Spectral Regularization for Support Estimation

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Abstract

In this paper we consider the problem of learning from data the support of a probability distribution when the distribution *does not* have a density (with respect to some reference measure). We propose a new class of regularized spectral estimators based on a new notion of reproducing kernel Hilbert space, which we call *"completely regular"*. Completely regular kernels allow to capture the relevant geometric and topological properties of an arbitrary probability space. In particular, they are the key ingredient to prove the universal consistency of the spectral estimators and in this respect they are the analogue of universal kernels for supervised problems. Numerical experiments show that spectral estimators compare favorably to state of the art machine learning algorithms for density support estimation.

1 Introduction

In this paper we consider the problem of estimating the support of an arbitrary probability distribution and we are more broadly motivated by the problem of learning from complex high dimensional data. The general intuition that allows to tackle these problems is that, though the initial representation of the data is often very high dimensional, in most situations the data are not uniformly distributed, but are in fact confined to a small (possibly low dimensional) region. Making such an intuition rigorous is the key towards designing effective algorithms for high dimensional learning.

The problem of estimating the support of a probability distribution is of interest in a variety of applications such as anomaly/novelty detection [8], or surface modeling [18]. From a theoretical point of view the problem has been usually considered in the setting where the probability distribution has a density with respect to a known measure (for example the Lebesgue measure in $\mathbb{R}^d$ or the volume measure on a manifold). Among others we mention [24, 5] and references therein. Algorithms inspired by Support Vector Machine (SVM), often called one-class SVM are have been proposed see [19, 22] and references therein. Another kernel method, related to the one we discuss in this paper, is presented in

[13]. More generally one of the main approaches to learning from high dimensional is the one considered in manifold learning. In this context the data are assumed to lie on a low dimensional Riemannian sub-manifold embedded (that is represented) in a high dimensional Euclidean space. This framework inspired algorithms to solve a variety of problems such as: semisupervised learning [3], clustering [25], data parameterization/dimensionality reduction [17, 23], to name a few. The basic assumption underlying manifold learning is often too restrictive to describe real data and this motivates considering other models, such as the setting where the data are assumed to be *essentially* concentrated around a low dimensional manifold as in [14], or can be modeled as samples from a metric space as in [12].
In this paper we consider a general scenario (see [20]) where the underlying model is a probability space (X, ρ) and we are given a (*similarity*) function K which is a reproducing kernel. The available training set is an i.i.d sample $x_1, \dots, x_n \sim \rho$. The geometry (and topology) in (X, ρ) is defined by the kernel K. While this framework is abstract and poses new challenges, by assuming the similarity function to be a reproducing kernel we can make full use of the good computational properties of kernel methods and the powerful theory of reproducing kernel Hilbert spaces (RKHS) [2]. Interestingly, the idea of using a reproducing kernel K to construct a metric on a set X is originally due to Schoenberg (see for example [4]).
Broadly speaking, in this setting we consider the problem of *finding a model of the smallest region X_ρ containing all the data*. A rigorous formalization of this problem requires: 1) defining the region X_ρ, 2) specifying the sense in which we model X_ρ. This can be easily done if the probability distribution has density p with respect to a known measure, in fact $X_\rho = \{x \in X \ : \ p(x) > 0\}$, but is otherwise a challenging question for a general distribution. Intuitively, X_ρ can be thought of as the region where the distribution is concentrated, that is $\rho(X_\rho) = 1$. However, there are many different sets having this property. If X is $\mathbb{R}^d$ (in fact any topological space), a natural candidate to define the region of interest, is the notion of *support* of a probability distribution– defined as the intersection of the closed subsets C of X, such that $\rho(C) = 1$. In an arbitrary probability space the support of the measure is not well defined since no topology is given.
The reproducing kernel K provides a way to solve this problem and also suggests a possible approach to model X_ρ. The first idea is to use the fact that under mild assumptions the kernel defines a metric on X [20], so that the concept of closed set, hence that of support, is well defined. The second idea is to use the kernel to construct a function F_ρ such that the level set corresponding to one is exactly the support X_ρ– in this case we say that the RKHS associated to K *separates* the support X_ρ. By doing this we are in fact imposing an assumption on X_ρ: given a kernel K, we can only separate certain sets. More precisely, our contribution is two-fold.

- We prove that F_ρ is uniquely defined by the null space of the integral operator associated to K. Given that the integral operator (and its spectral properties) can be approximated studying the kernel matrix on a sample, this result suggests a way to estimate the support empirically. However, a further complication arises from the fact that in general zero is not an isolated point of the spectrum, so that the estimation of a null space is an ill-posed problem (see for example [9]). Then, a regularization approach is needed in order to find a stable (hence generalizing) estimator. In this paper, we consider a spectral estimator based on a spectral regularization strategy, replacing the kernel matrix with its regularized version (Tikhonov regularization being one example).
- We introduce the notion of *completely regular RKHS*, that answer positively to the question whether there exist kernels that can separate the support of *any* distribution. Examples of completely regular kernels are presented and results suggesting how they can be constructed are given. The concept of completely regular RKHS plays a role similar to the concept of universal kernels in supervised learning, for example see [21].

Finally, given the above results, we show that the regularized spectral estimator enjoys a universal consistency property: the correct support can be asymptotically recovered for *any* problem (that is any probability distribution).
The plan of the paper is as follows. In Section 3 we introduce the notion of completely regular kernels and their basic properties. In Section 2 we present the proposed regularized algorithms. In Section 2.3 and 4 we provide a theoretical and empirical analysis, respectively. Proofs and further development can be found in the supplementary material.

2 Spectral Algorithms for Learning the Support

In this section, we first discuss our framework and our main assumptions. Then we present the proposed regularized spectral algorithms.
Motivated by the results in the previous section, we describe our framework which is given by a triple (X, ρ, K). We consider a probability space (X, ρ) and a training set $\mathbf{x} = (x_1 \ldots, x_n)$ sampled i.i.d. with respect to ρ. Moreover we consider a reproducing kernel K satisfying the following assumption.

