < \infty \) and \( \text{id} : \mathcal{R}(C^{\beta_1}) \to \mathcal{R}(C^{\beta_2}) \) is continuous, i.e., for any \( g \in \mathcal{R}(C^{\beta_1}) \),

\[
\| g \|_{\mathcal{R}(C^{\beta_2})} = \| (c_i) \|_{\ell_2(I, \alpha^{-2\beta_2})} = \sum_{i \in I} \frac{c_i^2}{\alpha_i^{2\beta}} \leq \sup_{i \in I} |\alpha_i|^{\beta_1-\beta_2} \| (c_i) \|_{\ell_2(I, \alpha^{-2\beta_1})} = \| C \|^{\beta_1-\beta_2} \| g \|_{\mathcal{R}(C^{\beta_1})} < \infty
\]

and so \( \mathcal{R}(C^{\beta_1}) \to \mathcal{R}(C^{\beta_2}) \). Similarly, we can show that \( \mathcal{R}(C) \to \mathcal{H} \). In the following, we first prove the result for \( 0 < \beta < 1 \) and then for \( \beta > 1 \).

(a) \( 0 < \beta < 1 \): For any \( f \in \mathcal{H} \) and \( g \in \mathcal{R}(C) \), we have

\[
\| f - g \|_{2\mathcal{H}}^2 = \left\| \sum_{i \in I \cup J} a_i \theta_i - \sum_{i \in I} c_i \phi_i \right\|_{2\mathcal{H}}^2 = \left\| \sum_{i \in I \cup J} (a_i - c_i) \theta_i \right\|^2_{2\mathcal{H}} = \| (a_i - c_i) \|^2_{\ell_2(I \cup J)}
\]

where we define \( c_i := 0 \) for \( i \in J \). For \( t > 0 \), we find

\[
K(f, t, \mathcal{H}, \mathcal{R}(C)) = \inf_{g \in \mathcal{R}(C)} \| f - g \|_{2\mathcal{H}} + t \| g \|_{\mathcal{R}(C)} = \inf_{(c_i) \in \ell_2(I, \alpha^{-2})} \| (a_i - c_i) \|^2_{\ell_2(I \cup J)} + t \| (c_i) \|^2_{\ell_2(I, \alpha^{-2})} = K(a, t, \ell_2(I \cup J), \ell_2(I, \alpha^{-2})).
\]

From this we immediately obtain the equivalence

\[
f \in [\mathcal{H}, \mathcal{R}(C)]_{\beta, 2} \iff (a_i) \in [\ell_2(I \cup J), \ell_2(I, \alpha^{-2})]_{\beta, 2}
\]
where $0 < \beta < 1$. Applying the second part of Lemma \[5.4\] to the counting measure on $I \cup J$ yields
\[
\ell_2(I \cup J), \ell_2(I, \alpha^{-2\beta})\beta,2 = \ell_2(I, \alpha^{-2\beta}).
\]
Since $\mathcal{R}(C^\beta)$ and $\ell_2(I, \alpha^{-2\beta})$ are isometrically isomorphic, we obtain $\mathcal{R}(C^\beta) = [\mathcal{H}, \mathcal{R}(C)]_{\beta, 2}$.

(b) $\beta > 1$ and $\beta \notin \mathbb{N}$: Define $\gamma := \lfloor \beta \rfloor$. Let $f \in \mathcal{R}(C^\gamma)$ and $g \in \mathcal{R}(C^{\gamma + 1})$, i.e., $\exists (c_i) \in \ell_2(I, \alpha^{-2\gamma})$ and $(d_i) \in \ell_2(I, \alpha^{-2\gamma - 2})$ such that $f = \sum_{i \in I} c_i \phi_i$ and $g = \sum_{i \in I} d_i \phi_i$. Since
\[
\|f - g\|_{\mathcal{R}(C^\gamma)} = \|(c_i - d_i)\|_{\ell_2(I, \alpha^{-2\gamma})},
\]
for $t > 0$, we have
\[
K(f, t, \mathcal{R}(C^\gamma), \mathcal{R}(C^{\gamma + 1})) = \inf_{g \in \mathcal{R}(C^{\gamma + 1})} \|f - g\|_{\mathcal{R}(C^\gamma)} + t\|g\|_{\mathcal{R}(C^{\gamma + 1})}
= \inf_{(d_i) \in \ell_2(I, \alpha^{-2\gamma - 2})} \|(c_i - d_i)\|_{\ell_2(I, \alpha^{-2\gamma})} + t\|(d_i)\|_{\ell_2(I, \alpha^{-2\gamma - 2})}
= K(c, t, \ell_2(I, \alpha^{-2\gamma}), \ell_2(I, \alpha^{-2\gamma - 2}))
\]
from which we obtain the following equivalence
\[
f \in [\mathcal{R}(C^\gamma), \mathcal{R}(C^{\gamma + 1})]_{\beta - \gamma, 2} \iff (c_i) \in \ell_2(I, \alpha^{-2\gamma}), \ell_2(I, \alpha^{-2\gamma - 2}) \beta - \gamma, 2 \Rightarrow \ell_2(I, \alpha^{-2\beta}),
\]
where $(\ast)$ follows from Lemma \[5.4\] and the result is obtained by noting that $\ell_2(I, \alpha^{-2\beta})$ and $\mathcal{R}(C^\beta)$ are isometrically isomorphic. \[\Box\]

### 8.12 Proof of Proposition \[5.4\]

**Observation 1**: By \[5.3\] Theorem 10.12, we have
\[
\mathcal{H} = \left\{ f \in L^2(\mathbb{R}^d) \cap C_b(\mathbb{R}^d) : \frac{f^\wedge}{\sqrt{\psi^\wedge}} \in L^2(\mathbb{R}^d) \right\},
\]
where $f^\wedge$ is defined in $L^2$ sense. Since
\[
\int |f^\wedge(\omega)| \, d\omega \leq \left( \int \frac{|f^\wedge(\omega)|^2}{\psi^\wedge(\omega)} \, d\omega \right)^{\frac{1}{2}} \left( \int \psi^\wedge(\omega) \, d\omega \right)^{\frac{1}{2}} < \infty
\]
where we used $\psi^\wedge \in L^1(\mathbb{R}^d)$ (see \[5.3\] Corollary 6.12), we have $f^\wedge \in L^1(\mathbb{R}^d)$. Hence Plancherel’s theorem and continuity of $f$ along with the inverse Fourier transform of $f^\wedge$ allow to recover any $f \in \mathcal{H}$ pointwise from its Fourier transform as
\[
f(x) = \frac{1}{(2\pi)^{d/2}} \int e^{ix^T\omega} f^\wedge(\omega) \, d\omega, \ x \in \mathbb{R}^d. \tag{31}
\]

