On Non-Inclusion of Certain Functions in Reproducing Kernel Hilbert Spaces

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Abstract

We use a classical characterisation to prove that functions which are bounded away from zero cannot be elements of reproducing kernel Hilbert spaces whose reproducing kernels decay to zero in a suitable way. The result is used to study Hilbert spaces on subsets of the real line induced by analytic translation-invariant kernels which decay to zero at infinity.

1 Introduction

The inclusion or non-inclusion of certain functions, often constants or polynomials, in reproducing kernel Hilbert spaces (RKHSs) has numerous implications in theory of statistical and machine learning algorithms. See Steinwart and Christmann (2008, p. 142); Lee et al. (2016, Assumption 2); and Karvonen et al. (2019, Proposition 6) for a few specific examples. Non-inclusion of polynomials in an RKHS also explains the phenomena observed in Xu and Stein (2017). Furthermore, error estimates for kernel-based approximations methods typically require that the target function be an element of the RKHS (Wendland, 2005, Chapter 11).

The RKHSs of a number of finitely smooth kernels, such as Matérn and Wendland kernels, are well understood, being norm-equivalent to Sobolev spaces (e.g., Wendland, 2005, Corollary 10.13). With the exception of power series kernels (Zwicknagl and Schaback, 2013), less is known about infinitely smooth kernels. Since the work of Steinwart et al. (2006) and Minh (2010), which is based on explicit computations involving an orthonormal basis of the RKHS, it has been known that the RKHS of the Gaussian kernel does not contain non-trivial polynomials. Recently, Dette and Zhigljavsky (2021) have proved that RKHSs of analytic translation-invariant kernels do not contain polynomials via connection to the classical Hamburger moment problem.

In this note we use a classical RKHS characterisation to furnish a simple proof for the fact that, roughly speaking, functions which are bounded away from zero (e.g., constant functions) cannot be elements of an RKHS whose kernel decays to zero in a certain manner. An analyticity assumption is used to effectively localise this result for domains \( \Omega \subset \mathbb{R} \) which contain an accumulation point. We then consider analytic translation-invariant kernels which decay to zero. Although quite simple, it seems that these results have not appeared in the literature.

Analyticity of functions in an RKHS has been previously studied by Saitoh (1997, pp. 41–43) and Sun and Zhou (2008). General results concerning existence of RKHSs containing given classes of functions can be found in Aronszajn (1950, Section I.13).\(^1\)

\(^1\)They do not state explicitly that their results apply to all analytic translation-invariant kernels, but this can be seen by inserting the standard bound \(|f^{(n)}(x)| \leq CR^n n!\) for analytic functions in their Equation (1.6) and using Stirling’s approximation.
2 Results

Let \( \Omega \) be a set. Recall that a function \( K : \Omega \times \Omega \to \mathbb{R} \) is a positive-semidefinite kernel if

\[
\sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m K(x_n, x_m) \geq 0
\]

for any \( N \geq 1, a_1, \ldots, a_N \in \mathbb{R}, \) and \( x_1, \ldots, x_N \in \Omega. \) By the Moore–Aronszajn theorem a positive-semidefinite kernel induces a unique reproducing kernel Hilbert space, \( H_K(\Omega) \), which consists of functions \( f : \Omega \to \mathbb{R}. \) The inner product and norm of this space are denoted \( \langle \cdot, \cdot \rangle_K \) and \( \|\cdot\|_K. \) The kernel is reproducing in \( H_K(\Omega) \), which is to say that \( f(x) = \langle f, K(\cdot, x) \rangle_K \) for every \( f \in H_K(\Omega) \) and \( x \in \Omega. \) The following theorem characterises the elements of an RKHS; see, for example, Section 3.4 in Paulsen and Raghupathi (2016) for a proof.

**Theorem 2.1** (Aronszajn). Let \( K \) be a positive-semidefinite kernel on \( \Omega. \) A function \( f : \Omega \to \mathbb{R} \) is contained in \( H_K(\Omega) \) if and only if

\[
R(x, y) = K(x, y) - c^2 f(x)f(y)
\]

defines a positive-semidefinite kernel on \( \Omega \) for some \( c > 0. \)

If \( \Theta \) is a subset of \( \Omega, \) the RKHS \( H_K(\Theta) \) contains those functions \( f : \Theta \to \mathbb{R} \) for which there exists an extension \( f_\epsilon \in H_K(\Omega) \) (i.e., \( f = f_\epsilon|_\Theta \)).