Assumption 1. *The reproducing kernel K is measurable and $K(x, x) = 1$, for all $x \in X$. Moreover K defines a completely regular and separable RKHS $\mathcal{H}$.*

We endow X with the metric d_K defined in (10), so that X becomes a separable metric space. The assumption of complete regularity ensures that any closed subset is separated by $\mathcal{H}$ and, hence, is measurable by Prop. 2. Then we can define the support X_ρ of the measure ρ, as the intersection of all the closed sets $C \subset X$, such that $\rho(C) = 1$. Clearly X_ρ is closed and $\rho(X_\rho) = 1$ (note that this last property depends on the separability of X, hence of $\mathcal{H}$).
Summarizing the key result in the previous section, under the above assumptions, X_ρ is the one level set of the function $F_\rho : X \to [0, 1]$

$$F_\rho(x) = \langle P_\rho K_x, K_x \rangle \,,$$

where P_ρ is a short notation for P_{X_ρ}. Since F_ρ depends on the unknown measure ρ, in practice it cannot be explicitly calculated. To design an effective empirical estimator we develop a novel characterization of the support of an arbitrary distribution that we describe in the next section.

2.1 A New Characterization of the Support

The key observation towards defining a learning algorithm to estimate X_ρ it is that the projection P_ρ can be expressed in terms of the integral operator defined by the kernel K.
To see this, for all $x \in X$, let $K_x \otimes K_x$ denote the rank one positive operator on $\mathcal{H}$, given by

$$(K_x \otimes K_x)(f) = \langle f, K_x \rangle \, K_x = f(x) K_x \qquad f \in \mathcal{H}.$$

Moreover, let $T : \mathcal{H} \to \mathcal{H}$ be the linear operator defined as

$$T = \int_X K_x \otimes K_x d\rho(x),$$

where the integral converges in the Hilbert space of Hilbert-Schmidt operators on $\mathcal{H}$ (see for example [7] for the proof). Using the reproducing property in $\mathcal{H}$ [2], it is straightforward to see that T is simply the integral operator with kernel K with domain and range in $\mathcal{H}$.
Then, one can easily see that the null space of T is precisely $(I - P_\rho)\mathcal{H}$, so that

$$P_\rho = T^\dagger T, \tag{1}$$

where $T^\dagger$ is the pseudo-inverse of T (see for example [9]). Hence

$$F_\rho(x) = \left\langle T^\dagger T K_x, K_x \right\rangle .$$

Observe that in general K_x does not belong to the domain of $T^\dagger$ and, if θ denotes the Heaviside function with $\theta(0) = 0$, then spectral theory gives that $P_\rho = T^\dagger T = \theta(T)$. The above observation is crucial as it gives a new characterization of the support of ρ in terms of the null space of T and the latter can be estimated from data.

2.2 Spectral Regularization Algorithms

Finally, in this section, we describe how to construct an estimator F_n of F_ρ. As we mentioned above, Eq. (1) suggests a possible way to learn the projection from finite data. In fact, we can consider the empirical version of the integral operator associated to K which is simply defined by

$$T_n = \frac{1}{n} \sum_{i=1}^{n} K_{x_i} \otimes K_{x_i}.$$

The latter operator is an unbiased estimator of T. Indeed, since $K_x \otimes K_x$ is a bounded random variable into the separable Hilbert space of Hilbert-Schmidt operators, one can use concentration inequalities for random variables in Hilbert spaces to prove that

$$\lim_{n\to+\infty} \frac{\sqrt{n}}{\log n} \|T - T_n\|_{\mathrm{HS}} = 0 \qquad \text{almost surely,} \tag{2}$$

where $\|\cdot\|_{\mathrm{HS}}$ is the Hilbert-Schmidt norm (see for example [16] for a short proof). However, in general $T_n^\dagger T_n$ does non converge to $T^\dagger T$ since 0 is an accumulation point of the spectrum of T or, equivalently, since $T^\dagger$ is not a bounded operator. Hence, a regularization approach is needed.
In this paper we study a spectral filtering approach which replaces $T_n^\dagger$ with an approximation $g_\lambda(T_n)$ obtained *filtering out* the components corresponding to the small eigenvalues of T_n. The function g_λ is defined by spectral calculus. More precisely if $T_n = \sum_j \sigma_j v_j \otimes v_j$ is a spectral decomposition of T_n, then $g_\lambda(T_n) = \sum_j g_\lambda(\sigma_j) v_j \otimes v_j$. Spectral regularization defined by linear filters is classical in the theory of inverse problems [9]. Intuitively, $g_\lambda(T_n)$ is an approximation of the generalized inverse $T_n^\dagger$ and it is such that the approximation gets better, but the condition number of $g_\lambda(T_n)$ gets worse as λ decreases. More formally these properties are captured by the following set of conditions.

Assumption 2. *For $\sigma \in [0,1]$, let $r_\lambda(\sigma) := \sigma g_\lambda(\sigma)$, then*

- $r_\lambda(\sigma) \in [0,1], \;\; \forall \lambda > 0,$
- $\lim_{\lambda \to 0} r_\lambda(\sigma) = 1, , \;\; \forall \sigma > 0$
- $|r_\lambda(\sigma) - r_\lambda(\sigma')| \leq L_\lambda |\sigma - \sigma'|, \forall \lambda > 0$, *where L_λ is a positive constant depending on λ.*

Examples of algorithms that fall into the above class include iterative methods– akin to boosting $g_\lambda(\sigma) = \sum_{k=0}^{m_\lambda} (1-\sigma)^k$, spectral cut-off $g_\lambda(\sigma) = \frac{1}{\sigma} \mathbf{1}_{\sigma > \lambda}(\sigma) + \frac{1}{\lambda} \mathbf{1}_{\sigma \leq \lambda}(\sigma)$, and Tikhonov regularization $g_\lambda(\sigma) = \frac{1}{\sigma + \lambda}$. We refer the reader to [9] for more details and examples, and, given the space constraints, will focus mostly on Tikhonov regularization in the following.
For a chosen filter, the regularized empirical estimator of F_ρ can be defined by

$$F_n(x) = \langle g_\lambda(T_n) T_n K_x, K_x \rangle \,. \tag{3}$$

One can see that that the computation of F_n reduces to solving a simple finite dimensional problem involving the empirical kernel matrix defined by the training data. Towards this end, it is useful to introduce the sampling operator $S_n : \mathcal{H} \to \mathbb{C}^n$ defined by $S_n f = (f(x_1), \ldots, f(x_n)), \;\; f \in \mathcal{H}$, which can be interpreted as the restriction operator which evaluates functions in $\mathcal{H}$ on the training set points. The adjoint $S_n^* : \mathbb{C}^n \to \mathcal{H}$ of S_n is given by $S_n^* \alpha = \sum_{i=1}^n \alpha_i K_{x_i}, \;\; \alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{C}^n$, and can be interpreted as the out-of-sample extension operator. A simple computation shows that $T_n = \frac{1}{n} S_n^* S_n$ and $S_n S_n^* = \mathbf{K}_n$ is the n by n kernel matrix, where the (i,j)-entry is $K(x_i, x_j)$. Then it is easy to see that $g_\lambda(T_n) T_n = g_\lambda(S_n^* S_n / n) S_n^* S_n / n = \frac{1}{n} S_n^* g_\lambda(\mathbf{K}_n / n) S_n$, so that

$$F_n(x) = \frac{1}{n} {\mathbf{k}_x}^T g_\lambda(\mathbf{K}_n / n) \mathbf{k}_x, \tag{4}$$

where $\mathbf{k}_x$ is the n-dimensional column vector $\mathbf{k}_x = S_n K_x = (K(x_1, x), \ldots, K(x_n, x))$. Note that Equation (4) plays the role of a representer theorem for the spectral estimator, in the sense that it reduces the problem of finding an estimator in an infinite dimensional space to a finite dimensional problem.

