

MATH 590: Meshfree Methods

Chapter 2 — Part 3: Native Space for Positive Definite Kernels

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Outline

- 1 Native Spaces for Positive Definite Kernels
- 2 Examples of Native Spaces for Popular RBFs



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First, we note that the definition of an RKHS tells us that $\mathcal{H}_K(\Omega)$ contains all functions of the form

$$f = \sum_{j=1}^N c_j K(\cdot, \mathbf{x}_j)$$

provided $\mathbf{x}_j \in \Omega$.



Using the properties of RKHSs established earlier along with the form of f just mentioned we have that

$$\|f\|_{\mathcal{H}_K(\Omega)}^2 = \langle f, f \rangle_{\mathcal{H}_K(\Omega)} = \left\langle \sum_{i=1}^N c_i K(\cdot, \mathbf{x}_i), \sum_{j=1}^N c_j K(\cdot, \mathbf{x}_j) \right\rangle_{\mathcal{H}_K(\Omega)}$$



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 &= \sum_{i=1}^N \sum_{j=1}^N c_i c_j K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{c}^T \mathbf{K} \mathbf{c}.
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So — for these special types of f — we can easily calculate the Hilbert space norm of f .

In particular, if $f = \mathbf{s}$ is a kernel-based interpolant, i.e., $\mathbf{c} = \mathbf{K}^{-1} \mathbf{y}$, then we also have

$$\|\mathbf{s}\|_{\mathcal{H}_K(\Omega)}^2 = \mathbf{y}^T \mathbf{K}^{-T} \mathbf{K} \mathbf{K}^{-1} \mathbf{y} = \mathbf{y}^T \mathbf{K}^{-1} \mathbf{y}.$$



Therefore, we **define** the (possibly infinite-dimensional) **space** of all **linear combinations**

$$H_K(\Omega) = \text{span}\{K(\cdot, \mathbf{z}) : \mathbf{z} \in \Omega\} \quad (1)$$

with an associated **bilinear form** $\langle \cdot, \cdot \rangle_K$ given by

$$\left\langle \sum_{i=1}^N c_i K(\cdot, \mathbf{x}_i), \sum_{j=1}^M d_j K(\cdot, \mathbf{z}_j) \right\rangle_K = \sum_{i=1}^N \sum_{j=1}^M c_i d_j K(\mathbf{x}_i, \mathbf{z}_j) = \mathbf{c}^T \mathbf{K} \mathbf{d}.$$

Remark

Note that this definition implies that a general element in $H_K(\Omega)$ has the form (where $N = \infty$ is allowed)

$$f = \sum_{j=1}^N c_j K(\cdot, \mathbf{x}_j).$$

*However, not **only** the coefficients c_j , but also the specific value of N and choice of points \mathbf{x}_j will vary with f .*

Theorem

If $K : \Omega \times \Omega \rightarrow \mathbb{R}$ is a symmetric strictly positive definite kernel, then the bilinear form $\langle \cdot, \cdot \rangle_K$ defines an inner product on $H_K(\Omega)$.



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Furthermore, $H_K(\Omega)$ is a *pre-Hilbert space* with reproducing kernel K .

Remark

A *pre-Hilbert space* is an inner product space whose completion is a Hilbert space.



Proof.

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The reproducing property follows from

$$\langle f, K(\cdot, \mathbf{x}) \rangle_K = \sum_{j=1}^N c_j K(\mathbf{x}, \mathbf{x}_j) = f(\mathbf{x}).$$



Since we just showed that $H_K(\Omega)$ is a pre-Hilbert space, i.e., need not be complete, we now first **form the completion** $\tilde{H}_K(\Omega)$ of $H_K(\Omega)$ with respect to the K -norm $\|\cdot\|_K$ ensuring that

$$\|f\|_K = \|f\|_{\tilde{H}_K(\Omega)} \quad \text{for all } f \in H_K(\Omega).$$



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In general, this completion will consist of equivalence classes of Cauchy sequences in $H_K(\Omega)$, so that we can obtain the **native space** $\mathcal{N}_K(\Omega)$ of K as a **space of continuous functions** with the help of the point evaluation functional (which extends continuously from $H_K(\Omega)$ to $\tilde{H}_K(\Omega)$), i.e., the (values of the) continuous functions in $\mathcal{N}_K(\Omega)$ are given via the right-hand side of

$$\delta_{\mathbf{x}}(f) = \langle f, K(\cdot, \mathbf{x}) \rangle_K, \quad f \in \tilde{H}_K(\Omega).$$



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Remark

The technical details concerned with this construction are discussed in [Wen05].