2.1 General Result

We begin with a result for general bounded kernels.

**Theorem 2.2.** Let \( K \) be a bounded positive-semidefinite kernel on \( \Omega \) and \((x_n)_{n=1}^{\infty} \) a sequence in \( \Omega \) such that

\[
\lim_{\ell \to \infty} |K(x_{\ell+n}, x_{\ell+m})| = 0 \quad \text{for any} \quad n \neq m. \tag{2.1}
\]

If \( f : \Omega \to \mathbb{R} \) satisfies either \( f(x_n) \geq \alpha \) or \( f(x_n) \leq -\alpha \) for some \( \alpha > 0 \) and all sufficiently large \( n, \) then \( f \notin H_K(\Omega). \)

**Proof.** Assume to the contrary that \( f \in H_K(\Omega). \) By Theorem 2.1 there exists \( c > 0 \) such that \( R(x, y) = K(x, y) - c^2 f(x)f(y) \) defines a positive-semidefinite kernel on \( \Omega. \) Therefore the quadratic form

\[
r_{N, \ell} = \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m R(x_{\ell+n}, x_{\ell+m})
\]

is non-negative for every \( N \geq 1 \) and \( \ell \geq 0 \) and any \( a_1, \ldots, a_N \in \mathbb{R}. \) By (2.1) it holds for all sufficiently large \( \ell \) that

\[
\max_{n, m \leq N} \left| K(x_{\ell+n}, x_{\ell+m}) \right| \leq \frac{1}{2} c^2 \alpha^2.
\]

Let \( C_K = \sup_{x \in \Omega} K(x, x) \) and set \( a_1 = \cdots = a_N = 1. \) Then, for sufficiently large \( \ell, \)

\[
r_{N, \ell} = \sum_{n=1}^{N} K(x_{\ell+n}, x_{\ell+n}) + \sum_{n \neq m} K(x_{\ell+n}, x_{\ell+m}) - c^2 \sum_{n=1}^{N} \sum_{m=1}^{N} f(x_{\ell+n})f(x_{\ell+m})
\]

\[
\leq C_K N + \frac{1}{2} c^2 \alpha^2 N^2 - c^2 \alpha^2 N^2
\]

\[
= \left( C_K - \frac{1}{2} c^2 \alpha^2 \right) N,
\]
which is negative if \( N > 2C_K/(c^2a^2) \). It follows that \( r_{N,e} \) is negative for sufficiently large \( N \) and \( e \) which contradicts the assumption that \( f \in H_K(\Omega) \).

An alternative way to prove a similar result in some settings is by appealing to integrability. For example, elements of the RKHS of an integrable translation-invariant kernel on \( \mathbb{R}^d \) are square-integrable [Wendland, 2005, Theorem 10.12]. Other integrability results can be found in Sun (2005) and Carmeli et al. (2006).

2.2 Analytic Functions

Next we use the fact that RKHSs which consist of analytic functions do not depend on the domain to prove a localised versions of the above results for certain subset of \( \mathbb{R} \). The classical results on real analytic functions that we use are collected in Section 1.2 of Krantz and Parks (2002).

**Lemma 2.3.** Let \( K \) be a positive-semidefinite kernel on \( \mathbb{R} \) and \( \Omega \) a subset of \( \mathbb{R} \) which has an accumulation point. If \( H_K(\mathbb{R}) \) consists of analytic functions and \( f: \mathbb{R} \to \mathbb{R} \) is analytic, then \( f \in H_K(\mathbb{R}) \) if and only if \( f\mid_\Omega \in H_K(\Omega) \).

**Proof.** If \( f \in H_K(\mathbb{R}) \), then \( f\mid_\Omega \in H_K(\Omega) \) by definition. Suppose then that \( f\mid_\Omega \notin H_K(\Omega) \). Hence there is an analytic function \( g \in H_K(\mathbb{R}) \) such that \( g\mid_\Omega = f\mid_\Omega \). The function \( f - g \) is analytic and vanishes on \( \Omega \). Because an analytic function which vanishes on a set with an accumulation point is identically zero, we conclude that \( g = f \) and therefore \( f \in H_K(\mathbb{R}) \).