2.3 Theoretical Analysis Consistency and Learning Rates

In this section we study the consistency property of spectral estimators. All the proofs of this section are reported in the supplementary material. We prove the results only for the filter corresponding to the classical Tikhonov regularization though the same results hold for the class of spectral filters described by Assumption 2. To study the consistency of the methods we need to choose an appropriate performance measure to compare F_n and F_ρ. Note that there is no natural notion of *risk*, since we have to compute the function *on* and *off* the support. Also note that standard metric used for support estimation

(see for example [24, 5]) cannot be used in our analsys since they rely on the existence of a reference measure μ (usually the Lebesgue measure) and the assumption that ρ is absolutely continuous with respect to μ.
The following preliminary result shows that we can control the convergence of the Tikhonov estimator F_n, defined by $g_\lambda(T) = (T_n + \lambda_n I)^{-1}$, to F_ρ uniformly on any compact set of X, provided a suitable sequence λ_n.

Theorem 1. *Let F_n be the estimator defined by Tikhonov regularization and choose a sequence λ_n so that*

$$\lim_{n\to\infty} \lambda_n = 0 \quad \textit{and} \quad \operatorname*{limsup}_{n\to\infty} \frac{\log n}{\lambda_n \sqrt{n}} < +\infty, \tag{5}$$

then

$$\lim_{n\to+\infty} \sup_{x\in C} |F_n(x) - F_\rho(x)| = 0, \qquad \textit{almost surely}, \tag{6}$$

for every compact subset C of X

Proof of Theorem 1. Without loss of generality, we can assume that the sequence (λ_n) is nondecreasing. For any n define $G_n : X \to \mathbb{R}$ as $G_n(x) = \langle (T + \lambda_n I)^{-1} T K_x, K_x \rangle$. Clearly, G_n is continuous. The idea of the proof is to split the error in an approximation error controlling the deviation of G_n from F_ρ and a sample error controlling the deviation of F_n from G_n.

We first deal with the approximation error. Since T is compact and positive, there exists an orthonormal basis (e_j) of eigenvectors of T with corresponding sequence (σ_j) of positive eigenvalues. Hence

$$G_n(x) = \sum_k \left(\frac{\sigma_j}{\sigma_j + \lambda_n}\right) |\langle K_x, e_j \rangle|^2.$$

It follows that $G_n(x)$ converges to $F_\rho(x)$ for all $x \in X$ and the sequence $(G_n(x))$ is nondecreasing. Dini's theorem implies that $\sup_{x\in C} |G_n(x) - F_\rho(x)|$ converges to zero for every compact set C.
For the sample error we can note that

$$(T + \lambda_n I)^{-1} T - (T_n + \lambda_n I)^{-1} T_n = \lambda_n (T + \lambda_n I)^{-1} (T_n - T)(T_n + \lambda_n I)^{-1},$$

and $\|(T + \lambda_n I)^{-1} K_x\| \le 1/\lambda_n$ as well as $\|(T_n + \lambda_n I)^{-1} K_x\| \le 1/\lambda_n$. Then $\sup_{x\in X} |G_n(x) - F_n(x)| \le \frac{1}{\lambda_n} \|T - T_n\|_{HS}$ and we can use the concentration results for $\|T - T_n\|_{HS}$ and the proposed regularization parameter choice to prove convergence of F_n to F_ρ. ☐

We add three comments. First, we note that, as we mentioned before, Tikhonov regularization can be replaced by a large class of filters. Second, we observe that a natural choice would be the regularization defined by kernel PCA [13], which corresponds to truncating the generalized inverse of the kernel matrix at some cutoff parameter λ. However, one can show that, in general, in this case it is not possible to choose λ so that the sample error goes to zero. In fact, for KPCA the sample error depends on the gap between the M-th and the $M+1$-th eigenvalue of T [1], where M-th and $M+1$-th are the eigenvalues around the cutoff parameter. Such a gap can go to zero with an arbitrary rate so that there exists *no* choice of the cut-off parameter ensuring convergence to zero of the sample error. Third, we note that the uniform convergence of F_n to F_ρ on compact subsets *does not* imply the convergence of the level sets of F_n to the corresponding level sets of F_ρ, for example with respect to the standard Hausdorff distance among closed subsets. In practice to have an effective decision rule, an off-set parameter τ_n can be introduced and the level set is replaced by

$$X_n = \{x \in X \mid F_n(x) \ge 1 - \tau_n\}$$

– recall that F_n takes values in $[0, 1]$. The following result will show that for a suitable choice of τ_n the Hausdorff distance between $X_n \cap C$ and $X_\rho \cap C$ goes to zero for all compact sets C. We recall that the Hausdorff distance between two subsets $A, B \subset X$ is

$$\mathrm{d}_H(A, B) = \max\{\sup_{a\in A} d_K(a, B), \sup_{b\in B} d_K(b, A)\}$$

Theorem 2. *If the sequence $(\tau_n)_{n\in\mathbb{N}}$ converges to zero in such a way that*

$$\limsup_{n\to\infty} \frac{\sup_{x\in C}|F_n(x)-F_\rho(x)|}{\tau_n} \leq 1, \qquad \textit{almost surely} \tag{7}$$

then,

$$\lim_{n\to+\infty} \mathrm{d}_H(X_n\cap C, X_\rho\cap C) = 0 \qquad \textit{almost surely},$$

for any compact subset C.

Proof of Theorem 2. Without loss of generality, we assume that X is itself compact and we prove the statement for $C = X$. The proof is split into two steps. First we show that

$$\lim_{n\to+\infty} \sup_{x\in X_\rho} d_K(x, X_n) = 0$$

Indeed the considered choice of τ_n implies that there exists $n_0 \in \mathbb{N}$ such that for all $n \geq n_0$

$$|F_n(x) - F_\rho(x)| \leq \tau_n \qquad \forall x \in X.$$

If $x \in X_\rho$,

$$F_n(x) - 1 = F_n(x) - F_\rho(x) \geq -|F_n(x) - F_\rho(x)| \geq -\tau_n,$$

so $x \in X_n$ and, hence, $d_K(x, X_n) = 0$ for all $n \geq n_0$.