**Observation 2**: Since $\psi^\wedge \in L^1(\mathbb{R}^d)$ and $\psi^\wedge \geq 0$, we have for all $j = 1, \ldots, d$,
\[
\left( \int |\omega_j | \psi^\wedge(\omega) \, d\omega \right)^2 \leq \left( \int \psi^\wedge(\omega) \, d\omega \right)^2 \left( \int |\omega_j |^2 \psi^\wedge(\omega) \, d\omega \right)^{\frac{1}{2}} \leq \left( \int \psi^\wedge(\omega) \, d\omega \right) \left( \int |\omega_j |^2 \psi^\wedge(\omega) \, d\omega \right)^{\frac{1}{2}} \leq \left( \int \psi^\wedge(\omega) \, d\omega \right) \left( \int \omega \|\|^{2} \psi^\wedge(\omega) \, d\omega \right)^{\frac{1}{2}} \leq \left( \int \psi^\wedge(\omega) \, d\omega \right) \left( \int \|\|^{2} \psi^\wedge(\omega) \, d\omega \right)^{\frac{1}{2}} < \infty,
\]
where we used Jensen’s inequality in $(\ast)$. This means $\omega_j \psi^\wedge(\omega) \in L^1(\mathbb{R}^d)$, $\forall \ j = 1, \ldots, d$ which ensures the existence of its Fourier transform and so
\[
\frac{\partial \psi(x)}{\partial x_j} = \frac{1}{(2\pi)^{d/2}} \int (i\omega_j) \psi^\wedge(\omega) e^{ix^T\omega} \, d\omega, \ x \in \mathbb{R}^d, \ \forall \ j = 1, \ldots, d. \tag{32}
\]
Observation 3: For $g \in \mathcal{H}$, we have for all $j = 1, \ldots, d$,
\[
\int |\omega_j|g^\wedge(\omega)| d\omega \leq \left( \int \frac{|g^\wedge(\omega)|^2}{\psi^\wedge(\omega)} d\omega \right)^{\frac{1}{2}} \left( \int |\omega_j|^2\psi^\wedge(\omega) d\omega \right)^{\frac{1}{2}} \leq \left( \int \frac{|g^\wedge(\omega)|^2}{\psi^\wedge(\omega)} d\omega \right)^{\frac{1}{2}} \left( \int \|\omega\|^2\psi^\wedge(\omega) d\omega \right)^{\frac{1}{2}} < \infty,
\]
which implies $\omega_j g^\wedge(\omega) \in L^1(\mathbb{R}^d), \forall j = 1, \ldots, d$. Therefore,
\[
\frac{\partial g(x)}{\partial x_j} = \frac{1}{(2\pi)^{d/2}} \int (i\omega_j)g^\wedge(\omega) e^{ix^T\omega} d\omega, \ x \in \mathbb{R}^d, \ \forall j = 1, \ldots, d. \quad (33)
\]
Observation 4: For any $g \in \mathfrak{S}$, we have
\[
\int \frac{|g^\wedge(\omega)|^2}{\psi^\wedge(\omega)} d\omega = \int \frac{|g^\wedge(\omega)|^2}{\phi^\wedge(\omega)} \frac{\phi^\wedge(\omega)}{\psi^\wedge(\omega)} d\omega \leq \|g\|_2 \left\| \frac{\phi^\wedge}{\psi^\wedge} \right\|_\infty < \infty,
\]
which implies $g \in \mathcal{H}$, i.e., $\mathfrak{S} \subset \mathcal{H}$.

We now use these observations to prove the result. Since $f_0 \in \mathcal{R}(C)$, there exists $g \in \mathcal{H}$ such that $f_0 = Cg$, which means
\[
f_0(y) = \int \sum_{j=1}^d \frac{\partial k(x, y)}{\partial x_j} \frac{\partial g(x)}{\partial x_j} \phi_0(x) \ dx = \int \sum_{j=1}^d \frac{1}{(2\pi)^{d/2}} \int e^{i(x-y)^T\omega}(i\omega_j)\phi^\wedge(\omega) \frac{\partial g(x)}{\partial x_j} \phi_0(x) \ dx
\]
\[
= \int \sum_{j=1}^d \frac{1}{(2\pi)^{d/2}} \int e^{i(x-y)^T\omega} \frac{\partial g(x)}{\partial x_j} \phi_0(x) \ dx \ (i\omega_j)\phi^\wedge(\omega) e^{-iy^T\omega} \ d\omega
\]
\[
= \frac{1}{(2\pi)^{d/2}} \int \sum_{j=1}^d (i\omega_j g^\wedge \ast \phi_0^\wedge)(\omega) \ (i\omega_j)\phi^\wedge(\omega) e^{-iy^T\omega} \ d\omega
\]
which from (82) means
\[
f_0^\wedge(\omega) = \sum_{j=1}^d (i\omega_j g^\wedge \ast \phi_0^\wedge)(\omega) \ (i\omega_j)\phi^\wedge(\omega), \quad (34)
\]
where we have invoked Fubini’s theorem in (1) and * represents the convolution. Define $\| \cdot \|_{L^r(\mathbb{R}^d)} := \| \cdot \|_r$. Consider
\[
\|f_0\|^2_B = \int \frac{|f_0^\wedge(\omega)|^2}{\phi^\wedge(\omega)} \ d\omega = \int \sum_{j=1}^d (i\omega_j g^\wedge \ast \phi_0^\wedge)(\omega) \ (i\omega_j)\phi^\wedge(\omega) \ d\omega \leq \int \sum_{j=1}^d |i\omega_j g^\wedge \ast \phi_0^\wedge| |(i\omega_j)| \phi^\wedge(\omega) \ d\omega \leq \int \sum_{j=1}^d |i\omega_j g^\wedge \ast \phi_0^\wedge|^2 \ d\omega \|\phi^\wedge(\omega)\|^2 \ (i\omega_j)^2 \|\phi^\wedge(\omega)\| \ d\omega \leq \left\| \int \sum_{j=1}^d |i\omega_j g^\wedge \ast \phi_0^\wedge|^2 (\cdot) \ |\cdot| \ d\omega \right\|_{L^2(\mathbb{R}^d)} \| \cdot \|_{L^2(\mathbb{R}^d)} < \infty, \quad (iii)
\]

31
where in the following we show that \( \sum_{j=1}^{d} |i\omega_j g^\wedge(\omega) * p_0^\wedge(\omega)|^2(\cdot) \in L^{\|r\|_{c}}(\mathbb{R}^d) \), i.e.,

\[
\left\| \sum_{j=1}^{d} |i\omega_j g^\wedge(\omega) * p_0^\wedge(\omega)|^2(\cdot) \right\|_{L^{\|r\|_{c}}} \leq \sum_{j=1}^{d} \left\| i\omega_j g^\wedge(\omega) * p_0^\wedge(\omega) \right\|^2_{L^{\|r\|_{c}}(\mathbb{R}^d)} = \sum_{j=1}^{d} \left\| i\omega_j g^\wedge(\omega) * p_0^\wedge(\omega) \right\|^2_{L^{\|r\|_{c}}(\mathbb{R}^d)} \leq \frac{(+)}{(**)} \left( \sum_{j=1}^{d} \left\| i\omega_j g^\wedge(\omega) \right\|^2_{L^{\|r\|_{c}}(\mathbb{R}^d)} \right) \leq \frac{(+)}{(**)} \left\| p_0 \right\|^2 \sum_{j=1}^{d} \left\| i\omega_j g^\wedge(\omega) \right\|^2_{L^{\|r\|_{c}}(\mathbb{R}^d)} < \infty,
\]

where we have invoked generalized Young’s inequality [13] Proposition 8.9 in \((*)\), Hausdorff-Young inequality [13] p. 253 in \((**)\), and observation 3 combined with \((iv)\) in \((1)\). This shows that \( f_0 \in \mathcal{R}(C) \Rightarrow f_0 \in \mathfrak{g}, \) i.e., \( \mathcal{R}(C) \subset \mathfrak{g} \). \( \square \)

### 8.13 Proof of Theorem 9

To prove Theorem 9 we need the following lemma [11] Lemma 5], which is due to Andreas Maurer.

