CHAPTER 12

Reproducing kernel Hilbert spaces

Many problems in statistics—among them interpolation, regression, density estimation, as well as non-parametric forms of dimension reduction and testing—involve optimizing over function spaces. Hilbert spaces include a reasonably broad class of functions, and enjoy a geometric structure similar to ordinary Euclidean space. A particular class of function-based Hilbert spaces are those defined by reproducing kernels, and these spaces—known as reproducing kernel Hilbert spaces—have attractive properties from both the computational and statistical points of view. In this chapter, we develop the basic framework of RKHSs, which are then applied to different problems in later chapters, including non-parametric least-squares (Chapter 13) and density estimation (Chapter 14).

■ 12.1 Basics of Hilbert spaces

Hilbert spaces are particular types of vector spaces, meaning that they are endowed with the operations of addition, and scalar multiplication. In addition, they have an inner product defined in the usual way:

Definition 12.1. An inner product on a vector space $\mathbb{V}$ is a mapping $\langle \cdot,\, \cdot \rangle_{\mathbb{V}} : \mathbb{V} \times \mathbb{V} \rightarrow \mathbb{R}$ such that

$$\langle f,\, g \rangle_{\mathbb{V}} = \langle g,\, f \rangle_{\mathbb{V}} \quad \text{for all } f, g \in \mathbb{V}. \tag{12.1a}$$

$$\langle f,\, f \rangle_{\mathbb{V}} \geq 0 \quad \text{for all } f \in \mathbb{V}, \text{ with equality iff } f = 0, \text{ and} \tag{12.1b}$$

$$\langle f + \alpha g,\, h \rangle_{\mathbb{V}} = \langle f,\, h \rangle_{\mathbb{V}} + \alpha \, \langle g,\, h \rangle_{\mathbb{V}} \quad \text{for all } f, g, h \in \mathbb{V} \text{ and } \alpha \in \mathbb{R}. \tag{12.1c}$$

A vector space equipped with an inner product is known as an *inner product space*. Note that any inner product induces a norm via $\|f\|_{\mathbb{V}} := \sqrt{\langle f,\, f \rangle_{\mathbb{V}}}$. Given this norm, we can then define the usual notion of *Cauchy sequence*—that is, a sequence $(f_n)_{n=1}^{\infty}$ with elements in $\mathbb{V}$ is Cauchy if for all $\epsilon > 0$, there exists some integer $N(\epsilon)$ such that

$$\|f_n - f_m\|_{\mathbb{V}} < \epsilon \qquad \text{for all } n,\, m \geq N(\epsilon).$$

Definition 12.2. A *Hilbert space* $\mathbb{H}$ is an inner product space $(\langle \cdot,\, \cdot \rangle_{\mathbb{H}}\,, \mathbb{H})$ in which every Cauchy sequence $\{f_n\}_{m=1}^{\infty}$ in $\mathbb{H}$ converges to some element $f^* \in \mathbb{H}$.

A metric space in which every Cauchy sequence $\{f_n\}_{n=1}^{\infty}$ converges to an element f^* of the space is known as *complete*. Thus, we can summarize by saying that a Hilbert space is a complete inner product space.

Example 12.1 (Sequence space $\ell^2(\mathbb{N})$)**.** Consider the space of square-summable real-valued sequences, namely

$$\ell^2(\mathbb{N}) := \Big\{ (\theta_j)_{j=1}^{\infty} \mid \sum_{j=1}^{\infty} \theta_j^2 < \infty \Big\}.$$

It becomes a Hilbert space when endowed with the inner product $\langle \theta,\, \gamma \rangle_{\ell^2(\mathbb{N})} = \sum_{j=1}^{\infty} \theta_j \gamma_j$. This sequence space plays important role in our discussion of eigenfunctions for reproducing kernel Hilbert spaces. Note that the Hilbert space $\mathbb{R}^m$, equipped with the usual Euclidean inner product, can be obtained as a finite-dimensional subspace of $\ell^2(\mathbb{N})$: in particular, the space $\mathbb{R}^m$ is isomorphic to the "slice"

$$\big\{ \theta \in \ell^2(\mathbb{N}) \mid \theta_j = 0 \quad \text{for all } j \geq m+1 \big\}.$$