Then, we prove that

$$\lim_{n\to+\infty} \sup_{x\in X_n} d_K(x, X_\rho) = 0$$

by contradiction. Assume the opposite, then there exists $\epsilon > 0$ such that for all $k \in \mathbb{N}$ there is $n_k \geq k$ and $\sup_{x\in X_{n_k}} d_K(x, X_\rho) \geq 2\epsilon$. Hence there is $x_k \in X_{n_k}$ such that

$$d_K(x_k, x) \geq \epsilon \qquad \text{for all } x \in X_\rho. \tag{8}$$

Since X is compact, possibly passing to a subsequence we can assume that $(x_k)_{k\in\mathbb{N}}$ converges to a x_0. We claim that $x_0 \in X_\rho$. Indeed

$$\begin{aligned}
|F_\rho(x_0) - 1| &\leq |F_\rho(x_0) - F_\rho(x_k)| + |F_\rho(x_k) - F_{n_k}(x_k)| + |F_{n_k}(x_k) - 1| \\
&\leq |F_\rho(x_0) - F_\rho(x_k)| + \sup_{x\in X}|F_\rho(x) - F_{n_k}(x)| + \tau_{n_k}
\end{aligned}$$

where the third term is due to the fact that $x_k \in X_{n_k}$ so that

$$1 + \tau_{n_k} \geq 1 \geq F_{n_k}(x_k) \geq 1 - \tau_{n_k}.$$

Since n_k goes to $+\infty$, F_ρ is continuous in x_0 and F_n converges to F_ρ uniformly, it follows that $F_\rho(x_0) = 1$, that is $x_0 \in X_\rho$. However, (8) implies that $d(x_0, x) \geq \epsilon$ for all $x \in X_\rho$, so that there is a contradiction. □

We add two comments. First, it is possible to show that, if the (normalized) kernel K is such that $\lim_{x'\to\infty} K_x(x') = 0$ for any $x \in X$ – as it happens for the Laplacian kernel, then Theorems 1 and 2 also hold by choosing $C = X$. Second, note that the choice of τ_n depends on the rate of convergence of F_n to F_ρ which will itself depend on some a-priori assumption on ρ. Developing learning rates and finite sample bound is a key question that we will tackle in future work.

2.4 A Priori Assumptions and Learning Rates

Inspecting the proof of the above Theorem 1 one can see that, the regularity of the distribution ρ is captured by the following condition

$$\sum_{j=1}^{\infty} \frac{|e_j(x)|^2}{\sigma_j^{2r}} \leq C, \quad \forall x \in X,$$

where $(\sigma_i, e_i)_j = 1^p$ are the eigenvalues and eigenvectors of T, $p \leq \infty$ and $r > 0$. The condition is satisfied if K is the linear kernel and in fact for any kernel inducing a finite dimensional RKHS. If we normalize the eigenfunctions with respect to the norm $\|f\|_\rho^2 = \int_X |f(x)|^d \rho(x)$, then we get rescaled functions $\phi_j \sqrt{\sigma_j} = e_j$, for all $j = 1, \ldots, \infty$. Using the rescaled functions the above condition becomes

$$\sum_{j=1}^{\infty} |\phi_j(x)|^2 \sigma_j^{1-2r}, \leq C, \quad \forall x \in X.$$

The latter condition is satisfied if the rescaled functions are uniformly bounded, the eigenvalues decay sufficiently fast and $0 < r < 1/2$.

3 Completely regular reproducing kernel Hilbert spaces

In this section we introduce the notion of a completely regular reproducing kernel Hilbert space. Such a space defines a geometry on a measurable space X which is compatible with the measurable structure. Furthermore it shows how to define a function F such that the one level set is the support of the probability distribution. The function is determined by the spectral projection associated with the null eigenvalue of the integral operator defined by the reproducing kernel. All the proofs of this section are reported in the supplementary material.

We assume X to be a measurable space with a probability measure ρ. We fix a complex[1] reproducing kernel Hilbert space $\mathcal{H}$ on X with a reproducing kernel $K : X \times X \to \mathbb{C}$ [2]. The scalar product and the norm are denoted by $\langle \cdot, \cdot \rangle$, linear in the first argument, and $\|\cdot\|$, respectively. For all $x \in X$, $K_x \in \mathcal{H}$ denotes the function $K(\cdot, x)$. For each function $f \in \mathcal{H}$, the reproducing property $f(x) = \langle f, K_x \rangle$ holds for all $x \in X$. When different reproducing kernel Hilbert spaces are considered, we denote by $\mathcal{H}_K$ the reproducing kernel Hilbert space with reproducing kernel K. Before giving the definition of completely regular RKHS, which is the key concept presented in this section, we need some preliminary definitions and results.

Definition 1. *A subset $C \subset X$ is* separated *by $\mathcal{H}$, if, for any $x_0 \notin C$, there exists $f \in \mathcal{H}$ such that*

$$f(x_0) \neq 0 \quad \text{and} \quad f(x) = 0 \qquad \forall x \in C. \tag{9}$$

For example, if $X = \mathbb{R}^d$ and $\mathcal{H}$ is the reproducing kernel Hilbert space with linear kernel $K(x, t) = x \cdot t$, the sets separated by $\mathcal{H}$ are precisely the hyperplanes containing the origin. In Eq. (9) the function f depends on x_0 and C, but Proposition 1 below will show that there is a function, possibly not in $\mathcal{H}$, whose one level set is precisely C (if $K(x, x) = 1$). Note that in [21] a different notion of *separating property* is given.
We need some further notation. For any set C, let $P_C : \mathcal{H} \to \mathcal{H}$ be the orthogonal projection onto the closure of the linear space generated by $\{K_x \mid x \in C\}$, so that $P_C^2 = P_C$, $P_C^* = P_C$ and

$$\ker P_C = \{K_x \mid x \in C\}^\perp = \{f \in \mathcal{H} \mid f(x) = 0, \ \forall x \in C\}.$$

Moreover let $F_C : X \to \mathbb{C}$ be defined by $F_C(x) = \langle P_C K_x, K_x \rangle$.