**Lemma 15.** Suppose \( A \) and \( B \) are self-adjoint Hilbert-Schmidt operators on a separable Hilbert space \( H \) with spectrum contained in the interval \([a, b]\), and let \((\sigma_i)_{i \in I}\) and \((\tau_j)_{j \in J}\) be the eigenvalues of \( A \) and \( B \), respectively. Given a function \( r : [a, b] \to \mathbb{R} \), if there exists a finite constant \( L \) such that \( |r(\sigma_i) - r(\tau_j)| \leq L|\sigma_i - \tau_j| \), \( \forall i \in I, j \in J \), then \( \|r(A) - r(B)\|_{HS} \leq L\|A - B\|_{HS} \).  

**Proof of Theorem 9** (i) The proof follows the ideas in the proof of Theorem 10 in [3], which is a more general result dealing with the smoothness condition, \( f_0 \in \mathcal{R}(\Theta(C)) \) where \( \Theta \) is operator monotone. Recall that \( \Theta \) is operator monotone on \([0, b]\) if for any pair of self-adjoint operators \( U, V \) with spectra in \([0, b]\) such that \( U \leq V \), we have \( \Theta(U) \leq \Theta(V) \), where \( \leq \) is the partial ordering for self-adjoint operators on some Hilbert space \( H \), which means for any \( f \in H \), \( \langle f, U f \rangle_H \leq \langle f, V f \rangle_H \). In our case, we adapt the proof for \( \Theta(C) = C^\beta \). Define \( r_\lambda(\alpha) := g_\lambda(\alpha)\alpha \) \( - 1 \). Since \( f_0 \in \mathcal{R}(C^\beta) \), there exists \( h \in \mathfrak{H} \) such that \( f_0 = C^\beta h \), which yields

\[
f_{g, \lambda, n} - f_0 = -g_\lambda(\hat{C})\hat{\xi} - f_0 = -g_\lambda(\hat{C})(\hat{\xi} + \hat{C} f_0) + r_\lambda(\hat{C})C^\beta h
= -g_\lambda(\hat{C})(\hat{\xi} + \hat{C} f_0) + r_\lambda(\hat{C})\hat{C}^\beta h + r_\lambda(\hat{C})(C^\beta - \hat{C}^\beta) h.
\]

so that

\[
\|f_{g, \lambda, n} - f_0\|_{2\xi} \leq \|g_\lambda(\hat{C})(\hat{\xi} + \hat{C} f_0)\|_{2\xi} + \|r_\lambda(\hat{C})C^\beta h\|_{2\xi} + \|r_\lambda(\hat{C})(C^\beta - \hat{C}^\beta) h\|_{2\xi}.
\]

We now bound \((A)\)-(C). Since \( (A) \leq \|g_\lambda(\hat{C})\|\|\hat{\xi} + \hat{C} f_0\|_{2\xi} \), we have \( (A) = O_{p_0}\left(\frac{1}{\lambda^{\max\{\lambda\}}\lambda}\right) \) where we used \((b)\) in \((E)\) and the bound on \( \|\hat{\xi} + \hat{C} f_0\|_{2\xi} \) from the proof of Theorem 8(i). Also, \((d)\) in \((E)\) implies that

\[
(B) \leq \|r_\lambda(\hat{C})\hat{C}^\beta\|\|h\|_{2\xi} \leq \max\{\gamma_\beta, \gamma_{\mathfrak{g}}\}\lambda^{\min\{\lambda, n\}}\|C^\beta - \hat{C}^\beta\|_{2\xi}.
\]

\((C)\) can be bounded as

\[
(C) \leq \|r_\lambda(\hat{C})\|\|C^\beta - \hat{C}^\beta\|\|C^{\beta - \hat{C}^\beta} f_0\|_{2\xi}.
\]

We now consider two cases:

\( \beta \leq 1 \): Since \( \alpha \mapsto \alpha^\theta \) is operator monotone on \([0, dE^2]\) for \( 0 \leq \theta \leq 1 \), by Theorem 1 in [3], there exists a constant \( c_\theta \) such that \( \|\hat{C}^\theta - C^\theta\| \leq c_\theta\|\hat{C} - C\|_{HS} \leq c_\theta\|\hat{C} - C\|_{HS} \) and so \( \|C\| = O_{p_0}(n^{1/2}) \). Since \( \lambda \geq n^{-1/2} \), we have \( \|C\| = O_{p_0}(\lambda^\beta) \).

\( \beta > 1 \): Since \( \alpha \mapsto \alpha^\theta \) is Lipschitz on \([0, dE^2]\) for \( \theta \geq 1 \), by Lemma 13 \( \|C^\beta - \hat{C}^\beta\| \leq \|C^\beta - \hat{C}^\beta\|_{HS} \leq \beta(dE^2)^{\beta - 1}\|C - \hat{C}\|_{HS} \) and therefore \( \|C\| = O_{p_0}(n^{1/2}) \).
Collecting all the above bounds, we obtain

\[ \|f_{g,\lambda, n} - f_0\|_{\mathcal{H}} \leq O_p\left( \frac{1}{\sqrt{n}} \right) + O_p\left( \lambda^{\min(\beta, n_0)} \right) \]

and the result follows. The proofs of the claims involving \( L^* \), \( h \) and \( KL \) follow exactly the same ideas as in the proof of Theorem \( \text{A.1} \) by using the above bound on \( \|f_{g,\lambda, n} - f_0\|_{\mathcal{H}} \) in Lemma \( \text{A.1} \).

(ii) We now bound \( J(p_0 \| p_{f_{g,\lambda, n}}) = \| \sqrt{C}(f_{g,\lambda, n} - f_0) \|_{\mathcal{H}}^2 \) as follows. Note that

\[ \sqrt{C}(f_{g,\lambda, n} - f_0) = \left( \sqrt{C} - \sqrt{C}(f_{g,\lambda, n} - f_0) + \sqrt{C}(f_{g,\lambda, n} - f_0) \right). \]

We bound \( \| (I') \|_{\mathcal{H}} \) as

\[ \| (I') \|_{\mathcal{H}} \leq \| \sqrt{C} - \sqrt{C}(f_{g,\lambda, n} - f_0) \|_{\mathcal{H}} \leq c_4 \sqrt{\| C - \sqrt{C} \|_{HS}} \| f_{g,\lambda, n} - f_0 \|_{\mathcal{H}} \]

\[ = O_p\left( \frac{1}{\sqrt{n}} \right) + O_p\left( \lambda^{\min(\beta, n_0)} \right), \]

where we used the fact that \( \alpha \mapsto \sqrt{\alpha} \) is operator monotone along with \( \lambda \geq n^{-1/2} \). Using (33), \( \| (I') \|_{\mathcal{H}} \) can be bounded as

\[ \| (II') \|_{\mathcal{H}} \leq \| \sqrt{C} g_\lambda(\hat{C}) \| \| \hat{C} f_0 \|_{\mathcal{H}} + \| \sqrt{C} r_\lambda(\hat{C}) \| \| C^{-\beta} f_0 \|_{\mathcal{H}} + \| \sqrt{C} r_\lambda(\hat{C}) \| \| C^{-\beta} f_0 \|_{\mathcal{H}} \]

where \( \| \sqrt{C} g_\lambda(\hat{C}) \| \leq \sqrt{\frac{\lambda_1 \varepsilon}{\lambda_2}} \), \( \| \sqrt{C} r_\lambda(\hat{C}) \| \leq (\frac{\gamma_0}{\gamma_0}) \lambda^{\min(\beta, n_0)} \) and \( \| \sqrt{C} r_\lambda(\hat{C}) \| \leq (\frac{\gamma_0}{\gamma_0}) \lambda^{\min(\beta, n_0)} \) with \( \| \hat{C} f_0 \|_{\mathcal{H}} \) and \( \| C^{-\beta} \|_{\mathcal{H}} \) bounded as in part (i) above. Here \( (a \lor b) := \max\{a, b\} \). Combining \( \| (I') \|_{\mathcal{H}} \) and \( \| (II') \|_{\mathcal{H}} \), we obtain the required result.