In summary, we now know that the native space $\mathcal{N}_K(\Omega)$ is given by (continuous functions in) the completion of

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In the **special case** when we are dealing with strictly positive definite (**translation invariant**) functions $\Phi(\mathbf{x} - \mathbf{z}) = K(\mathbf{x}, \mathbf{z})$ and when $\Omega = \mathbb{R}^d$ we get a **characterization of native spaces in terms of Fourier transforms**.



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We present the following theorem without proof (for details see [Wen05]).



Theorem

Suppose $\Phi \in C(\mathbb{R}^d) \cap L_1(\mathbb{R}^d)$ is a real-valued strictly positive definite function. Define

$$\mathcal{G} = \{f \in L_2(\mathbb{R}^d) \cap C(\mathbb{R}^d) : \frac{\hat{f}}{\sqrt{\hat{\Phi}}} \in L_2(\mathbb{R}^d)\}$$

and equip this space with the bilinear form

$$\langle f, g \rangle_{\mathcal{G}} = \frac{1}{\sqrt{(2\pi)^d}} \left\langle \frac{\hat{f}}{\sqrt{\hat{\Phi}}}, \frac{\hat{g}}{\sqrt{\hat{\Phi}}} \right\rangle_{L_2(\mathbb{R}^d)} = \frac{1}{\sqrt{(2\pi)^d}} \int_{\mathbb{R}^d} \frac{\hat{f}(\omega) \overline{\hat{g}(\omega)}}{\hat{\Phi}(\omega)} d\omega.$$

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Then \mathcal{G} is a real Hilbert space with inner product $\langle \cdot, \cdot \rangle_{\mathcal{G}}$ and reproducing kernel $\Phi(\cdot - \cdot)$. Hence, \mathcal{G} is the native space of Φ on \mathbb{R}^d , i.e., $\mathcal{G} = \mathcal{N}_{\Phi}(\mathbb{R}^d)$ and both inner products coincide.

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In particular, every $f \in \mathcal{N}_{\Phi}(\mathbb{R}^d)$ can be recovered from its Fourier transform $\hat{f} \in L_1(\mathbb{R}^d) \cap L_2(\mathbb{R}^d)$.

Mercer's theorem allows us to construct the native space/RKHS $\mathcal{H}_K(\Omega)$ for any continuous positive definite kernel K by representing the functions in \mathcal{H}_K as infinite linear combinations of the eigenfunctions φ_n of the Hilbert–Schmidt integral operator \mathcal{K} , i.e.,

$$\mathcal{H}_K = \left\{ f : f = \sum_{n=1}^{\infty} c_n \varphi_n \right\}.$$

Thus the eigenfunctions $\{\varphi_n\}_{n=1}^{\infty}$ of \mathcal{K} provide an alternative basis for $\mathcal{H}_K(\Omega)$ instead of the standard $\{K(\cdot, \mathbf{z}) : \mathbf{z} \in \Omega\}$.

For any fixed \mathbf{x} , the corresponding “basis transformation” is given by the Mercer series

$$K(\cdot, \mathbf{z}) = \sum_{n=1}^{\infty} \lambda_n \varphi_n \varphi_n(\mathbf{z}).$$

This shows that indeed $K(\cdot, \mathbf{z}) \in \mathcal{H}_K(\Omega)$.