Proposition 1. *For any subset $C \subset X$, the following facts are equivalent*

(i) the set C is separated by $\mathcal{H}$;

(ii) for all $x \notin C$, $K_x \notin \operatorname{Ran} P_C$;

(iii) $C = \{x \in X \mid F_C(x) = K(x, x)\}$.

If one of the above conditions is satisfied, then $K(x, x) \neq 0 \qquad \forall x \notin C$.

[1]Considering complex valued RKHS allows to use the theory of Fourier transform and for practical problems we can simply consider real valued kernels.

Proof of Proposition 1. We prove that (i) implies (ii). Given $x_0 \notin C$, by contradiction, assume there is $f \in \mathcal{H}$ such that $f(x_0) \neq 0$, $f(x) = 0$ for all $x \in C$ and $K_{x_0} \in \operatorname{Ran} P_C$. Clearly, $f \in \ker P_C = \operatorname{Ran} P_C^{\perp}$, so that $f(x_0) = \langle f, K_{x_0} \rangle = 0$, which is a contradiction.
We prove that (ii) implies (iii). If $x \in C$, then $K_x \in \operatorname{Ran} P_C$ by definition of P_C, so that $F_C(x) = K(x,x)$, hence $C \subset \{x \in X \mid K(x,x) = F_C(x)\}$. If $x \notin C$, by assumption $(I - P_C)K_x \neq 0$, thus $K(x,x) - F_C(x) = \|(I - P_C)K_x\|^2 \neq 0$ and $C \supset \{x \in X \mid K(x,x) = F_C(x)\}$.
We prove that (iii) implies (i). If $x_0 \notin C$, define $f = (I - P_C)K_{x_0} \in \ker P_C$, so that $f(x) = 0$ for all $x \in C$. Furthermore, $f(x_0) = K(x_0, x_0) - F_C(x_0) \neq 0$.
Clearly, (ii) implies that $K(x,x) \neq 0$ for all $x \notin C$. □

A natural and minimal requirement on $\mathcal{H}$ is to be able to separates any pairs of distinct points and this implies that $K_x \neq K_t$ if $x \neq t$ and $K(x,x) \neq 0$. The first condition ensures the metric given by

$$d_K(x,y) = \|K_x - K_t\| \qquad x, t \in X. \tag{10}$$

to be well defined. Then (X, d_K) is a metric space and the sets separated by $\mathcal{H}$ are always d_K-closed, see Prop. 2 below. This last property is not enough to ensure that we can evaluate ρ on the set separated by RKHS $\mathcal{H}$. In fact the σ-algebra generated by the metric d might not be contained in the σ-algebra on X. The next result shows that assuming the kernel to be measurable is enough to solve this problem.

Proposition 2. *Assume that $K_x \neq K_t$ if $x \neq t$, then the sets separated by $\mathcal{H}$ are closed with respect to d_K. Moreover, if $\mathcal{H}$ is separable and the kernel is measurable, then the sets separated by $\mathcal{H}$ are measurable.*

Proof of Proposition 2. To prove that the sets separated by $\mathcal{H}$ are closed with respect to d_K , note that by definition of the metric d_K, the map $x \mapsto K_x$ is continuous from X, endowed with the metric d_K, into $\mathcal{H}$, so that $x \mapsto K(x,x) - F_C(x)$ is a continuous map, hence its zero level set is a closed subset of X.
To show that if $\mathcal{H}$ is separable and the kernel is measurable, then the sets separated by $\mathcal{H}$ are measurable, we first observe that the map $x \mapsto K_x$ is measurable from X into $\mathcal{H}$ since $\mathcal{H}$ is separable and K is a measurable kernel (Proposition 3.1 in [7]). As above, it follows that $x \mapsto K(x,x) - F_C(x)$ is a measurable map, so that its zero level set is a measurable subset of X. □

Given the above premises, the following is the key definition that characterizes the reproducing kernel Hilbert spaces which are able to separate the *largest* family of subsets of X.

Definition 2 (Completely Regular RKHS)**.** *A reproducing kernel Hilbert space $\mathcal{H}$ with reproducing kernel K such that $K_x \neq K_t$ if $x \neq t$ is called completely regular if $\mathcal{H}$ separates all the subsets $C \subset X$ which are closed with respect to the metric* (10)*.*

The term *completely regular* is borrowed from topology, where a topological space is called completely regular if, for any closed subset C and any point $x_0 \notin C$, there exists a continuous function f such that $f(x_0) \neq 0$ and $f(x) = 0$ for all $x \in C$. In the supplementary material, several examples of completely regular reproducing kernel Hilbert spaces are given, as well as a discussion on how such spaces can be constructed. A particular case is when X is already a metric space with a distance function d_X. If K is continuous with respect to d_X, the assumption of complete regularity forces the metrics d_K and d_X to have the same closed subsets. Then, the supports defined by d_K and d_X are the same. Furthermore, since the closed sets of X are independent of $\mathcal{H}$, the complete regularity of $\mathcal{H}$ can be proved by showing that a suitable family of *bump*[2] functions is contained in $\mathcal{H}$.

Corollary 1. *Let X be a separable metric space with respect to a metric d_X. Assume that the kernel K is a continuous function with respect to d_X and that the space $\mathcal{H}$ separates every subset C which is closed with respect to d_X. Then*

(i) The space $\mathcal{H}$ is separable and K is measurable with respect to the Borel σ-algebra generated by d_X.

(ii) The metric d_K defined by (10) *is equivalent to d_X, that is, a set is closed with respect to d_K if and only if it is closed with respect to d_X.*

[2]Given an open subset U and a compact subset $C \subset U$, a bump function is a continuous compactly supported function which is one on C and its support is contained in U.

(iii) The space $\mathcal{H}$ is completely regular.

Proof of Corollary 1. (i) This follows from Proposition 12 and Corollary 3 in [7].

(ii) Condition (a) states that, for any sequence $(x_j)_{j\in\mathbb{N}}$ such that $\lim_j d_X(x_j, x) = 0$ for some $x \in X$, then $\lim_j d_K(x_j, x) = 0$. Hence, the d_K-closed subsets are d_X-closed, too. Conversely, if C is d_X-closed, (b) implies that $C = \{x \in X \mid K(x, x) - F_C(x) = 0\}$, which is a d_K-closed subset by (i) of Proposition 2.

(iii) It follows from (ii) and (b). Note that, since the points are closed sets for d_X, condition (b) implies that $K_x \neq K_t$ if $x \neq t$.

