FURTHER PROPERTIES OF GAUSSIAN REPRODUCING KERNEL HILBERT SPACES

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Abstract. We generalize the orthonormal basis for the Gaussian RKHS described in [3] to an infinite, continuously parametrized, family of orthonormal bases, along with some implications. The proofs are direct generalizations of those in [3].

1. Main Results

Notation 1. Let \( \alpha = (\alpha_1, \ldots, \alpha_n) \in (\mathbb{N} \cup \{0\})^n \), \( |\alpha| = \sum_{j=1}^{n} \alpha_j \), \( x^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n} \), and \( C_\alpha^d = \frac{d!}{\alpha_1! \cdots \alpha_n!} \), the multinomial coefficients. Also, by writing \( L^p(X) \), \( dx \), we assume that the Lebesgue measure is being used.

Theorem 1. Let \( X \subset \mathbb{R}^n \) be any set with non-empty interior. Let \( K(x,t) = \exp(-\frac{|x-t|^2}{\sigma^2}) \). Let \( c \in \mathbb{R}^n \) be fixed but otherwise arbitrary. Let \( H_K \) be the RKHS induced by \( K \). Then \( \dim(H_K) = \infty \) and

\[
H_K = \{ f = e^{-\frac{|x-c|^2}{\sigma^2}} \sum_{|\alpha|=0}^{\infty} w_\alpha (x-c)^\alpha : \|f\|^2_K = \sum_{k=0}^{\infty} \frac{k!}{(2/\sigma^2)^k} \sum_{|\alpha|=k}^{\infty} \frac{w_\alpha^2 C_\alpha^k}{k!} < \infty \}. 
\]

The inner product \( \langle \cdot, \cdot \rangle_K \) on \( H_K \) is given by

\[
\langle f, g \rangle_K = \sum_{k=0}^{\infty} \frac{k!}{(2/\sigma^2)^k} \sum_{|\alpha|=k}^{\infty} \frac{w_\alpha v_\alpha C_\alpha^k}{k!} 
\]

for \( f = e^{-\frac{|x-c|^2}{\sigma^2}} \sum_{|\alpha|=0}^{\infty} w_\alpha (x-c)^\alpha, \ g = e^{-\frac{|x-c|^2}{\sigma^2}} \sum_{|\alpha|=0}^{\infty} v_\alpha (x-c)^\alpha \in H_K \). An orthonormal basis for \( H_K \) is

\[
\{ \phi_{\alpha,c}(x) = \sqrt{\frac{(2/\sigma^2)^k C_\alpha^k}{k!}} e^{-\frac{|x-c|^2}{\sigma^2}} (x-c)^\alpha \}_{|\alpha|=k,k=0}^{\infty} 
\]

Remark 1. By varying \( c \) through \( \mathbb{R}^n \), we obtain a continuously parametrized family of orthonormal bases of \( H_K \) - there are uncountably many of them. In particular, for \( c = 0 \), we obtain the orthonormal basis \( \{ \phi_\alpha(x) = \sqrt{\frac{(2/\sigma^2)^k C_\alpha^k}{k!}} e^{-\frac{|x|^2}{\sigma^2}} x^\alpha \}_{|\alpha|=k,k=0}^{\infty} 
\)

already described in [4] and [3].

Let us discuss some immediate implications of Theorem 1. Consider the function

\[ \phi_{0,c}(x) = \exp\left(-\frac{|x-c|^2}{\sigma^2}\right). \]
**Corollary 1.** For any \( c \in \mathbb{R}^n \) and any set \( X \subset \mathbb{R}^n \) with non-empty interior, \( \phi_{0,c} \in \mathcal{H}_{K,\sigma}(X) \), with

\[
\| \phi_{0,c} \|_{\mathcal{H}_{K,\sigma}(X)} = 1.
\]