♣

Example 12.2 (The space $L^2[0,1]$)**.** Any element of the space $L^2[0,1]$ is a function $f : [0,1] \rightarrow \mathbb{R}$ that is Lebesgue integrable, and satisfies $\|f\|_{L^2[0,1]}^2 = \int_0^1 f^2(x)dx < \infty$. Since this norm does not distinguish between functions that differ only on a set of Lebesgue zero, we are implicitly identifying all such functions. The space $L^2[0,1]$ is a Hilbert space when equipped with the inner product $\langle f,\, g \rangle_{L^2[0,1]} = \int_0^1 f(x)g(x)dx$. When the space $L^2[0,1]$ is clear from context, we omit the subscript in the inner product notation. In a certain sense, the space $L^2[0,1]$ is equivalent to the sequence space $\ell^2(\mathbb{N})$. In particular, let $(\phi_j)_{j=1}^{\infty}$ be any complete orthonormal basis of $L^2[0,1]$. By definition, the basis functions satisfy $\|\phi_j\|_{L^2[0,1]} = 1$ for all $j \in \mathbb{N}$, and $\langle \phi_i,\, \phi_j \rangle = 0$ for all $i \neq j$, and moreover, any function $f \in L^2[0,1]$ has the representation $f = \sum_{j=1}^{\infty} a_j \phi_j$, where $a_j := \langle f,\, \phi_j \rangle$ is the j^{th} basis coefficient. By Parseval's theorem, we have

$$\|f\|_{L^2[0,1]}^2 = \sum_{j=1}^{\infty} a_j^2,$$

so that $f \in L^2[0,1]$ if and only if the sequence $a = (a_j)_{j=1}^{\infty} \in \ell^2(\mathbb{N})$. The correspondence $f \longleftrightarrow (a_j)_{j=1}^{\infty}$ thus defines an isomorphism between $L^2[0,1]$ and $\ell^2(\mathbb{N})$. ♣

All of the preceding examples are instances of *separable Hilbert spaces*, for which there is a countable dense subset. For such Hilbert spaces, we can always find a collection of functions $(\phi_j)_{j=1}^{\infty}$, orthonormal in the Hilbert space (meaning that $\langle \phi_i, \, \phi_j \rangle_{\mathbb{H}} = \delta_{ij}$ for all positive integers i, j) such that any $f \in \mathbb{H}$ can be written in the form $f = \sum_{j=1}^{\infty} a_j \phi_j$ for some sequence of coefficients $(a_j)_{j=1}^{\infty} \in \ell^2(\mathbb{N})$. Although there do exist non-separable Hilbert spaces, here we focus primarily on the separable case.

The notion of a linear functional plays an important role in characterizing reproducing kernel Hilbert spaces. A *linear functional* on a Hilbert space $\mathbb{H}$ is a mapping $L : \mathbb{H} \rightarrow \mathbb{R}$ that is linear, meaning that $L(f + \alpha g) = L(f) + \alpha L(g)$ for all $f, g \in \mathbb{H}$ and $\alpha \in \mathbb{R}$. A linear functional is said to be *bounded* if there exists some $M < \infty$ such that $|L(f)| \leq M \|f\|_{\mathbb{H}}$ for all $f \in \mathbb{H}$. Given any $g \in \mathbb{H}$, the mapping $f \mapsto \langle f, \, g \rangle_{\mathbb{H}}$ defines a linear functional. It is bounded, since by the Cauchy-Schwarz inequality, we have $|\langle f, \, g \rangle_{\mathbb{H}}| \leq M \, \|f\|_{\mathbb{H}}$ for all $f \in \mathbb{H}$, where $M := \|g\|_{\mathbb{H}}$. The Riesz representation theorem guarantees that every bounded linear functional arises in exactly this way.

Theorem 12.1 (Riesz representation theorem)**.** Let L be a bounded linear functional on a Hilbert space. Then there exists a unique $g \in \mathbb{H}$ such that $L(f) = \langle f, \, g \rangle_{\mathbb{H}}$ for all $f \in \mathbb{H}$.