□

As a consequence of the above result, many classical reproducing kernel Hilbert spaces are completely regular. For example, if $X = \mathbb{R}^d$ and $\mathcal{H}$ is the Sobolev space of order s with $s > d/2$, then $\mathcal{H}$ is completely regular. This is due to the fact that the space of smooth compactly supported functions is contained in $\mathcal{H}$. In fact, a standard result of analysis ensures that, for any closed set C and any $x_0 \notin C$ there exists a smooth bump function such that $f(x_0) = 1$ and its support is contained in the complement of C. Interestingly enough, if $\mathcal{H}$ is the reproducing kernel Hilbert space with the Gaussian kernel, it is known that the elements of $\mathcal{H}$ are analytic functions, see Cor. 4.44 in [21]. Clearly $\mathcal{H}$ can not be completely regular. Indeed, if C is a closed subset of $\mathbb{R}^d$ with not empty interior and $f \in \mathcal{H}$ is such that $f(x) = 0$ for all $x \in C$, a standard result of complex analysis implies that $f(x) = 0$ for every $x \in \mathbb{R}^d$. Finally, the next result shows that the reproducing kernel can be normalized to one on the diagonal under the mild assumption that $K(x, x) \neq 0$ for all $x \in X$.

Lemma 1. *Assume that $K(x, x) > 0$ for all $x \in X$. Then the reproducing kernel Hilbert space with the normalized kernel $K'(x, t) = \dfrac{K(x, t)}{\sqrt{K(x, x)K(t, t)}}$ separates the same sets as $\mathcal{H}$.*

Proof of Lemma 1. Denote by $\mathcal{H}'$ the reproducing kernel Hilbert space with kernel K', and define the map $\Phi : X \to \mathcal{H}$, $\Phi(x) = K_x/\|K_x\|$. It is simple to check that $\langle\Phi(y), \Phi(x)\rangle = K'(x, y)$ and $\Phi(X)^\perp = \{0\}$, so that the map $\Phi_* : \mathcal{H} \to \mathcal{H}'$

$$(\Phi_* f)(x) = \langle f, \Phi(x)\rangle$$

is a unitary operator with $K'_x = \Phi_*\Phi(x)$. Clearly, for any $f \in \mathcal{H}$ and $x \in X$

$$\langle\Phi_* f, K'_x\rangle_{\mathcal{H}'} = \langle\Phi_* f, \Phi_*\Phi(x)\rangle_{\mathcal{H}'} = \frac{\langle f, K_x\rangle_{\mathcal{H}}}{\|K_x\|}.$$

The above equality shows that $\mathcal{H}$ and $\mathcal{H}'$ separate the same sets. □

Finally we briefly mention some examples and refer to the supplementary material for further developments. In particular, we prove that both the Laplacian kernel $K(x, y) = e^{-\frac{\|x-y\|_2}{\sqrt{2}\sigma}}$ and ℓ_1-exponential kernel $K(x, y) = e^{-\frac{\|x-y\|_1}{\sqrt{2}\sigma}}$ defined on $\mathbb{R}^d$ are completely regular for any $\sigma > 0$ and $d \in \mathbb{N}$.

4 Empirical Analysis

In this section we describe some preliminary experiments aimed at testing the properties and the performances of the proposed methods both on simlauted and real data. Again for space constraints we will only discuss spectral algorithms induced by Tikhonov regularization. Note that while computations can be made efficient in several ways, we consider a simple algorithmic protocol and leave a more refined computational study for future work. Following the discussion in the last section, Tikhonov regularization defines an estimator $F_n(x) = \mathbf{k}_x{}^T(\mathbf{K}_n + n\lambda I)^{-1}\mathbf{k}_x$ and a point is labeled as belonging to the support if $F_n(x) \geq 1 - \tau$. The computational cost for the algorithm is, in the worst case, of order n^3, like standard regularized least squares, for training and order Nn^2 if we have to predict the value of F_n at N test points. In practice, one has to choose a good value for the regularization parameter λ and this requires computing multiple solutions, a so called *regularization path*. As noted in [15], if we

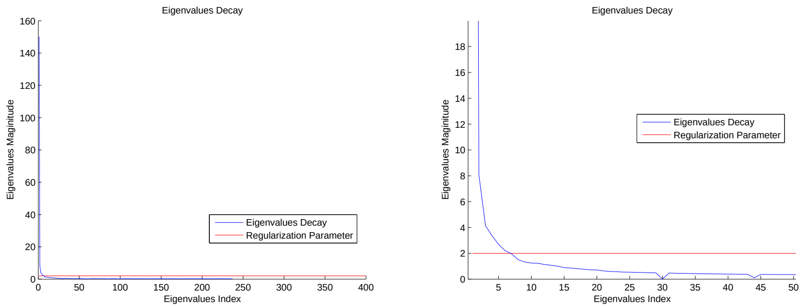

Figure 1: Decay of the eigenvalues of the kernel matrix ordered in decreasing magnitude and corresponding regularization parameter (Left) and a detail of the first 50 eigenvalues (Right).

form the inverse using the eigendecomposition of the kernel matrix the price of computing the full regularization path is essentially the same as that of computing a single solution (note that the cost of the eigen-decomposition of $\mathbf{K}_n$ is also of order n^3 though the constant is worse). This is the strategy that we consider in the following. In our experiments we considered two data-sets the MNIST data-set and the CBCL face database. For the digits we considered a reduced set consisting of a training set of 5000 images and a test set of 1000 images. In the first experiment we trained on 500 images for the digit 3 and tested on 200 images of digits 3 and 8. Each experiment consists of training on one class and testing on two different classes and was repeated for 20 trials over different training set choices. The performance is evaluated computing ROC curve (and the corresponding AUC value) for varying τ, τ', τ''. For all our experiments we considered the Laplacian kernel. Note that, in this case the algorithm requires to choose 3 parameters: the regularization parameter λ, the kernel width σ and the threshold τ. In supervised learning cross validation is typically used for parameter tuning, but cannot be used in our setting since support estimation is an unsupervised problem. Then, we considered the following heuristics. The kernel width is chosen as the median of the distribution of distances of the K-th nearest neighbor of each training set point for $K = 10$. Fixed the kernel width, we choose regularization parameter in correspondence of the maximum curvature in the eigenvalue behavior– see Figure 1, the rational being that after this value the eigenvalues are relatively small. For comparison we considered a Parzen window density estimator and one-class SVM (1CSVM)as implemented by [6]. For the Parzen window estimator we used the same kernel used in the spectral algorithm, that is the Laplacian kernel and use the same width used in our estimator. Given a kernel width an estimate of the probability distribution is computed and can be used to estimate the support by fixing a threshold τ'. For the one-class SVM we considered the Gaussian kernel, so that we have to fix the kernel width and a regularization parameter ν. We fix the kernel width to be the same used by our estimator and fixed $\nu = 0.9$. For the sake of comparison, also for one-class SVM we considered a varying offset τ''. The ROC curves on the different tasks are reported (for one of the trial) in Figure 2, Left. The mean and standard deviation of the AUC