**Theorem 2.4.** Let \( K \) be a bounded positive-semidefinite kernel on \( \mathbb{R} \) such that \( H_K(\mathbb{R}) \) consists of analytic functions, \( \Omega \) a subset of \( \mathbb{R} \) which has an accumulation point, and \( (x_n)_{n=1}^\infty \) a sequence in \( \Omega \) such that

\[
\lim_{\ell \to \infty} |K(x_{\ell+n}, x_{\ell+m})| = 0 \quad \text{for any} \quad n \neq m.
\]

Then a function \( f: \Omega \to \mathbb{R} \) is not an element of \( H_K(\Omega) \) if there exist an analytic function \( f_\alpha : \mathbb{R} \to \mathbb{R} \) and \( \alpha > 0 \) such that \( f\mid_\Omega = f_\alpha \mid_\Omega \) and either \( f_\alpha(x_n) \geq \alpha \) or \( f_\alpha(x_n) \leq -\alpha \) for all sufficiently large \( n \).

**Proof.** By Lemma 2.3 \( f \in H_K(\Omega) \) if and only if \( f_\alpha \in H_K(\mathbb{R}) \). But by Theorem 2.2 \( f_\alpha \) cannot be an element of \( H_K(\mathbb{R}) \). This proves the claim.

Note that the requirement that \( H_K(\mathbb{R}) \) consist of analytic function cannot be simply removed. For example, by Proposition 2.3 the RKHS of the non-analytic kernel \( K(x, y) = \exp(-|x - y|) \) on \( \mathbb{R} \) does not contain non-trivial polynomials. However, if \( \Omega \) is a bounded interval, then \( H_K(\Omega) \) is norm-equivalent to the first-order standard Sobolev space and therefore contains all polynomials.

2.3 Translation-Invariant Kernels

A kernel \( K \) on \( \mathbb{R} \) is translation-invariant if there is a function \( \varphi: [0, \infty) \to \mathbb{R} \) such that

\[
K(x, y) = \varphi((x - y)^2) \quad \text{for all} \quad x, y \in \mathbb{R}.
\]

For translation-invariant kernels the decay assumption (2.1) can be cast into a less abstract form.

**Proposition 2.5.** Let \( K \) be a translation-invariant positive-semidefinite kernel on \( \mathbb{R} \) for \( \varphi \geq 0 \) such that \( \lim_{r \to \infty} \varphi(r) = 0 \). Then a function \( f: \mathbb{R} \to \mathbb{R} \) is not an element of \( H_K(\mathbb{R}) \) if there is \( R \in \mathbb{R} \) such that (a) \( f \) does not change sign on \( [R, \infty) \) and \( \lim_{x \to \infty} |f(x)| > 0 \) or (b) \( f \) does not change sign on \( (-\infty, R] \) and \( \lim_{x \to -\infty} |f(x)| > 0 \).
which implies that $f$ for every $x \in \mathbb{R}$. The claim follows from Theorem 2.7 by selecting a sequence $(x_n)_{n=1}^{\infty}$ such that $|x_{\ell+n} - x_{\ell+m}| \to \infty$ as $\ell \to \infty$ for any $n \neq m$ and $x_n \to \infty$ (or $x_n \to -\infty$). For example, $x_n = 1 + \cdots + n$ (or $x_n = -(1 + \cdots + n)$) suffices since then

$$|x_{\ell+n} - x_{\ell+m}| = \frac{|n - m| (2\ell + n + m + 1)}{2} \geq \ell.$$ 

\[\square\]

Note that this proposition could be slightly generalised by requiring only that $f(x_n)$ be bounded away from zero for large $n$. For example, the function $f(x) = \sin(\pi(x + \frac{1}{2}))^2$, which is not covered by Proposition 2.5, satisfies $f(x_n) = 1$ for all $n$ if $x_n = \pm (1 + \cdots + n)$.

Let $\varphi^{(n)}_+(0)$ denote the $n$th derivative from right of $\varphi$ at the origin and define

$$D^n K_x(y) = \frac{\partial^n}{\partial v^n} K(v, y) \bigg|_{v=x} \quad \text{and} \quad D^{n,n} K(x, y) = \frac{\partial^{2n}}{\partial v^n \partial w^n} K(v, w) \bigg|_{v=x, w=y}.$$ 

The following lemma has been essentially proved by Sun and Zhou (2008). For completeness we supply a simple proof.

**Lemma 2.6.** If $K$ is a translation-invariant positive-semidefinite kernel on $\mathbb{R}$ for $\varphi$ which is analytic on $\mathbb{R}$, then all elements of $H_K(\mathbb{R})$ are analytic.