(iii) The proof follows the ideas in the proof of Theorems 5 and 6. Consider \( f_{g,\lambda, n} - f_0 = -g_\lambda(\hat{C})(\hat{C} f_0 + \hat{\xi}) + r_\lambda(\hat{C}) f_0 \) so that

\[ \|f_{g,\lambda, n} - f_0\|_{\mathcal{H}} \leq \| C^{-1} \| \| C g_\lambda(\hat{C}) \| \| \hat{C} f_0 + \hat{\xi} \|_{\mathcal{H}} + \| C^{-1} \| \| r_\lambda(\hat{C}) \| \| f_0 \|_{\mathcal{H}} \]

\[ \leq \| C^{-1} \| \| \hat{C} f_0 + \hat{\xi} \|_{\mathcal{H}} + \| \| C^{-1} \| \| g_\lambda(\hat{C}) \| \| \hat{C} - C \| \| f_0 \|_{\mathcal{H}} \]

Therefore \( \|f_{g,\lambda, n} - f_0\|_{\mathcal{H}} = O_p(n^{-1/2}) + O(\lambda^{\min(1, n_0)}) \) where we used the fact that \( \lambda \geq n^{-1/2} \) and the result follows.

\[ \square \]

8.14 Proof of Theorem 10

Before studying \( J(p_0 \| p_{f_{g,\lambda, n}}) \), let us consider \( J(p_0 \| p_f) \) for any \( p_f \in \mathcal{P} \),

\[ J(p_0 \| p_f) = \frac{1}{2} \int p_0(x) \left( \frac{\partial}{\partial x} \log p_0(x) - \frac{\partial f}{\partial x} \right)^2 dx = \frac{1}{2} \int p_0(x) \left( \frac{\partial}{\partial x} \log p_0(x) \right)^2 dx, \]

where the last equality is obtained by using a calculation similar to the one in the proof of Theorem 3 with \( C := \int p_0(x) \sum_{i=1}^d \frac{\partial f(x)}{\partial x_i} \wedge \frac{\partial f(x)}{\partial x_i} dx \) and \( \zeta := \int p_0(x) \sum_{i=1}^d \frac{\partial \log p_0(x)}{\partial x_i} \frac{\partial \log p_0(x)}{\partial x_i} dx \). From Theorem 3(i), it is clear that \( C \) is a compact, positive, self-adjoint operator. Since \( f^* \in \arg \inf_{f \in \mathcal{F}} J(p_0, p_f) \), it is easy to check that \( f^* \) satisfies \( C f^* = \zeta \). Also note that for any \( f \in \mathcal{H} \),

\[ \langle f, \zeta \rangle_{\mathcal{H}} = \int p_0(x) \sum_{i=1}^d \frac{\partial f(x)}{\partial x_i} \left( \frac{\partial \log p_0(x)}{\partial x_i} - \frac{\partial \log p_0(x)}{\partial x_i} \right) dx \]

\[ = \int \sum_{i=1}^d \frac{\partial f(x)}{\partial x_i} \frac{\partial p_0(x)}{\partial x_i} dx - \int p_0(x) \sum_{i=1}^d \frac{\partial f(x)}{\partial x_i} \frac{\partial \log p_0(x)}{\partial x_i} dx \]
\[\begin{align*}
\equiv & - \int p_0(x) \sum_{i=1}^{d} \frac{\partial^2 f(x)}{\partial x_i^2} \, dx - \int p_0(x) \sum_{i=1}^{d} \left( \frac{\partial f(x)}{\partial x_i} \frac{\partial \log q_0(x)}{\partial x_i} \right) \, dx \\
= & - \int p_0(x) \sum_{i=1}^{d} \left( f_i \frac{\partial^2 k(\cdot,x)}{\partial x_i^2} + \frac{\partial k(\cdot,x)}{\partial x_i} \frac{\partial \log q_0(x)}{\partial x_i} \right) \, dx \\
= & - \left\langle f, \int p_0(x) \sum_{i=1}^{d} \left( \frac{\partial^2 k(\cdot,x)}{\partial x_i^2} + \frac{\partial k(\cdot,x)}{\partial x_i} \frac{\partial \log q_0(x)}{\partial x_i} \right) \, dx \right\rangle_{\mathcal{H}},
\end{align*}\]

where \((*)\) follows from partial integration. Hence

\[J(p_0\| p_f) = \frac{1}{2} \langle f, C f \rangle_{\mathcal{H}} + \langle f, \xi \rangle_{\mathcal{H}} + \frac{1}{2} \int p_0(x) \left\| \frac{\partial}{\partial x} \log \frac{p_0}{q_0} \right\|_2^2 \, dx. \quad (36)\]

Similar to Theorem 3, it can be shown that

\[f_\lambda := -(C + \lambda I)^{-1} \xi \in \mathcal{H} \quad (37)\]

is the unique minimizer of \(J(p_0\| p_f) + \frac{1}{2} \| f \|_{\mathcal{H}}^2\) where \(\lambda > 0\). By replacing \(C\) and \(\xi\) by \(\hat{C}\) and \(\hat{\xi}\) respectively, it is interesting to note that minimizing

\[\frac{1}{2} \langle f, \hat{C} f \rangle_{\mathcal{H}} + \langle f, \hat{\xi} \rangle_{\mathcal{H}} + \frac{1}{2} \int p_0(x) \left\| \frac{\partial}{\partial x} \log \frac{p_0}{q_0} \right\|_2^2 \, dx + \frac{\lambda}{2} \| f \|_{\mathcal{H}}^2\]

over \(f \in \mathcal{H}\) yields the same estimator \(f_{\lambda,n} := (\hat{C} + \lambda I)^{-1} \hat{\xi}\) that is obtained in Theorems 3 and 4. Given this estimator, \(f_{\lambda,n}\), one can construct \(p_{f_{\lambda,n}}\) as a plug-in estimator. Before we analyze \(J(p_0\| p_{f_{\lambda,n}})\), we need a small calculation for notational convenience.

For any probability densities \(p, q \in C^1\), it is clear that \(\sqrt{2J(p\| q)} = \left\| \frac{\partial \log p}{\partial x} - \frac{\partial \log q}{\partial x} \right\|_{L^2(\mu)}\). We generalize this by defining

\[\sqrt{2J(p\| q)} := \left\| \frac{\partial \log p}{\partial x} - \frac{\partial \log q}{\partial x} \right\|_{L^2(\mu)}.\]

Clearly, if \(\mu = p\), then \(J(p\| q)\) matches with \(J(p\| q)\). Therefore, for probability densities \(p, q, r \in C^1\),

\[\sqrt{J(p\| r)} \leq \sqrt{J(p\| q) + J(q\| r)}. \quad (38)\]