Proof. Consider the null space $\mathbb{N}(L) = \{h \in \mathbb{H} \mid L(h) = 0\}$. Since L is a bounded linear operator, the null space is closed. (See Exercise 12.1.) Moreover, as we show in Exercise 12.3, for any such closed subspace, we have the direct sum decomposition $\mathbb{H} = \mathbb{N}(L) + [\mathbb{N}(L)]^{\perp}$ where $[\mathbb{N}(L)]^{\perp}$ consists of all $g \in \mathbb{H}$ such that $\langle h, \, g \rangle_{\mathbb{H}} = 0$ for all $h \in \mathbb{N}(L)$. If $\mathbb{N}(L) = \mathbb{H}$, then we take $g = 0$. Otherwise, there must exist a non-zero element $g_0 \in [\mathbb{N}(L)]^{\perp}$. Define $h = L(f) g_0 - L(g_0) f$, and note that $L(h) = 0$ by construction. Consequently, we must have $\langle h, \, g_0 \rangle_{\mathbb{H}} = 0$, or equivalently $L(f) = \langle g, \, f \rangle_{\mathbb{H}}$, where $g := \frac{L(g_0)}{\|g_0\|_{\mathbb{H}}^2} \, g_0$. As for uniqueness, suppose that there exist $g, g' \in \mathbb{H}$ such that $\langle g, \, f \rangle_{\mathbb{H}} = L(f) = \langle g', \, f \rangle_{\mathbb{H}}$ for all $f \in \mathbb{H}$. Re-arranging yields $\langle g - g', \, f \rangle_{\mathbb{H}} = 0$ for all $f \in \mathbb{H}$, and setting $f = g - g'$ shows that $\|g - g'\|_{\mathbb{H}}^2 = 0$, and hence $g = g'$ as claimed.

□

■ 12.2 Reproducing kernel Hilbert spaces

We now turn to the notion of a reproducing kernel Hilbert space, or RKHS for short. These Hilbert spaces are particular types of function spaces—more specifically, functions f with domain $\mathcal{X}$ mapping to the real line $\mathbb{R}$. One way to define an RKHS—which we pursue in the following section—is via boundedness of the functionals $x \mapsto f(x)$.

These evaluation functions are particularly relevant in statistical settings, since many applications involve sampling a function at a subset of points on its domain.

12.2.1 Representer of evaluation

For a given point $x \in \mathcal{X}$, the *evaluation functional* at x is the mapping $L_x : \mathbb{H} \to \mathbb{R}$ that performs the operation $f \mapsto f(x)$. Note that L_x is a linear functional, since

$$L_x(f + \alpha g) = (f + \alpha g)(x) = f(x) + \alpha g(x) \; = \; L_x(f) + \alpha L_x(g)$$

for every pair of functions $f, g \in \mathbb{H}$ and scalar $\alpha \in \mathbb{R}$.

Definition 12.3. A *reproducing kernel Hilbert space* $\mathbb{H}$ is a Hilbert space of real-valued functions on $\mathcal{X}$ such that for each $x \in \mathcal{X}$, the evaluation functional $L_x : \mathbb{H} \to \mathbb{R}$ is bounded (i.e., there exists some $M < \infty$ such that $|L_x(f)| \leq M \|f\|_{\mathbb{H}}$ for all $f \in \mathbb{H}$).

When L_x is a bounded linear functional, the Riesz representation (Theorem 12.1) implies that there must exist some element R_x of the Hilbert space $\mathbb{H}$ such that

$$f(x) \; = \; L_x(f) = \langle f, \, R_x \rangle_{\mathbb{H}} \quad \text{for all } f \in \mathbb{H}. \tag{12.2}$$

This element of $\mathbb{H}$ is known as the *representer of evaluation* at $x \in \mathcal{X}$.

The boundedness of R_x has a very important consequence: in particular, it ensures that convergence of a sequence of functions in an RKHS implies pointwise convergence. Indeed, if $f_n \to f^*$ in the Hilbert space norm, then for any $x \in \mathcal{X}$, we have

$$\big|f_n(x) - f^*(x)\big| = \big|\langle R_x, \, f_n - f^* \rangle_{\mathbb{H}}\big| \; \leq \; \|R_x\|_{\mathbb{H}} \, \|f_n - f^*\|_{\mathbb{H}} \; \to 0, \tag{12.3}$$

where we have applied the Cauchy-Schwarz inequality. This property is not shared by an arbitrary Hilbert space, with $L^2[0,1]$ being one case where this property fails (see Example 12.4).