To illustrate the result of Corollary 1, we note that by Aronszajn’s Restriction Theorem (see [1], section 5), for any set \( X \subset \mathbb{R}^n \),

\[
\mathcal{H}_{K,\sigma}(X) = \{ f : X \rightarrow \mathbb{R} \mid \exists F \in \mathcal{H}_{K,\sigma}(\mathbb{R}^n) : f = F|_X \},
\]

with corresponding norm

\[
\| f \|_{\mathcal{H}_{K,\sigma}(X)} = \min\{ \| F \|_{\mathcal{H}_{K,\sigma}(\mathbb{R}^n)} : f = F|_X \}.
\]

In particular, this implies that \( \phi_{0,c}(x) = \exp\left( -\frac{||x-c||^2}{\sigma^2} \right) \in \mathcal{H}_{K,\sigma}(X) \) for all \( c \in \mathbb{R}^n \),

\[
\| \phi_{0,c} \|_{\mathcal{H}_{K,\sigma}(X)} \leq \| \phi_{0,c} \|_{\mathcal{H}_{K,\sigma}(\mathbb{R}^n)} = \| K_c \|_{\mathcal{H}_{K,\sigma}(\mathbb{R}^n)} = 1.
\]

In particular, for \( c \in X \), we have

\[
\| \phi_{0,c} \|_{\mathcal{H}_{K,\sigma}(X)} = \| K_c \|_{\mathcal{H}_{K,\sigma}(X)} = 1.
\]

**Remark 2.** We wish to emphasize that one can only write \( \phi_{0,c}(x) = \exp\left( -\frac{||x-c||^2}{\sigma^2} \right) \) = \( K_c(x) \) when \( c \in X \): the function \( \exp\left( -\frac{||x-c||^2}{\sigma^2} \right) \) is always defined on any \( X \subset \mathbb{R}^n \) and for any \( c \in \mathbb{R}^n \), but we cannot talk about \( K_c \) if \( c \notin X \). Thus the Restriction Theorem only allows us to conclude that \( \| \phi_{0,c} \|_{\mathcal{H}_{K,\sigma}(X)} \leq 1 \) when \( c \notin X \).

The power of the Orthonormal Basis Theorem (Theorem 3) is clearly illustrated in the proof of Theorem 1. Note that there is no need for us to consider the larger set \( \mathbb{R}^n \) or embedding maps between \( \mathcal{H}_{K,\sigma}(X) \) and \( \mathcal{H}_{K,\sigma}(\mathbb{R}^n) \). We automatically have \( \phi_{0,c} \in \mathcal{H}_{K,\sigma}(X) \) without having to invoke the Restriction Theorem.

**Theorem 2.** Let \( X \subset \mathbb{R}^n \) be any set with non-empty interior. Let \( K(x, z) = \exp(\frac{-||x-z||^2}{\sigma^2}) \). Let \( c \in \mathbb{R}^n \) be arbitrary. The Hilbert space \( \mathcal{H}_K \) induced by \( K \) on \( X \) contains the function \( \exp(\frac{-\mu||x-c||^2}{\sigma^2}) \) if and only if \( 0 < \mu < 2 \). For such \( \mu \), the corresponding functions have norms given by

\[
\left\| \exp\left( -\frac{\mu||x-c||^2}{\sigma^2} \right) \right\|_{\mathcal{H}_{K,\sigma}(X)}^2 = \left[ \frac{1}{\mu(2-\mu)} \right]^{\frac{n}{2}}.
\]