Based on (38), we have

\[\begin{align*}
\inf_{p \in P} J(p_0\| p) & \leq \sqrt{J(p_0\| p_{f_{\lambda,n}}\| p_0) + J(p_{f^{*}}\| p_{f_{\lambda,n}}\| p_0)} \\
& = \sqrt{\inf_{p \in P} J(p_0\| p) + \sqrt{J(p_{f^{*}}\| p_{f_{\lambda,n}}\| p_0)}} \\
& = \sqrt{\inf_{p \in P} J(p_0\| p) + \frac{1}{\sqrt{2}} \sqrt{\| f_{\lambda,n} - f^{*}, C(f_{\lambda,n} - f^{*}) \|_{\mathcal{H}}}} \\
& = \sqrt{\inf_{p \in P} J(p_0\| p) + \frac{1}{\sqrt{2}} \sqrt{\mathcal{A}_{\| \mathcal{H}}(f_{\lambda,n} - f^{*})}} \\
& = \sqrt{\inf_{p \in P} J(p_0\| p) + \frac{1}{\sqrt{2}} \sqrt{\mathcal{A}_{\| \mathcal{H}}(f_{\lambda,n} - f^{*})} + \frac{1}{\sqrt{2}} \mathcal{A}^{*}(\lambda), \quad (39)\end{align*}\]

where \(\mathcal{A}^{*}(\lambda) = \| \sqrt{\mathcal{C}}(f_{\lambda,n} - f^{*}) \|_{\mathcal{H}}\). The result simply follows from the proof of Theorem 6 where we showed that \(\| \sqrt{\mathcal{C}}(f_{\lambda,n} - f_{\lambda}) \|_{\mathcal{H}} = O_{p_0}(\frac{1}{\sqrt{n}})\) and \(\mathcal{A}^{*}(\lambda) = O(\lambda^{-\frac{1}{2} + \frac{1}{2} < 1})\) as \(\lambda \to 0\), \(n \to \infty\) if \(f_0 \in R(C^{\beta})\) for \(\beta \geq 0\). When \(|C^{-1}| < \infty\), we bound \(\| \sqrt{\mathcal{C}}(f_{\lambda,n} - f^{*}) \|_{\mathcal{H}}\) in (38) as \(\| \sqrt{\mathcal{C}}(f_{\lambda,n} - f^{*}) \|_{\mathcal{H}}\) where \(f_{\lambda,n} - f^{*}\) is in turn bounded as in (19).
8.15 Proof of Proposition \[\text{[11]}\]

For \(f \in \mathcal{H}\), we have
\[
\|f\|_{W_2}^2 = \int \left( \sum_{i=1}^{d} \left( \frac{\partial f}{\partial x_i} \right)^2 \right) p_0(x) \, dx \leq \|f\|_{\mathcal{H}}^2 \int \left( \sum_{i=1}^{d} \left| \frac{\partial k(\cdot, x)}{\partial x_i} \right| \right)^2 p_0(x) \, dx < \infty,
\]
which means \(f \in W_2(p_0)\) and therefore \([f]_\sim \in W_2(p_0)\). Since \(\|I_k f\|_{W_2} = \|f\|_{W_2} = \|f\|_{\mathcal{H}} \leq c \|f\|_{\mathcal{H}} < \infty\) where \(c\) is some constant, it is clear that \(I_k\) is a continuous map from \(\mathcal{H}\) to \(W_2(p_0)\). The adjoint \(S_k : W_2(p_0) \to \mathcal{H}\) of \(I_k : \mathcal{H} \to W_2(p_0)\) is defined by the relation \((S_k f, g)_{\mathcal{H}} = (f, I_k g)_{W_2}\), \(f \in W_2(p_0)\), \(g \in \mathcal{H}\). If \(f := [h]_\sim \in W_2^{-\infty}\), then
\[
(h, I_k g)_{W_2} = \sum_{|\alpha|=1} (\partial^\alpha h)(x) (\partial^\alpha g)(x) p_0(x) \, dx.
\]
For \(y \in \Omega\) and \(g = k(\cdot, y)\), this yields
\[
S_k[h]_\sim(y) = (S_k[h]_\sim, k(\cdot, y))_{\mathcal{H}} = (h, I_k k(\cdot, y))_{W_2} = \int \sum_{i=1}^{d} \frac{\partial k(y, x)}{\partial x_i} (\partial^\alpha h)(x) p_0(x) \, dx.
\]
We now show that \(I_k\) is Hilbert-Schmidt. Since \(\mathcal{H}\) is separable, let \((e_l)_{l \geq 1}\) be an ONB of \(\mathcal{H}\). Then we have
\[
\sum_{l} \|I_k e_l\|_{W_2}^2 = \sum_{l} \int \sum_{i=1}^{d} \left( \frac{\partial e_l(x)}{\partial x_i} \right)^2 p_0(x) \, dx = \int \sum_{i=1}^{d} \sum_{l} \left( \frac{\partial k(x, \cdot)}{\partial x_i} \right)_{\mathcal{H}}^2 p_0(x) \, dx = \int \sum_{i=1}^{d} \left( \frac{\partial k(x, \cdot)}{\partial x_i} \right)_{\mathcal{H}}^2 p_0(x) \, dx < \infty,
\]
which proves that \(I_k\) is Hilbert-Schmidt (hence compact) and therefore \(S_k\) is also Hilbert-Schmidt and compact. The other assertions about \(S_k I_k\) and \(I_k S_k\) are straightforward. \(\square\)

8.16 Proof of Theorem \[\text{[12]}\]

By slight abuse of notation, \(f_\ast\) is used to denote \([f_\ast]_\sim\) in the proof for simplicity. For \(f \in \mathcal{F}\), we have
\[
J(p_0\|p_f) = \frac{1}{2} \|I_k f - f_\ast\|_{W_2}^2 = \frac{1}{2} (E_k f, f)_{\mathcal{H}} - (S_k f_\ast, f)_{\mathcal{H}} + \frac{1}{2} \|f_\ast\|_{W_2}^2.
\]
Since \(k\) satisfies (C) it is easy to verify that \((S_k f_\ast, f)_{\mathcal{H}} = (f_\ast, -\xi)_{\mathcal{H}}\), \(\forall f \in \mathcal{H}\). This implies \(S_k f_\ast = -\xi\), and
\[
J(p_0\|p_f) = \frac{1}{2} (E_k f, f)_{\mathcal{H}} + (f, \xi)_{\mathcal{H}} + \frac{1}{2} \|f_\ast\|_{W_2}^2,
\]
where \(\xi\) is defined in Theorem \[\text{[8]} ii]\), and \(E_k\) is precisely the operator \(C\) defined in Theorem \[\text{[8]} ii]\). Following the proof of Theorem \[\text{[8]} ii]\), for \(\lambda > 0\), it is easy to show that the unique minimizer of the regularized objective, \(J(p_0\|p_f) + \frac{\lambda}{2} \|f\|_{\mathcal{H}}^2\), exists and is given by
\[
f_\lambda = -(E_k + \lambda I)^{-1} \xi = (E_k + \lambda I)^{-1} S_k f_\ast. \tag{41}
\]
We would like to reiterate that \[\text{[10]}\] and \[\text{[11]}\] also match with their counterparts in Theorem \[\text{[8]}\] and therefore as in Theorem \[\text{[8]} iv\], an estimator of \(f_\ast\) is given by \(f_{\lambda,n} = -(\hat{E}_k + \lambda I)^{-1} \hat{\xi}\). In other words, this is the same as in Theorem \[\text{[8]} iv\] since \(\hat{E}_k = \hat{C}\), and can be solved by a simple linear system provided in Theorem \[\text{[4]}\] Here \(\hat{E}_k\) is the empirical estimator of \(E_k\). Now consider
\[
\sqrt{2} J(p_0\|p_{f_{\lambda,n}}) = \|I_k f_{\lambda,n} - f_\ast\|_{W_2} \leq \|I_k (f_{\lambda,n} - f_\lambda)\|_{W_2} + \|I_k f_{\lambda} - f_\ast\|_{W_2} = \|\sqrt{\hat{E}_k} (f_{\lambda,n} - f_\lambda)\|_{\mathcal{H}} + B(\lambda), \tag{42}
\]
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where \( \mathcal{B}(\lambda) := \| I_k f_{\lambda} - f_{\star} \|_{W_2} \). The proof now proceeds using the following decomposition, equivalent to the one used in the proof of Theorem 6(i), i.e.,