12.2.2 Some examples

In this section, we discuss some examples of Hilbert spaces, considering both those that are reproducing kernel Hilbert spaces, and some that are not. Let us begin with a simple example of an RKHS.

Example 12.3 (Linear functions on $\mathbb{R}^m$)**.** We start with the simplest example of an RKHS, namely the set of all linear functions on $\mathbb{R}^m$. Any such function has the form $f_\beta(\cdot) = \langle \cdot, \, \beta \rangle$ for some vector $\beta \in \mathbb{R}^m$, and the set of all such functions forms a vector space. We can define an inner product on this function space in the obvious way—namely, $\langle f_\beta, f_{\widetilde{\beta}}\rangle_{\mathbb{H}} := \langle \beta, \widetilde{\beta}\rangle$—and the completeness of this inner product space follows from the completeness of $\mathbb{R}^m$. Let us now verify the boundedness of the evaluation functional. For any $x \in \mathbb{R}^m$ and $f_\beta \in \mathbb{H}$, the Cauchy-Schwarz inequality on $\mathbb{R}^m$ implies that

$$|L_x(f_\beta)| = |\langle x, \beta\rangle| \;\leq\; \|x\|_2 \, \|\beta\|_2.$$

By definition of our inner product, we have $\|f_\beta\|_{\mathbb{H}} = \|\beta\|_2$, so that we have shown that $|L_x(f_\beta)| \leq \|x\|_2 \, \|f_\beta\|_{\mathbb{H}}$. Consequently, the evaluation functional is bounded. Finally, let us verify that for any $x \in \mathbb{R}^m$, the representer of evaluation R_x is the function $f_x(\cdot) = \langle \cdot, x\rangle$. By the definition of our inner product $\langle \cdot, \cdot\rangle_{\mathbb{H}}$, we have

$$\langle f_\beta, f_x\rangle_{\mathbb{H}} = \langle \beta, x\rangle \;=\; f_\beta(x), \quad \text{valid for any } f_\beta \in \mathbb{H},$$

which provides an explicit demonstration of the Riesz representation (12.2) of the evaluation functional L_x. ♣

We now turn to an infinite-dimensional Hilbert space that is *not* an RKHS.

Example 12.4 (The space $L^2[0,1]$ is not an RKHS)**.** Consider the sequence of functions $f_n(x) = x^n$ for $n = 1, 2, \ldots$. Since $\int_0^1 f_n^2(x)dx = \frac{1}{2n+1}$, this sequence is contained in $L^2[0,1]$, and moreover $\|f_n\|_{L^2[0,1]} \to 0$. However, $f_n(1) = 1$ for all $n = 1, 2, \ldots$, so that this norm convergence does not imply pointwise convergence. Thus, if $L^2[0,1]$ were an RKHS, then this would contradict inequality (12.3). More abstractly, we could argue directly that $L^2[0,1]$ cannot be an RKHS, since it actually consists of equivalence classes of functions, where we identify any pair of functions that differ only on a set of Lebesgue measure zero. Consequently, elements of $L^2[0,1]$ are not defined in a pointwise sense.

An alternative way to see that $L^2[0,1]$ is not an RKHS is to ask whether it is possible to find functions a family of functions $\{R_x \in L^2[0,1],\ x \in [0,1]\}$ such that

$$\int_0^1 f(y) R_x(y) dy = f(x) \qquad \text{for all } f \in L^2[0,1].$$

This identity will hold if we define R_x to be a "delta-function"—that is, infinite at x and zero elsewhere. However, such objects certainly do not belong to $L^2[0,1]$, and exist only in the sense of generalized functions. ♣

Although $L^2[0,1]$ itself is not an RKHS, we can obtain an RKHS by imposing further restrictions on our functions. One way to do so is by imposing constraints on functions and their derivatives. The *Sobolev spaces* form an important class that arise in this way: the following example describes a first-order Sobolev space that is an RKHS.