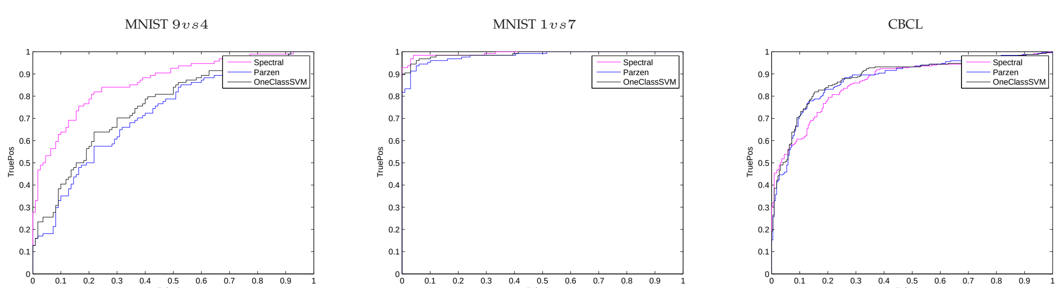

Figure 2: ROC curves for the different estimator in three different tasks: digit 9vs 4 Left, digit 1vs 7 Center, CBCL Right.

	3vs 8	8vs 3	1vs 7	9vs 4	CBCL
Spectral	0.8371 ± 0.0056	0.7830 ± 0.0026	$0.9921 \pm 4.7283e-04$	0.8651 ± 0.0024	0.8682 ± 0.0023
Parzen	0.7841 ± 0.0069	0.7656 ± 0.0029	$0.9811 \pm 3.4158e-04$	$0.0.7244 \pm 0.0030$	0.8778 ± 0.0023
1CSVM	0.7896 ± 0.0061	0.7642 ± 0.0032	$0.9889 \pm 1.8479e-04$	0.7535 ± 0.0041	0.8824 ± 0.0020

Table 1: Average and standard deviation of the AUC for the different estimators on the considered tasks.

for the 3 methods is reported in Table 4. Similar experiments were repeated considering other pairs of digits, see Table 4. Also in the case of the CBCL data sets we considered a reduced data-set consisting of 472 images for training and other 472 for test. On the different test performed on the Mnist data the spectral algorithm always achieves results which are better- and often substantially better - than those of the other methods. On the CBCL dataset SVM provides the best result, but spectral algorithm still provides a competitive performance.

5 Conclusions

In this paper we presented a new approach to estimate the support of an arbitrary probability distribution. Unlike previous work we drop the assumption that the distribution has a density with respect to a (known) reference measure and consider a general probability space. To overcome this problem we introduce a new notion of RKHS, that we call completely regular, that captures the relevant geometric properties of the probability distribution. Then, the support of the distribution can be characterized as the null space of the integral operator defined by the kernel and can be estimated using a spectral filtering approach. The proposed estimators are proven to be universally consistent and have good empirical performances on some benchmark data-sets. Future work will be devoted to derive finite sample bounds, to develop strategies to scale-up the algorithms to massive data-sets and to a more extensive experimental analysis.

A Complete Regularity: sufficient conditions and examples

In this section we provide some sufficient conditions characterizing completely regular reproducing kernel Hilbert spaces and we give some examples of such spaces.

The first result is about translation invariant kernels on $\mathbb{R}^d$. We show that if Fourier transform of the kernel satisfies a suitable growth condition, then the corresponding reproducing kernel Hilbert space is completely regular. In the following $L^1(\mathbb{R}^d)$ is the space of integrable functions with respect to the Lebesgue measure dx in $\mathbb{R}^d$ and $\hat{f}$ is the Fourier transform of $f \in L^1(\mathbb{R}^d)$, defined as

$$\hat{f}(\omega) = \int e^{-2\pi i \omega \cdot x} f(x) dx$$

Theorem. *Let $K : \mathbb{R}^d \to \mathbb{C}$ be a continuous function in $L^1(\mathbb{R}^d)$ such that*

$$\hat{K}(\omega) \geq \frac{a}{(1 + b\|\omega\|^m)^n} \qquad \forall \omega \in \mathbb{R}^d \tag{11}$$

for suitable $m, n \in \mathbb{N}$ and $a, b > 0$. Then,

(i) the translation invariant kernel $K(x,t) = K(x - t)$ is positive definite and continuous;

(ii) the corresponding reproducing kernel Hilbert space $\mathcal{H}$ is completely regular.

The proof depends on an explicit characterization of the reproducing kernel Hilbert space $\mathcal{H}$ given by the following result.

Proposition. *Let $K : \mathbb{R}^d \to \mathbb{C}$ be a continuous function in $L^1(\mathbb{R}^d)$ such that $\hat{K} = \hat{K}$ is strictly positive, then the kernel $K(x,t) = K(x - t)$ is positive definite and the corresponding reproducing kernel is*

$$\mathcal{H} = \left\{ f \in L^2 \mid \int \hat{K}(\omega)^{-1} |\hat{f}(\omega)|^2 d\omega < \infty \right\} \tag{12}$$

Proof. Denote by $L^2 = L^2(\mathbb{R}^d)$ the space of square integrable functions with scalar product $\langle \cdot, \cdot \rangle_2$ and recall that $\mathcal{F}$ is a unitary operator in L^2. We claim that K is a positive definite kernel and $\hat{K} \in L^1(\mathbb{R}^d)$. Let L_K be the integral operator of kernel K with respect to the Lebesgue measure, namely

$$(L_K f)(t) = \int K(t-x) f(x)\, dx = (K * f)(t),$$

which is a bounded operator on L^2 since $K \in L^1(\mathbb{R}^d)$. Since L_K is a convolution operator, the Fourier transform makes L_K unitary equivalent to the multiplicative operator by $\hat{K}$. It follows that

$$\langle L_K f, f \rangle_2 = \left\langle \hat{K} \cdot \hat{f}, \hat{f} \right\rangle_2 \geq 0 \qquad \forall\, f \in L^2(\mathbb{R}^d)$$