\[
\begin{align*}
  f_{\lambda,n} - f_{\lambda} &= -(\hat{E}_k + \lambda I)^{-1}(\hat{\xi} - f_{\lambda}) \\
  &= -(\hat{E}_k + \lambda I)^{-1}(\hat{\xi} + \hat{E}_k f_{\lambda} + \lambda f_{\lambda}) \\
  &\stackrel{(\dagger)}{=} -(\hat{E}_k + \lambda I)^{-1}(\hat{\xi} + \hat{E}_k f_{\lambda} + S_k f_{\star} - E_k f_{\lambda} + \hat{S}_k f_{\star} + \hat{S}_k f_{\star}),
\end{align*}
\]

where we used (\(\dagger\)) \(\hat{S}_k f_{\star}\) is well-defined as it is the empirical version of the restriction of \(S_k\) to \(W_2^\perp(p_0)\). Since \(S_k f_{\star} - E_k f_{\star} = S_k (f_{\star} - I_k f_{\star})\) and \(S_k f_{\star} - E_k f_{\star} = \hat{S}_k (f_{\star} - I_k f_{\star})\), we have

\[
f_{\lambda,n} - f_{\lambda} = -(\hat{E}_k + \lambda I)^{-1}(\hat{\xi} + \hat{S}_k f_{\star}) + (\hat{E}_k + \lambda I)^{-1}(\hat{S}_k - S_k)(f_{\star} - I_k f_{\star})
\]

and so

\[
\| \sqrt{E_k}(f_{\lambda,n} - f_{\lambda})\|_{\mathcal{C}} \leq \Theta \| \hat{\xi} + \hat{S}_k f_{\star} \|_{\mathcal{C}} + \Theta \| (\hat{S}_k - S_k)(f_{\star} - I_k f_{\star})\|_{\mathcal{C}}, \tag{43}
\]

where \(\Theta := \| \sqrt{E_k}(\hat{E}_k + \lambda I)^{-1}\|\). As in the proof of Theorem 6 it can be shown that if \(\lambda \geq \frac{4(\sqrt{n}+1)^2}{\sqrt{n}}\), then \(\| \sqrt{E_k}(\hat{E}_k + \lambda I)^{-1}\| \leq \frac{2}{\sqrt{n}}\). Following the proof of Theorem 6(i), we have

\[
\mathbb{E}\| \hat{\xi} + \hat{S}_k f_{\star} \|_{\mathcal{C}}^2 = \frac{n-1}{n} \| \xi + S_k f_{\star} \|_{\mathcal{C}}^2 + \frac{1}{n} \int \left( \sum_{i=1}^{d} \frac{\partial k_i(x)}{\partial x_i} \frac{\partial f_{\star}}{\partial x_i} + \| \xi \|_{\mathcal{C}} \right)^2 p_0(x) \, dx \]

wherein the first term is zero as \(S_k f_{\star} + \xi = 0\) and the second term is finite since \(\| \sum_{i=1}^{d} \frac{\partial k_i(x)}{\partial x_i} \frac{\partial f_{\star}}{\partial x_i} + \| \xi \|_{\mathcal{C}} \|_{\mathcal{C}}^2 \leq 2 \| \xi \|_{\mathcal{C}}^2 + 2dE_k^2 \sum_{i=1}^{d} \left| \frac{\partial f_{\star}}{\partial x_i} \right|^2 \). Therefore, an application of Chebyshev’s inequality yields \(\| \hat{\xi} + \hat{S}_k f_{\star} \|_{\mathcal{C}} = O_{p_0}(n^{-1/2})\). To this end, define \(g := f_{\star} - I_k f_{\lambda}\) and consider

\[
\mathbb{E}_p_0 \| \hat{S}_k g - S_k g \|_{\mathcal{C}}^2 = \frac{\int \| \sum_{i=1}^{d} \frac{\partial k_i(x)}{\partial x_i} \frac{\partial g}{\partial x_i} \|_{\mathcal{C}}^2 p_0(x) \, dx - \| S_k g \|_{\mathcal{C}}^2}{n} \leq \frac{dE_k^2}{n} \| g \|_{W_2}^2,
\]

which therefore yields the claim through an application of Chebyshev’s inequality. Using this in \(\mathcal{B}(\lambda)\) and combining it with \(\mathcal{B}(\lambda)\) yields

\[
\sqrt{2 J(p_0\|p_{f_{\lambda,n}})} \leq O_{p_0} \left( \frac{1}{\sqrt{n}} + \frac{\mathcal{B}(\lambda)}{\sqrt{n}} \right) + \mathcal{B}(\lambda). \tag{44}
\]

(i) We bound \(\mathcal{B}(\lambda)\) as follows. First note that \(\mathcal{B}(\lambda) = \| I_k (S_k k + \lambda I)^{-1} S_k f_{\star} - f_{\star} \|_{W_2} = \| (T_k + \lambda I)^{-1} T_k f_{\star} - f_{\star} \|_{W_2}\) and so for any \(h \in \mathcal{K}\), we have

\[
\mathcal{B}(\lambda) = \| (T_k + \lambda I)^{-1} T_k f_{\star} - f_{\star} \|_{W_2} \leq \|((T_k + \lambda I)^{-1} T_k - I)(f_{\star} - I_k h)\|_{W_2} + \| (T_k + \lambda I)^{-1} T_k I_k h - I_k h \|_{W_2}. \tag{45}
\]

Since \(T_k\) is a self-adjoint compact operator, there exists \((\alpha_l)_{l \in \mathbb{N}}\) and ONB \((\phi_l)_{l \in \mathbb{N}}\) of \(\mathcal{R}(T_k)\) so that \(T_k = \sum_l \alpha_l \langle \phi_l, \cdot \rangle_{W_2} \phi_l\). Let \((\psi_j)_{j \in \mathbb{N}}\) be the orthonormal basis of \(\mathcal{N}(T_k)\). Then we have

\[
(I)^2 = \sum_l \left( \frac{\alpha_l}{\alpha_l + \lambda} - 1 \right)^2 \| f_{\star} - I_k h, \phi_l \|_{W_2}^2 + \sum_j \| f_{\star} - I_k h, \psi_j \|_{W_2}^2 \]

\[
\leq \sum_l \| f_{\star} - I_k h, \phi_l \|_{W_2}^2 + \sum_j \| f_{\star} - I_k h, \psi_j \|_{W_2}^2 = \| f_{\star} - I_k h \|_{W_2}^2. \tag{46}
\]

From \((T_k + \lambda I)^{-1} T_k = I_k (E_k + \lambda I)^{-1} S_k\) and \(S_k I_k h = E_k h\), we have

\[
(II) = \| I_k (E_k + \lambda I)^{-1} E_k h - I_k h \|_{W_2} = \| \sqrt{E_k}(E_k + \lambda I)^{-1} E_k h - \sqrt{E_k} h \|_{\mathcal{C}} \leq \| h \|_{\mathcal{C}} \sqrt{\lambda}, \tag{47}
\]
where the inequality follows from Proposition A.2 ii). Using (46) and (47) in (45), we obtain $\mathcal{B}(\lambda) \leq \|f_\ast - I_k h\|_{W_2} + \|h\|_{C(\sqrt{\lambda})}$, using which in (44) yields

$$\sqrt{2} J(p_0\|p_{f_\ast\ast}) \leq \|f_\ast - I_k h\|_{W_2} + O_{p_0} \left( \frac{1}{\sqrt{n}} \right) + \|h\|_{C(\sqrt{\lambda})}.$$