Example 12.5 (A simple Sobolev space)**.** A function f over $[0,1]$ is said to be *absolutely continuous* if its derivative f' exists almost everywhere and is Lebesgue integrable, and we have $f(x) = f(0) + \int_0^x f'(z)dz$ for all $x \in [0,1]$. Now consider the set of functions

$$\mathbb{H}^1[0,1] := \big\{ f : [0,1] \to \mathbb{R} \mid f(0) = 0, \text{ and } f \text{ is absolutely continuous with } f' \in L^2[0,1] \big\}. \tag{12.4}$$

We define an inner product on this space via $\langle f,\, g \rangle_{\mathbb{H}^1} := \int_0^1 f'(z)g'(z)dz$, and claim that the resulting Hilbert space is an RKHS. In order to verify this claim, we need to exhibit a a representer of evaluation: for any $x \in [0,1]$, consider the function $R_x(z) = \min\{x, z\}$. It is differentiable at every point $z \in [0,1] \backslash \{x\}$, and we have $R_x'(z) = \mathbb{I}_{[0,x]}(z)$. Moreover, for any $z \in [0,1]$, it is easy to verify that

$$\min\{x, z\} = \int_0^z \mathbb{I}_{[0,x]}(u)du,$$

so that R_x is absolutely continuous by definition. Since $R_x(0) = 0$, we conclude that R_x is an element of $\mathbb{H}^1[0,1]$. Finally, to verify that R_x is the representer of evaluation, we calculate

$$\langle f,\, R_x \rangle_{\mathbb{H}^1} = \int_0^1 f'(z)R_x'(z)dz \;=\; \int_0^x f'(z)dz \;=\; f(x),$$

where the final equality uses the fundamental theorem of calculus. ♣

Another standard way in which to generate reproducing kernel Hilbert spaces is via some type of basis expansion.

Example 12.6 (RKHS via sinusoidal Fourier expansion)**.** Define the sinusoidal Fourier basis functions $\phi_j(x) := \sin\big(\frac{(2j-1)\pi x}{2}\big)$ for $j \in \mathbb{N} := \{1, 2, \ldots\}$. By construction, we have $\int_0^1 \phi_j(x)dx = 0$ for all $j \in \mathbb{N}$, and

$$\int_0^1 \phi_j(x)\phi_k(x)dx = \begin{cases} 1 & \text{if } j = k \\ 0 & \text{otherwise.} \end{cases}$$

Consequently, the functions $(\phi_j)_{j=1}^\infty$ are orthonormal within $L^2[0,1]$. We define a class of functions in terms of expansions of the form $f = \sum_{j=1}^\infty a_j \phi_j$, for a suitably chosen sequence of coefficients $(a_j)_{j=1}^\infty$. In particular, given a nonnegative sequence $\mu_1 \geq \mu_2 \geq \mu_3 \geq \ldots \geq 0$ such that $\sum_{j=1}^\infty \mu_j < \infty$, let us consider the function class

$$\mathbb{H} := \Big\{ f = \sum_{j=1}^\infty a_j \phi_j \mid \sum_{j=1}^\infty a_j^2 < \infty,\, \sum_{j=1}^\infty \frac{a_j^2}{\mu_j} < \infty \Big\}. \tag{12.5}$$

(If $\mu_j = 0$ for some j, then we interpret the constraint to mean that $a_j = 0$.) Given two functions in $\mathbb{H}$, say $f = \sum_{j=1}^{\infty} a_j \phi_j$ and $g = \sum_{j=1}^{\infty} b_j \phi_j$, we define their inner product $\langle f,\, g \rangle_{\mathbb{H}} := \sum_{j=1}^{\infty} a_j b_j / \mu_j$. It can be verified that $\mathbb{H}$ is a Hilbert space using this inner product; moreover, we claim that it is in fact an RKHS.