since $\hat{K} \geq 0$ by assumption. Hence L_K is a positive operator, so that K is positive definite. Indeed, let $\{\varphi_n\}_{n\in\mathbb{N}}$ be a Dirac sequence in 0 and, for each $x \in X$ define φ_n^x as $\varphi_n^x(t) = \varphi_n(t-x)$. Fixed $\{x_i\}_{i=1,2\ldots N} \subset \mathbb{R}^d$ and $\{c_i\}_{i=1,2\ldots N} \subset \mathbb{C}$, set $\phi_n = \sum_{i=1}^n c_i \varphi_n^{x_i}$, then

$$0 \leq \langle L_K \phi_n, \phi_n \rangle_2 = \sum_{i,j=1}^n c_i \overline{c_j} \left\langle L_K \varphi_n^{x_i}, \varphi_n^{x_j} \right\rangle \underset{n\to\infty}{\longrightarrow} \sum_{i,j=1}^n c_i \overline{c_j} K(x_i, x_j),$$

where the last equality is due to the continuity of K. Since K is a positive definite function, the Fourier inversion theorem in $L^1(\mathbb{R}^d)$ implies that $\hat{K} \in L^1(\mathbb{R}^d)$, see [10].
Finally, let $\mathcal{H}$ be the corresponding reproducing kernel Hilbert space. Since the support of the Lebesgue measure is $\mathbb{R}^d$, a generalization of the Mercer theorem [7] implies that $L_K^{1/2}$ is a unitary isomorphism of L^2 onto $\mathcal{H}$. Clearly $\widehat{L_K^{1/2} f} = \hat{K}^{1/2} \hat{f}$, so that the (12) follows. □

The first part of the above proposition is a converse result of Bochner theorem [10]. Given the above proposition, the proof of the Theorem is straightforward.

Proof of the Theorem. Condition (11) implies that $\hat{K}$ is strictly positive, so that (i) is proved by Proposition A. In particular, from (12) we see that $f \in \mathcal{H}$ if and only if $f \in L^2$ and

$$\int \hat{K}(\omega)^{-1} |\hat{f}(\omega)|^2 d\omega < \infty.$$

Clearly, if $f \in C_c^\infty(\mathbb{R}^d)$, then $\hat{f}$ is a Schwartz function on $\mathbb{R}^d$, so that $f \in \mathcal{H}$ by (11). □

A second result gives a very simple tool to construct completely regular reproducing kernel Hilbert spaces on high dimensional spaces.

Proposition. *If X_i, $i = 1, 2 \ldots d$, are sets and $\mathcal{H}_{K_i}$ are completely regular reproducing kernel Hilbert spaces on X_i for all $i = 1, 2 \ldots d$, then $\mathcal{H}_K$ is completely regular on the product space $X = X_1 \times X_2 \ldots X_d$, where K is the product kernel $K = K_1 K_2 \ldots K_d$.*

Proof. Each set X_i and X are endowed with the metric d_K induced by the corresponding kernel. We claim that in this way X is the topological product of the X_i's. Indeed, $\mathcal{H}_K = \mathcal{H}_{K_1} \otimes \ldots \otimes \mathcal{H}_{K_d}$, and, if $x = (x_1, \ldots, x_d) \in X$, then $K_x = K_{x_1} \otimes \ldots \otimes K_{x_d}$. It follows that, if $\{x_{i,k}\}_{k\in\mathbb{N}}$ is a sequence in X_i such that $\lim_k x_{i,k} = x_i$, then

$$\begin{aligned}
\lim_k d_K\left((x_{1,k}, \ldots, x_{d,k}), (x_1, \ldots, x_d)\right)^2 &= \lim_k \|K_{(x_{1,k},\ldots,x_{d,k})} - K_{(x_1,\ldots,x_d)}\|^2 \\
&= \lim_k K(x_{1,k}, x_{1,k}) \ldots K(x_{d,k}, x_{d,k}) - 2\mathrm{Re}\left(K(x_{1,k}, x_1) \ldots K(x_{d,k}, x_d)\right) \\
&\quad + K(x_1, x_1) \ldots K(x_d, x_d)
\end{aligned}$$

Since $\lim_k K(x_{i,k}, x_{i,k}) = \lim_k K(x_{i,k}, x_i) = K(x_i, x_i)$, the claim follows.
If $C \subset X$ is closed and $x = (x_1, \ldots, x_d) \in X \setminus C$, let U_i, $i = 1, \ldots d$, be open neighborhoods of x_i in X_i such that $U = U_1 \times \ldots \times U_d$ is disjoint from C. Pick $f_i \in \mathcal{H}_{K_i}$ such that $f_i(x_i) \neq 0$ and $f_i|_{X_i \setminus U_i} = 0$. Then the product function $f(x_1, \ldots, x_d) = f_1(x_1) \ldots f_d(x_d)$ is in $\mathcal{H}_K$, and satisfies $f(x) \neq 0$ and $f|_C = 0$. □

We end the section by presenting wo classes of completely regular reproducing kernel Hilbert spaces with exponential kernels. The first result is about exponential kernels defined by a euclidean metric.

Proposition. *Let*

$$K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}, \qquad K(x, y) = e^{-\alpha\|x-y\|},$$

with $\alpha > 0$. Then K is a positive definite kernel and the corresponding reproducing kernel Hilbert space $\mathcal{H}$ is completely regular for all $d \in \mathbb{N} \setminus \{0\}$.

Proof. Since K is a radial function, its Fourier transform is

$$\begin{aligned} \hat{K}(\omega) &= \frac{2\pi}{\|\omega\|^{\frac{d-2}{2}}} \int_0^\infty e^{-\alpha r} r^{\frac{d}{2}} J_{\frac{d-2}{2}}(2\pi\|\omega\|r)dr \\ &= 2^d \pi^{\frac{d-1}{2}} \alpha \Gamma(\frac{d+1}{2}) \left(\alpha^2 + 4\pi^2\|\omega^2\|\right)^{-\frac{d+1}{2}}, \end{aligned} \tag{13}$$

where J_n is the Bessel function of order n, Γ is Euler gamma function, and we used formula 6.623(2) p. 712 in [11] to evaluate the integral. The claim then follows from the above Theorem. $\square$

Eqs. (13) shows that (up to a constant rescaling of norms)

$$\mathcal{H} = W^{\frac{d+1}{2}}(\mathbb{R}^d),$$

where W^s is the Sobolev space of order s.

Finally, we consider the exponential kernel defined by the ℓ_1-norm, that is

$$K(x, y) = e^{-\alpha\|x-y\|_1} \qquad \|(x_1, x_2 \dots x_d)\|_1 = |x_1| + |x_2| + \dots + |x_d|.$$

For $d = 1$, the last proposition shows that $\mathcal{H}_K$ is completely regular. The same is true for arbitrary $d \geq 2$ as a consequence of the previous results.

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