Since the above inequality holds for any $h \in \mathcal{H}$, we therefore have

$$\sqrt{2} J(p_0\|p_{f_\ast\ast}) \leq \inf_{h \in \mathcal{H}} \left( \|f_\ast - I_k h\|_{W_2} + \sqrt{\lambda} \|h\|_{C(\sqrt{\lambda})} \right) + O_{p_0} \left( \frac{1}{\sqrt{n}} \right)$$

$$= K(f_\ast, \sqrt{\lambda}, W_2(p_0), I_k(\mathcal{H})) + O_{p_0} \left( \frac{1}{\sqrt{n}} \right) \quad (48)$$

where the $K$-functional is defined in (30). Note that $I_k(\mathcal{H}) \cong \mathcal{H}/\mathcal{H} \cap \mathbb{R}$ is continuously embedded in $W(p_0)$. From (30), it is clear that the $K$-functional as a function of $t$ is an infimum over a family of affine linear and increasing functions and therefore is concave, continuous and increasing w.r.t. $t$. This means, in (48), as $\lambda \to 0$, $K(f_\ast, \sqrt{\lambda}, W_2(p_0), I_k(\mathcal{H})) \to \inf_{f \in \mathcal{H}} \|f_\ast - I_k h\|_{W_2} = \sqrt{2} \inf_{p \in \mathcal{T}} J(p_0\|p)$. Since $J(p_0\|p_{f_\ast\ast}) \geq \inf_{p \in \mathcal{T}} J(p_0\|p)$, we have that $J(p_0\|p_{f_\ast\ast}) \to \inf_{p \in \mathcal{T}} J(p_0\|p)$ as $\lambda \to 0$, $\lambda n \to \infty$ and $n \to \infty$.

(ii) Recall $\mathcal{B}(\lambda)$ from (i). From Proposition A.2(i) it follows that $\mathcal{B}(\lambda) \to 0$ as $\lambda \to 0$ if $f_\ast \in \mathcal{R}(T_k)$. Therefore, (44) reduces to $\sqrt{2} J(p_0\|p_{f_\ast\ast}) \leq O_{p_0} \left( \frac{1}{\sqrt{n}} \right) + \mathcal{B}(\lambda)$ and the consistency result follows. If $f_\ast \in \mathcal{R}(T_k^\beta)$ for some $\beta > 0$, then the rates follow from Proposition A.2 by noting that $\mathcal{B}(\lambda) \leq \max\{1, \|T_k\|^{\beta-1}\lambda^{\min\{1,\beta\}}\|T_k^{-\beta} f_\ast\|_{W_2}$ and choosing $\lambda = n^{-\max\{1, \frac{1}{\beta-1}\}}$.

(iii) This simply follows from an analysis similar to the one used in the proof of Theorem 5(iii).

\[\square\]

8.17 Denseness of $I_k^\mathcal{H}$ in $W_2(p)$

In this section, we discuss the denseness of $I_k^\mathcal{H}$ in $W_2(p)$ for a given $p \in \mathcal{P}_{FD}$, where $\mathcal{P}_{FD}$ is defined in Theorem 13 which is equivalent to the injectivity of $S_k$ (see [30] Theorem 4.12]). To this end, in the following result we show that under certain conditions on a bounded continuous translation invariant kernel on $\mathbb{R}^d$, the restriction of $S_k$ to $W_2^\infty(p)$ is injective when $d = 1$, while the result for any general $d > 1$ is open. However, even for $d = 1$, this does not guarantee the injectivity of $S_k$ (which is defined on $W_2(p)$). Therefore, the question of characterizing the injectivity of $S_k$ (or equivalently the denseness of $I_k^\mathcal{H}$ in $W_2(p)$) is open.

Proposition 8.6. Suppose $k(x, y) = \psi(x - y), x, y \in \mathbb{R}^d$ where $\psi \in C_b(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$, $\int \|\psi\|^2 \omega(\omega) d\omega < \infty$ and supp$(\psi^\wedge) = \mathbb{R}^d$. If $d = 1$, then the restriction of $S_k$ to $W_2^\infty(p)$ is injective for any $p \in \mathcal{P}_{FD}$.

Proof. Fix any $p \in \mathcal{P}_{FD}$. We need to show that for $[f]_\sim \in W_2^\infty(p)$, $S_k[f]_\sim = 0$ implies $[f]_\sim = 0$. From Proposition 11 we have

$$S_k[f]_\sim = \int \sum_{j=1}^d \frac{\partial \psi(\cdot, x)}{\partial x_j} (\partial_j f)(x) p(x) dx = \int \sum_{j=1}^d \frac{\partial \psi(\cdot, x)}{\partial x_j} (\partial_j f)(x) p(x) dx$$

$$= \int \sum_{j=1}^d \frac{1}{(2\pi)^{d/2}} \int i\omega_j \psi^\wedge(\omega) e^{i(\omega, \cdot - x)} d\omega (\partial_j f)(x) p(x) dx = \int \sum_{j=1}^d \phi_j(\omega) \psi^\wedge(\omega) e^{i(\omega, \cdot)} d\omega$$

where

$$\phi_j(\omega) := \frac{1}{(2\pi)^{d/2}} \int (i\omega_j) e^{-i(\omega, x)} (\partial_j f)(x) p(x) dx.$$

$S_k f = 0$ implies $\sum_{j=1}^d \phi_j(\omega) \psi^\wedge(\omega) = 0$ for all $\omega \in \mathbb{R}^d$. Since supp$(\psi^\wedge) = \mathbb{R}^d$, we have $\sum_{j=1}^d \phi_j(\omega) = 0$ a.e., i.e., for $\omega$-a.e.,

$$0 = \int (i\omega_j)(\partial_j f)(x) p(x) e^{-i(\omega, x)} dx = \sum_{j=1}^d (i\omega_j)(p(\partial_j f))^\wedge(\omega).$$

For $d = 1$, this implies $(\partial_j f)p = 0$ a.e. and so $\|f\|_{W_2} = 0$. \[\square\]
Examples of kernels that satisfy the conditions in Proposition 3.6 include the Gaussian, Matérn (with $\beta > 1$) and inverse multiquadrics on $\mathbb{R}$.

### 8.18 Proof of Proposition 13

For any $p \in \mathcal{P}_{\text{PD}}$, define $f := \log \frac{p}{q_0}$, which implies that $[f]_\sim \in W_2(p)$. Since $I_k(\mathcal{H})$ is dense in $W_2(p)$, we have for any $\epsilon > 0$, there exists $g \in \mathcal{H}$ such that $\|[f]_\sim - I_k g\|_{W_2} \leq \sqrt{2\epsilon}$. For a given $g \in \mathcal{H}$, pick $p_g \in \mathcal{P}$. Therefore,

$$J(p\|p_g) = \frac{1}{2} \int p(x) \left\| \frac{\partial \log p}{\partial x} - \frac{\partial \log p_g}{\partial x} \right\|^2 dx = \frac{1}{2} \|[f]_\sim - I_k g\|_{W_2}^2 \leq \epsilon$$

and the result follows. $\square$

### A Appendix: Supplementary Results

In this section, we present some technical results that are used in the proofs.

#### A.1 Bounds on various distances between $p_f$ and $p_g$

In the following result, claims (iii) and (iv) are quoted from Lemma 3.1 of [40].