For a given $x \in [0,1]$, define the function $R_x := \sum_{j=1}^{\infty} \widetilde{x}_j \phi_j$ where $\widetilde{x}_j := \mu_j \phi_j(x)$ for $j \in \mathbb{N}$. Since $|\phi_j(x)| \leq 1$ for all $x \in [0,1]$ and $j \in \mathbb{N}$, we have

$$\|R_x\|^2_{L^2[0,1]} = \sum_{j=1}^{\infty} \widetilde{x}_j^2 \; = \; \sum_{j=1}^{\infty} \mu_j^2 \phi_j^2(x) \; \leq \; \sum_{j=1}^{\infty} \mu_j^2 < \infty,$$

where the final inequality uses the fact that $\sum_{j=1}^{\infty} \mu_j^2 \leq \big(\sum_{j=1}^{\infty} \mu_j \big)^2$. Similarly, we have

$$\|R_x\|^2_{\mathbb{H}} = \sum_{j=1}^{\infty} \widetilde{x}_j^2 / \mu_j \; = \; \sum_{j=1}^{\infty} \mu_j \phi_j(x) < \infty,$$

showing that $R_x \in \mathbb{H}$. Finally, the representer property is easily checked, since for any $f = \sum_{j=1}^{\infty} a_j \phi_j \in \mathbb{H}$, we have

$$\langle f,\, R_x \rangle_{\mathbb{H}} = \sum_{j=1}^{\infty} \frac{a_j \mu_j \phi_j(x)}{\mu_j} \; = \; \sum_{j=1}^{\infty} a_j \phi_j(x) \; = \; f(x).$$

♣

Although it might not be obvious at this point, it turns out that—for an appropriate choice of the weights $\{\mu_j\}_{j=1}^{\infty}$—the first-order Sobolev space from Example 12.5 is an instance of the sinusoidal basis RKHS just defined. More generally, as will be clarified later, if we allow for arbitrary basis functions (generalizing the sinusoids), then Example 12.6 is in a certain sense generic: a large class of RKHSs can be represented in terms of a suitable orthonormal basis and weight sequence $(\mu_j)_{j=1}^{\infty}$. We return to this connection in later sections.

Let us now turn to some higher-order generalizations of the first-order Sobolev space from Example 12.5.

Example 12.7 (Higher-order Sobolev spaces and smoothing splines)**.** For some fixed integer $\alpha \geq 1$, consider the class $\mathbb{H}^{\alpha}[0,1]$ of real-valued functions on $[0,1]$ that are α-times differentiable (almost everywhere), with the α-derivative $f^{(\alpha)}$ being Lebesgue integrable, and such that $f(0) = f^{(1)}(0) = \cdots = f^{(\alpha-1)}(0) = 0$. (Here $f^{(k)}$ denotes the k^{th} order derivative of f.) We may define an inner product on this space via

$$\langle f,\, g \rangle_{\mathbb{H}} := \int_0^1 f^{(\alpha)}(z) g^{(\alpha)}(z)\, dz. \tag{12.6}$$

Note that this set-up generalizes Example 12.5, which corresponds to the case $\alpha = 1$.

We now claim that this inner product defines an RKHS, and more specifically, that the representer of evaluation is given by

$$R_x(y) = \int_0^1 \frac{(x-z)_+^{\alpha-1}}{(\alpha-1)!} \frac{(y-z)_+^{\alpha-1}}{(\alpha-1)!} dz,$$

where $(t)_+ := \max\{0, t\}$. Note that R_x is α-times differentiable almost everywhere on $[0,1]$ with $R_x^{(\alpha)}(y) = (x-y)_+^{\alpha-1}/(\alpha-1)!$. To verify that R_x acts as the representer of evaluation, recall that any function $f : [0,1] \to \mathbb{R}$ that is α-times differentiable almost everywhere has the Taylor series expansion

$$f(x) = \sum_{\ell=0}^{\alpha-1} f^{(\ell)}(0) \frac{x^\ell}{\ell!} + \int_0^1 f^{(\alpha)}(z) \frac{(x-z)_+^{\alpha-1}}{(\alpha-1)!} \, dz. \tag{12.7}$$

Using the previously mentioned properties of R_x and the definition (12.6) of the inner product, we obtain

$$\langle R_x, \, f \rangle_{\mathbb{H}} = \int_0^1 f^{(\alpha)}(z) \frac{(x-z)_+^{\alpha-1}}{(\alpha-1)!} dz \; = \; f(x),$$

where the final equality uses the Taylor series expansion (12.7), and the fact that the first $\alpha - 1$ derivatives of f vanish at 0.