The inner product for $\mathcal{H}_K(\Omega)$ can now be written as

$$\langle \mathbf{f}, \mathbf{g} \rangle_{\mathcal{H}_K(\Omega)} = \left\langle \sum_{m=1}^{\infty} c_m \varphi_m, \sum_{n=1}^{\infty} d_n \varphi_n \right\rangle_{\mathcal{H}_K(\Omega)} = \sum_{n=1}^{\infty} \frac{c_n d_n}{\lambda_n},$$

where we used the fact that the eigenfunctions are not only L_2 -orthonormal, but also orthogonal in $\mathcal{H}_K(\Omega)$, i.e.,

$$\langle \varphi_m, \varphi_n \rangle_{\mathcal{H}_K(\Omega)} = \frac{\delta_{mn}}{\sqrt{\lambda_m} \sqrt{\lambda_n}}.$$



We can also verify that K is indeed the reproducing kernel of \mathcal{H}_K since the Mercer series of K and the orthogonality of the eigenfunctions imply

$$\langle f, K(\cdot, \mathbf{x}) \rangle_{\mathcal{H}_K(\Omega)} = \left\langle \sum_{m=1}^{\infty} c_m \varphi_m, \sum_{n=1}^{\infty} \lambda_n \varphi_n \varphi_n(\mathbf{x}) \right\rangle_{\mathcal{H}_K(\Omega)}$$



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 &= \sum_{n=1}^{\infty} c_n \varphi_n(\mathbf{x}) \\
 &= f(\mathbf{x}).
 \end{aligned}$$



Finally (cf. [Wen05]), we can also describe the RKHS \mathcal{H}_K as

$$\mathcal{H}_K(\Omega) = \left\{ f \in L_2(\Omega) : \sum_{n=1}^{\infty} \frac{1}{\lambda_n} |\langle f, \varphi_n \rangle_{L_2(\Omega)}|^2 < \infty \right\}$$

with inner product

$$\langle f, g \rangle_{\mathcal{H}_K(\Omega)} = \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \langle f, \varphi_n \rangle_{L_2(\Omega)} \langle g, \varphi_n \rangle_{L_2(\Omega)}, \quad f, g \in \mathcal{H}_K(\Omega).$$



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Remark

Since $\mathcal{H}_K(\Omega)$ is a subspace of $L_2(\Omega)$ this latter interpretation corresponds to the *identification of the coefficients in the eigenfunction expansion of an $f \in \mathcal{H}_K(\Omega)$ with the generalized Fourier coefficients of f , i.e., $c_n = \langle f, \varphi_n \rangle_{L_2(\Omega)}$.*

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For $m > d/2$ the **Sobolev space** W_2^m can be defined as (see, e.g., [AF03])

$$W_2^m(\mathbb{R}^d) = \{f \in L_2(\mathbb{R}^d) \cap C(\mathbb{R}^d) : \hat{f}(\cdot)(1 + \|\cdot\|_2^2)^{m/2} \in L_2(\mathbb{R}^d)\}. \quad (2)$$



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Remark

One also frequently sees the definition

$$W_2^m(\Omega) = \{f \in L_2(\Omega) \cap C(\Omega) : D^\alpha f \in L_2(\Omega) \text{ for all } |\alpha| \leq m, \alpha \in \mathbb{N}^d\}, \quad (3)$$

which applies whenever $\Omega \subset \mathbb{R}^d$ is a bounded domain.



Example

Using the notation $r = \|\mathbf{x}\|$ and **modified Bessel functions of the second kind** $K_{d/2-\beta}$, the **Matérn kernels**

$$\kappa_{\beta}(r) = \frac{K_{d/2-\beta}(r)}{r^{d/2-\beta}}, \quad \beta > \frac{d}{2},$$

have Fourier transform

$$\hat{\kappa}_{\beta}(\|\boldsymbol{\omega}\|) = \left(1 + \|\boldsymbol{\omega}\|^2\right)^{-\beta}.$$

So it can immediately be seen that **their native space is**

$$\mathcal{N}_{\mathcal{K}}(\mathbb{R}^d) = W_2^{\beta}(\mathbb{R}^d) \quad \text{with } \beta > d/2,$$

which is why some people refer to the Matérn kernels as Sobolev splines.

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Example

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The native space of Gaussians was recently characterized in [FY11] in terms of an (infinite) vector of differential operators. In fact, the native space of Gaussians is contained in the Sobolev space $W_2^m(\mathbb{R}^d)$ for any m .

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Band-limited functions play an important role in sampling theory.



References I

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- [Wen05] H. Wendland, *Scattered Data Approximation*, Cambridge Monographs on Applied and Computational Mathematics, vol. 17, Cambridge University Press, 2005.