In [3], it is shown that \( f_0(x) = \exp(-\frac{\mu||x||^2}{\sigma^2}) \in \mathcal{H}_{K,\sigma}(X) \) if and only if \( 0 < \mu < 2 \). If \( X = \mathbb{R}^n \), then it follows immediately from the translation-invariant property that \( f_c(x) = \exp(-\frac{\mu||x-c||^2}{\sigma^2}) \in \mathcal{H}_{K,\sigma}(X) \) if and only if \( 0 < \mu < 2 \). Specifically, in terms of the Fourier Transform,

\[
\| f_0 \|_{\mathcal{H}_{K,\sigma}(\mathbb{R}^n)}^2 = \frac{1}{(2\pi)^n (\sigma \sqrt{\pi})^n} \int_{\mathbb{R}^n} e^{\frac{-2\pi^2 \xi^2}{\sigma^2}} |\widehat{f}_0(\xi)|^2 d\xi
\]

\[
= \frac{1}{(2\pi)^n (\sigma \sqrt{\pi})^n} \int_{\mathbb{R}^n} e^{\frac{-2\pi^2 \xi^2}{\sigma^2}} |\widehat{f}_c(\xi)|^2 d\xi = \| f_c \|_{\mathcal{H}_{K,\sigma}(\mathbb{R}^n)}^2.
\]

If \( X \neq \mathbb{R}^n \), the Restriction Theorem gives

\[
\| f_c \|_{\mathcal{H}_{K,\sigma}(X)}^2 \leq \| f_c \|_{\mathcal{H}_{K,\sigma}(\mathbb{R}^n)}^2.
\]
So if $0 < \mu < 2$, then we can conclude that $f_c \in \mathcal{H}_{K,\sigma}(X)$. But we cannot say more about $\|f_c\|^2_{\mathcal{H}_{K,\sigma}(X)}$. We cannot make a statement on the reverse direction either: if $f_c \in \mathcal{H}_{K,\sigma}(X)$, we cannot infer that $0 < \mu < 2$ using the Restriction Theorem. This is what Theorem 2 gives us.

2. Proofs of Main Results

2.1. The Weyl Inner Product and Orthonormal Basis of the Gaussian RKHS. Let us prove Theorem 1. It was shown in [2] that for $X = \mathbb{R}^n$, $n \in \mathbb{N}$, and $K(x,t) = \langle x, t \rangle^d$, $d \in \mathbb{N}$, we have $\mathcal{H}_K = \mathcal{H}_d(\mathbb{R}^n)$, the linear space of all homogeneous polynomials of degree $d$ in $\mathbb{R}^n$, with the inner product $\langle \cdot, \cdot \rangle$ being the Weyl inner product on $\mathcal{H}_d(\mathbb{R}^n)$:

$$\langle f, g \rangle_K = \sum_{|\alpha| = d} \frac{w_\alpha v_\alpha}{C_\alpha^d},$$

for $f = \sum_{|\alpha| = d} w_\alpha t^\alpha$, $g = \sum_{|\alpha| = d} v_\alpha t^\alpha \in \mathcal{H}_K$.

**Theorem 3** (Aronszajn). Let $H$ be a separable Hilbert space of functions over $X$ with orthonormal basis $\{\phi_k\}_{k=0}^{\infty}$. $H$ is a reproducing kernel Hilbert space iff

$$\sum_{k=0}^{\infty} |\phi_k(x)|^2 < \infty$$

for all $x \in X$. The unique kernel $K$ is defined by

$$K(x,y) = \sum_{k=0}^{\infty} \phi_k(x)\phi_k(y).$$

**Proof of Theorem 3.** We will show that the inner product $\langle \cdot, \cdot \rangle_K$ in $\mathcal{H}_K$ is simply a generalization of the Weyl inner product for the homogeneous polynomial space $\mathcal{H}_d(\mathbb{R}^n)$, $d \in \mathbb{N}$. Consider the following expansion

$$K(x,t) = \exp \left( -\frac{||x-t||^2}{\sigma^2} \right) = \exp \left( -\frac{||x-c||^2 - ||c-t||^2}{\sigma^2} \right) = \exp \left( -\frac{||x-c||^2}{\sigma^2} \right) \exp \left( -\frac{||t-c||^2}{\sigma^2} \right) \sum_{k=0}^{\infty} \frac{(2/\sigma^2)^k}{k!} \sum_{|\alpha|=k} C_\alpha^k (x-c)^\alpha (t-c)^\alpha. $$