In Example 12.21 to follow, we show how to augment the Hilbert space so as to remove the constraint on the first $\alpha - 1$ derivatives of the functions f. ♣

■ 12.3 Kernel functions

In this section, we turn to the connection between RKHSs and the notion of a positive semidefinite kernel function. These kernel functions are a natural generalization of the idea of a positive semidefinite matrix, and are defined as follows.

Definition 12.4 (Positive semidefinite kernel function)**.** A symmetric bivariate function $\mathcal{K} : \mathcal{X} \times \mathcal{X} \to [0, \infty)$ is positive semidefinite (PSD) if for all integers $n \geq 1$ and elements $\{x_i\}_{i=1}^n \subset \mathcal{X}$, the $n \times n$ matrix with elements $\mathbf{K}_{ij} := \mathcal{K}(x_i, \, x_j)$ is positive semidefinite.

This notion is best understood via some examples.

Example 12.8 (Linear kernels)**.** When $\mathcal{X} = \mathbb{R}^d$, we can define the linear kernel function $\mathcal{K}(x, \, x') := \langle x, \, x' \rangle$. It is clearly a symmetric function of its arguments. In order to verify the positive semidefiniteness, let $\{x_i\}_{i=1}^n$ be an arbitrary collection of points in $\mathbb{R}^d$, and consider the matrix $\mathbf{K} \in \mathbb{R}^{n \times n}$ with entries $K_{ij} = \langle x_i, \, x_j \rangle$. For any real vector

$\alpha \in \mathbb{R}^n$, we have

$$\alpha^T \mathbf{K} \alpha = \sum_{i,j=1}^{n} \alpha_i \alpha_j \langle x_i, \, x_j \rangle \; = \; \Big\| \sum_{i=1}^{n} a_i x_i \Big\|_2^2 \geq 0.$$

Since $n \in \mathbb{N}$, $\{x_i\}_{i=1}^n$, and $\alpha \in \mathbb{R}^n$ were all arbitrary, we conclude that $\mathcal{K}$ is positive semidefinite. ♣

Example 12.9 (Polynomial kernels)**.** A natural generalization of the linear kernel is the *homogeneous polynomial kernel* $\mathcal{K}(x, \, x') = (\langle x, \, x' \rangle)^m$ of degree $m \geq 2$. Let us demonstrate the positive semidefiniteness of this function in the special case $m = 2$. Note that we have

$$\mathcal{K}(x, \, x') = \big(\sum_{j=1}^{d} x_j x_j' \big)^2 \; = \; \sum_{j=1}^{d} x_j^2 (x_j')^2 + 2 \sum_{i<j} x_i x_j (x_i' x_j').$$

Let us define a mapping $\Phi : \mathbb{R}^d \to \mathbb{R}^D$ where $D = d + \binom{d}{2}$, in particular with entries

$$\Phi(x) = \begin{bmatrix} x_j^2, \; j = 1, 2, \ldots, d \\ \sqrt{2} x_i x_j, \qquad\qquad i < j \end{bmatrix}, \tag{12.8}$$

corresponding to all polynomials of degree two in $(x_1, \ldots, x_d)$. With this definition, we see that $\mathcal{K}$ can be expressed as a Gram matrix—namely, $\mathcal{K}(x, \, x') = \langle \Phi(x), \, \Phi(x') \rangle_{\mathbb{R}^D}$. Following the same argument as Exercise (12.8), it is straightforward to verify that this Gram representation ensures that $\mathcal{K}$ must be positive semidefinite. As a side comment, we note that the mapping $x \mapsto \Phi(x)$ is often referred to as the *feature mapping* for the polynomial kernel, since it captures the sense in which the kernel function embeds the original data into a higher-dimensional space.

An extension of the homogeneous polynomial kernel is the *inhomogeneous polynomial kernel* $\mathcal{K}(x, \, x') = \big(1 + \langle x, \, x' \rangle\big)^m$, which is based on all polynomials of degree m or less. We leave it as an exercise for the reader to verify that it is also a positive semidefinite kernel function.

♣

The preceding examples provided some particular instances of kernels, and used Gram matrix constructions to verify the positive semidefiniteness. At their heart lies a generic way of constructing a positive semidefinite kernel function from any RKHS, which we now describe.