**Lemma A.1.** Define $\mathcal{P}_\infty := \left\{ p_f = \frac{e^{f}q_0}{\int_0^\infty e^{f}q_0 dx} : f \in \ell^\infty(\Omega) \right\}$, where $q_0$ is a probability density on $\Omega \subset \mathbb{R}^d$ and $\ell^\infty(\Omega)$ is the space of bounded measurable functions on $\Omega$. Then for any $p_f, p_g \in \mathcal{P}_\infty$, we have

1. $\|p_f - p_g\|_{L_r(\Omega)} \leq 2e^{2\|f-g\|_\infty} e^{\min\{\|f\|_\infty, \|g\|_\infty\}} \|f - g\|_\infty q_0 \|L_r(\Omega)\|$ for any $1 \leq r \leq \infty$;
2. $\|p_f - p_g\|_{L_1(\Omega)} \leq 2e^{\|f-g\|_\infty} \|f - g\|_\infty$;
3. $KL(p_f\|p_g) \leq \|f - g\|_\infty^2 e^{\|f-g\|_\infty} (1 + \|f - g\|_\infty)$;
4. $h(p_f, p_g) \leq e^{\|f-g\|_\infty^2/2} \|f - g\|_\infty$.

**Proof.** (i) Define $A(f) := \int e^f q_0 dx$. Consider

$$\|p_f - p_g\|_{L_r(\Omega)} = \left\| \frac{e^f q_0}{A(f)} - e^g q_0 \right\|_{L_r(\Omega)} = \frac{\left\| e^f q_0 A(g) - e^g q_0 A(f) \right\|_{L_r(\Omega)}}{A(f) A(g)}$$

$$\leq \frac{\left\| e^f q_0 (A(g) - A(f)) + (e^f - e^g) q_0 A(f) \right\|_{L_r(\Omega)}}{A(f) A(g)}$$

$$\leq \frac{\left\| A(g) - A(f) \right\| e^f q_0 \|L_r(\Omega)\|}{A(g) A(f)} + \frac{\left\| (e^f - e^g) q_0 A(f) \right\|_{L_r(\Omega)}}{A(f) A(g)}.$$  \hspace{1cm} (A.1)

Observe that

$$|A(f) - A(g)| \leq \int |e^f - e^g| q_0 dx = \int e^g |e^f - e^g - 1| q_0 dx \leq e^{\|f-g\|_\infty} \|f - g\|_\infty A(g)$$

since $|e^{u-v} - 1| \leq |u - v|e^{u-v}$ for any $u, v \in \mathbb{R}$. Similarly,

$$\left\| (e^f - e^g) q_0 \right\|_{L_r(\Omega)} \leq e^{\|f-g\|_\infty} \|f - g\|_\infty e^g q_0 \|L_r(\Omega)\|.$$
Using these above, we obtain

\[ \|p_f - p_g\|_{L^r(\Omega)} \leq e^{\|f-g\|_{\infty}} \left( \frac{\|e^f q_0\|_{L^r(\Omega)}}{A(f)} + \frac{\|e^g q_0\|_{L^r(\Omega)}}{A(g)} \right). \]  

(A.2)

Since \( \|e^f q_0\|_{L^r(\Omega)} \leq e^{\|f\|_{\infty}} q_0 \) and \( A(f) \geq e^{-\|f\|_{\infty}} \), from (A.2) we obtain

\[ \|p_f - p_g\|_{L^r(\Omega)} \leq e^{\|f-g\|_{\infty}} q_0 \left( e^{2\|f\|_{\infty}} + e^{2\|g\|_{\infty}} \right). \]

\[ \leq 2e^{\|f-g\|_{\infty}} \|f - g\|_{\infty} q_0 \|q_0\|_{L^r(\Omega)} e^{2\min\{\|f\|_{\infty}, \|g\|_{\infty}\}} \]

where we used \( \max\{a, b\} \leq \min\{a, b\} + |a - b| \) for \( a, b \geq 0 \) in the last line above.

(ii) This simply follows from (A.2) by using \( r = 1 \).

A.2 Bounds on approximation errors, \( A_0(\lambda) \) and \( A_{\frac{1}{2}}(\lambda) \)

The following result is quite well-known in the theory of linear inverse problems [12].

**Proposition A.2.** Let \( C \) be a bounded, self-adjoint compact operator on a separable Hilbert space \( H \). For \( \lambda > 0 \) and \( f \in H \), define \( f_\lambda := (C + \lambda I)^{-1} Cf \) and \( A_\theta(\lambda) := \|C^\theta(f_\lambda - f)\|_H \) for \( \theta \geq 0 \). Then the following hold.

(i) \( A_\theta(\lambda) \to 0 \) as \( \lambda \to 0 \) for any \( \theta > 0 \) and \( A_\theta(\lambda) \to 0 \) as \( \lambda \to 0 \) if \( f \in \overline{R(C)} \).

(ii) If \( f \in R(C^{\beta}) \) for \( \beta \geq 0 \) and \( \beta + \theta > 0 \), then

\[ A_\theta(\lambda) \leq \max\{1, \|C\|^{\beta+\theta-1}\lambda^{\min\{1,\beta+\theta\}}\|C^{-\beta} f\|_H. \]

**Proof.** (i) Since \( C \) is bounded, compact and self-adjoint, Hilbert-Schmidt theorem [Theorems VI.16, VI.17][28] ensures that

\[ C = \sum_i \alpha_i \phi_i \langle \phi_i, \cdot \rangle_H, \]

where \( (\alpha_i)_{i \in \mathbb{N}} \) are the positive eigenvalues and \( (\phi_i)_{i \in \mathbb{N}} \) are the corresponding unit eigenvectors that form an ONB for \( R(C) \). Let \( \theta = 0 \). Since \( f \in \overline{R(C)} \),

\[ A_0^2(\lambda) = \| (C + \lambda I)^{-1} C f - f \|_H^2 = \left\| \sum_i \frac{\alpha_i}{\alpha_i + \lambda} \langle f, \phi_i \rangle_H \phi_i - \sum_i \langle f, \phi_i \rangle_H \phi_i \right\|_H^2 \]

\[ = \left\| \sum_i \frac{\lambda}{\alpha_i + \lambda} \langle f, \phi_i \rangle_H \phi_i \right\|_H^2 = \sum_i \left( \frac{\lambda}{\alpha_i + \lambda} \right)^2 \|f, \phi_i\|_H^2 \to 0 \]

as \( \lambda \to 0 \).

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(ii) If $f \in R(C^\beta)$, then there exists $g \in H$ such that $f = C^\beta g$. This yields

$$A^2_0(\lambda) = \left\| C^\theta (C + \lambda I)^{-1} C f - C^\theta f \right\|^2_H = \left\| C^\theta (C + \lambda I)^{-1} C^{\beta+1} g - C^\theta g \right\|^2_H$$

$$= \left\| \sum_i \lambda \alpha_i^{\theta+\beta} (g, \phi_i)_H \phi_i \right\|^2_H = \sum_i \left( \frac{\lambda \alpha_i^{\theta+\beta}}{\alpha_i + \lambda} \right)^2 \langle g, \phi_i \rangle^2.$$  \hspace{1cm} (A.4)

Suppose $0 < \beta + \theta < 1$. Then

$$\frac{\alpha_i^{\theta+\beta}}{\alpha_i + \lambda} = \left( \frac{\alpha_i}{\alpha_i + \lambda} \right)^{\theta+\beta} \left( \frac{\lambda}{\alpha_i + \lambda} \right)^{-\theta+\beta} \leq \lambda^{\theta+\beta}.$$

On the other hand, for $\beta + \theta \geq 1$, we have

$$\frac{\alpha_i^{\theta+\beta}}{\alpha_i + \lambda} = \left( \frac{\alpha_i}{\alpha_i + \lambda} \right)^{\theta+\beta} \leq \| C\|^\beta \theta^{-1} \lambda.$$

Using the above in (A.4) yields the result. \hfill \Box

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