Let $H_0 = \{ f \in \mathcal{H}_d : \sum_{|\alpha|=0}^{\infty} w_\alpha (x-c)^\alpha | \sum_{k=0}^{\infty} \frac{k!}{(2/\sigma^2)^k} \sum_{|\alpha|=k} w_\alpha^2 C_\alpha^k < \infty \}$. For $f \in H_0$, $g \in H_0$, we define the inner product

$$\langle f, g \rangle_{K,0} = \sum_{k=0}^{\infty} \frac{k!}{(2/\sigma^2)^k} \sum_{|\alpha|=k} \frac{w_\alpha v_\alpha}{C_\alpha^k}. $$

Let us show that $H_0$ is itself a Hilbert space under $\langle \cdot, \cdot \rangle_{K,0}$. For simplicity let $n = 1$. Then

$$H_0 = \{ f = e^{-\frac{||x-c||^2}{\sigma^2}} \sum_{k=0}^{\infty} w_k (x-c)^k | \sum_{k=0}^{\infty} \frac{k!}{(2/\sigma^2)^k} \sum_{|\alpha|=k} w_\alpha^2 C_\alpha^k < \infty \}. $$

It is clear that $H_0$ is an inner product space under $\langle \cdot, \cdot \rangle_{K,0}$. Its completeness under the induced norm $\| \cdot \|_{K,0}$ is equivalent to the completeness of the weighted $\ell^2$ sequence space

$$\ell^2_w = \{ (w_k)_{k=0}^{\infty} : \| (w_k)_{k=0}^{\infty} \|_{\ell^2_w} = \left( \sum_{k=0}^{\infty} \frac{k!}{(2/\sigma^2)^k} w_k^2 \right)^{1/2} \}. $$

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which is itself a Hilbert space. Thus \((H_0, \| \cdot \|_{K_0})\) is a Hilbert space.

If \(X \subset \mathbb{R}^n\) has non-empty interior, then the monomials \((x - c)^\alpha, |\alpha| \geq 0,\) are all distinct. It follows from the definition of the inner product \(\langle \cdot, \cdot \rangle_{K_0}\) that the \(\phi_{\alpha, c}'s,\) as given in \((2),\) are orthonormal under \(\langle \cdot, \cdot \rangle_{K_0}\). Since \(H_0 = \text{span}\{\phi_{\alpha, c}\}_\alpha\), it follows that the \(\phi_{\alpha, c}'s\) form an orthonormal basis for \((H_0, \| \cdot \|_{K_0}).\) By Theorem \(3\) and the relations

\[
\sum_{k=0}^\infty \sum_{|\alpha|=k} \phi_{\alpha, c}(x)\phi_{\alpha, c}(t) = K(x, t),
\]

\[
\sum_{k=0}^\infty \sum_{|\alpha|=k} |\phi_{\alpha, c}(x)|^2 = K(x, x) = 1 < \infty,
\]

it follows that \((H_0, \| \cdot \|_{K_0})\) is a reproducing kernel Hilbert space of functions on \(X\) with kernel \(K(x, t).\) Since the RKHS induced by a kernel \(K\) on a set \(X\) is unique, we must have \((H_0, \| \cdot \|_{K_0}) = (\mathcal{H}_K, \| \cdot \|_K).\)

\[\text{Proof of Theorem} \ (2)\] Let us first consider the case \(n = 1.\) Then

\[
\mathcal{H}_K = \{f = e^{-\frac{(x-c)^2}{\sigma^2}} \sum_{k=0}^\infty w_k(x-c)^k : \|f\|^2_K = \sum_{k=0}^\infty \frac{2^k k!}{2^k} w_k^2 < \infty\}
\]