**Proof.** Because $K$ is infinitely differentiable on $\mathbb{R}$, every $f \in H_K(\mathbb{R})$ is infinitely differentiable and satisfies

$$|f^{(n)}(x)| = |\langle f, D^n K_x \rangle_K| \leq \|f\|_K \|D^n K_x\|_K = \|f\|_K \sqrt{|D^{n,n} K(x, x)|}$$

for every $n \geq 0$ and $x \in \mathbb{R}$ (Steinwart and Christmann, 2008, Corollary 4.36). From the Taylor expansion

$$K(x, y) = \sum_{n=0}^{\infty} \frac{\varphi^{(n)}_+(0)}{n!} (x - y)^2n$$

it is straightforward to compute that, for any $x \in \mathbb{R}$,

$$D^{n,n} K(x, x) = (-1)^n \frac{(2n)!}{n!} \varphi^{(n)}_+(0).$$

Since $\varphi$ is analytic, there are positive constants $C$ and $R$ such that $|\varphi^{(n)}_+(0)| \leq CR^n n!$ for every $n \geq 0$. It follows that

$$|f^{(n)}(x)| \leq \|f\|_K \sqrt{\frac{(2n)!}{n!} \varphi^{(n)}_+(0)} \leq \|f\|_K \sqrt{CR^n (2n)!} \leq \sqrt{C} \|f\|_K (2\sqrt{R})^n n!,$$

which implies that $f$ is analytic on $\mathbb{R}$.

\[\square\]

**Theorem 2.7.** Let $K$ be a translation-invariant positive-semidefinite kernel on $\mathbb{R}$ for $\varphi \geq 0$ which is analytic on $[0, \infty)$ and satisfies $\lim_{r \to \infty} \varphi(r) = 0$ and $\Omega$ a subset of $\mathbb{R}$ which has an accumulation point. Then a function $f : \Omega \to \mathbb{R}$ is not an element of $H_K(\Omega)$ if there exists an analytic function $f_c : \mathbb{R} \to \mathbb{R}$ such that $f_c |\Omega = f$ and

$$\liminf_{x \to \infty} |f_c(x)| > 0 \quad \text{or} \quad \liminf_{x \to \infty} |f_c(x)| > 0.$$ 

**Proof.** The claim follows from Lemmas 2.3 and 2.6 and Proposition 2.5. The requirement in Proposition 2.5 that the function should not change sign follows from continuity and (2.2).

\[\square\]
3 Examples

Standard examples of analytic translation-invariant kernels are the Gaussian kernel

\[ K(x, y) = \varphi((x - y)^2) \quad \text{for} \quad \varphi(r) = \exp(-r) \]

and the inverse quadratic

\[ K(x, y) = \varphi((x - y)^2) \quad \text{for} \quad \varphi(r) = \frac{1}{1 + r}. \]

It is known that the RKHSs of these kernels do not contain non-trivial polynomials \( \text{Minh, 2010} \) \( \text{Dette and Zhigljavsky, 2021} \) on bounded intervals. These results are special cases of Theorem 2.7 which can be applied to any analytic function whose analytic continuation is bounded away from zero at infinity. For example, the function

\[ f(x) = \exp \left( -\sin(x)^2 + \frac{1}{\sqrt{1 + x^2}} \right) \]

is in the RKHS of no translation-invariant kernel for which \( \varphi \geq 0 \) decays to zero at infinity.

The exponential kernel

\[ K(x, y) = \exp(xy) \]

serves as a good example that \( \lim_{x \to \infty} K(x, y) = 0 \) for infinitely many \( y \) is not a sufficient condition for Theorem (2.7) to hold. The RKHS on \( \mathbb{R} \) of the exponential kernel consists of analytic functions and contains all polynomials. For any \( y < 0 \) it holds that \( \lim_{x \to \infty} K(x, y) = 0 \). However, it is not possible to select a sequence \( (x_n)_{n=1}^{\infty} \) for which \( K \) satisfies (2.1). For clearly \( x_{\ell+n} \) and \( x_{\ell+m} \) would have to have had opposite signs for all sufficiently large \( \ell \) if \( n \neq m \). But this would in particular imply that \( \text{sgn}(x_{\ell+1}) \neq \text{sgn}(x_{\ell+2}) \), \( \text{sgn}(x_{\ell+1}) \neq \text{sgn}(x_{\ell+3}) \), and \( \text{sgn}(x_{\ell+2}) \neq \text{sgn}(x_{\ell+3}) \) for sufficiently large \( \ell \), which is not possible.

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