Consider the function \(e^{-\frac{\mu(x-c)^2}{\sigma^2}}\), which is

\[
e^{-\frac{\mu(x-c)^2}{\sigma^2}} = e^{-\frac{(x-c)^2}{\sigma^2}} \cdot e^{-\frac{(\mu-1)(x-c)^2}{\sigma^2}} = e^{-\frac{(x-c)^2}{\sigma^2}} \sum_{k=0}^\infty (-1)^k \frac{(\mu-1)^k(x-c)^{2k}}{\sigma^{2k} k!}.
\]

Thus \(w_{2k} = \frac{(-1)^k(\mu-1)^k}{\sigma^{2k} k!}\) and \(w_j = 0\) for \(j \neq 2k.\) Then

\[
\sum_{k=0}^\infty \frac{\sigma^{2k} k!}{2^k} w_k^2 = \sum_{k=0}^\infty \frac{\sigma^{2k} k!}{2^k} \frac{(\mu-1)^{2k}}{\sigma^{4k} k!} \frac{(2k)!}{(2k)!} = \sum_{k=0}^\infty \frac{(\mu-1)^{2k}(2k)!}{2^{2k} k!}.
\]

If \(\mu \leq 0\) or \(\mu \geq 2,\) then

\[
\sum_{k=0}^\infty \frac{(\mu-1)^{2k}(2k)!}{2^{2k} k!} \geq \sum_{k=0}^\infty \frac{(2k)!}{2^{2k} k!} = \infty
\]

showing that \(f \notin \mathcal{H}_K\) in those cases. If \(0 < \mu < 2,\) then

\[
\sum_{k=0}^\infty \frac{(\mu-1)^{2k}(2k)!}{2^{2k} k!} = 1 + \sum_{k=1}^\infty \frac{(\mu-1)^{2k}(2k-1)!!}{(2k-1)!!},
\]

which converges by the Ratio Test. Hence we have \(\sum_{k=0}^\infty \frac{\sigma^{2k} k!}{2^k} w_k^2 < \infty,\) showing that \(e^{-\frac{(x-c)^2}{\sigma^2}} e^{-\frac{(x-c)^2}{\sigma^2}} \in \mathcal{H}_K\) for \(0 < \mu < 2,\) with norm

\[
\|e^{-\frac{(x-c)^2}{\sigma^2}}\|^2_K = \sum_{k=0}^\infty \frac{(\mu-1)^{2k}(2k)!}{2^{2k} k!} = \frac{1}{\sqrt{1 - (\mu-1)^2}} = \frac{1}{\sqrt{\mu(2-\mu)}}.
\]

For any \(n \in \mathbb{N},\) we have

\[
e^{-\frac{(x-c)^2}{\sigma^2}} e^{-\frac{(x-c)^2}{\sigma^2}} e^{-\frac{(x-c)^2}{\sigma^2}} = e^{-\frac{(x-c)^2}{\sigma^2}} \prod_{i=1}^n \sum_{k_i=0}^\infty w_{k_i} (x_i - c_i)^{k_i}
\]

\[
= e^{-\frac{(x-c)^2}{\sigma^2}} \sum_{\{k_1, \ldots, k_n\} = 0}^\infty \prod_{i=1}^n w_{k_i} (x_i - c_i)^{k_i},
\]

\[
\|e^{-\frac{(x-c)^2}{\sigma^2}}\|^2_K = \sum_{k=0}^\infty \frac{(\mu-1)^{2k}(2k)!}{2^{2k} k!} = \frac{1}{\sqrt{1 - (\mu-1)^2}} = \frac{1}{\sqrt{\mu(2-\mu)}}.
\]
\[ \| e^{-\frac{\|x-c\|^2}{2\sigma^2}} \|_K^2 = \sum_{k_1, \ldots, k_n \geq 0} \prod_{i=1}^{n} \frac{\sigma^2 k_i!}{2^{k_i} k_i^2 w_{k_i}^2} = \prod_{i=1}^{n} \sum_{k_i=0}^{\infty} \frac{\sigma^2 k_i!}{2^{k_i} k_i^2 w_{k_i}^2}. \]

The result then follows from the one dimensional case above by symmetry. \( \square \)

References

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