Example 12.10 (PSD kernel from representer of evaluation)**.** The representers of evaluation $\{R_x\}_{x \in \mathbb{H}}$ associated with any RKHS can be used to define a positive semidefinite kernel function. In particular, let us define a bivariate function $\mathcal{K} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ via

$\mathcal{K}(x, x') := \langle R_x, R_{x'} \rangle_{\mathbb{H}}$. Symmetry of the inner product ensures that $\mathcal{K}$ is a symmetric function, so that it remains to show that $\mathcal{K}$ is positive semidefinite. For any $n \geq 1$, let $\{x_i\}_{i=1}^n \subset \mathcal{X}$ be an arbitrary collection of points, and consider the $n \times n$ matrix with elements $K_{ij} = \mathcal{K}(x_i, x_j)$. For an arbitrary vector $\alpha \in \mathbb{R}^n$, we have

$$\alpha^T \mathbf{K} \alpha = \sum_{j,k=1}^n \alpha_j \alpha_k \mathcal{K}(x_j, x_k) \; = \; \langle \sum_{j=1}^n \alpha_j R_{x_j}, \sum_{j=1}^n \alpha_j R_{x_j} \rangle_{\mathbb{H}} \; = \; \| \sum_{j=1}^n \alpha_j R_{x_j} \|_{\mathbb{H}}^2 \; \geq \; 0,$$

which proves the positive semidefiniteness. For any $x \in \mathbb{H}$, the object $\mathcal{K}(\cdot, x)$ can be considered as an element of our Hilbert space. Indeed, it can be identified with R_x, since

$$\langle \mathcal{K}(\cdot, x), \mathcal{K}(\cdot, x) \rangle_{\mathbb{H}} \; = \; \mathcal{K}(x, x) = \langle R_x, \mathcal{K}(\cdot, x) \rangle_{\mathbb{H}}$$

for all $x \in \mathcal{X}$. Consequently, the function $\mathcal{K}(\cdot, x)$ is said to satisfy the *reproducing kernel property*, namely

$$\langle \mathcal{K}(\cdot, x), f \rangle_{\mathbb{H}} = f(x) \qquad \text{for all } f \in \mathbb{H}. \tag{12.9}$$

Thus, we have shown that any RKHS can be equipped with a symmetric positive semidefinite kernel satisfying the reproducing property (12.9). In Exercise 12.4, we show that the reproducing kernel of an RKHS must be unique. ♣

The preceding example illustrates one direction of a fundamental correspondence between the set of all RKHSs and the set of positive semidefinite kernel functions. In the other direction, given a positive semidefinite kernel function, we can define an associated Hilbert space of functions by considering all expansions of the form

$$f(\cdot) := \sum_{i=1}^n \alpha_i \, \mathcal{K}(\cdot, x_i),$$

where $n \in \mathbb{N}$ is arbitrary, and we are also free to choose the coefficient vector $\alpha \in \mathbb{R}^n$ and the sequence $\{x_i\}_{i=1}^n \subset \mathcal{X}$. In order to make such a set of functions into a Hilbert space, we need to define an inner product (and hence a Hilbert norm), and also take the completion of the space (by adjoining to it all possible functions that are obtained as limits of Cauchy sequences). This argument is made more precise in the proof of the following correspondence result:

Theorem 12.2. Given any reproducing kernel Hilbert space $\mathbb{H}$ of functions $f : \mathcal{X} \to \mathbb{R}$, there exists a unique positive semidefinite kernel function $\mathcal{K} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. Conversely, given any positive semidefinite kernel function $\mathcal{K}$, we can define an RKHS in which $\mathcal{K}$ acts as the representer of evaluation.

Proof. In Example 12.10, we showed how the representers $\{R_x\}_{x \in \mathcal{X}}$ induce a positive semidefinite kernel function $\mathcal{K}$. Combined with the uniqueness shown in Exercise 12.4, we conclude that any RKHS is associated with a unique reproducing kernel.

In the other direction, suppose that $\mathcal{K}$ is a positive semidefinite function on $\mathcal{X} \times \mathcal{X}$. Consider the space $\widetilde{\mathbb{H}}$ of functions of the form $f(\cdot) = \sum_{j=1}^n \alpha_j \mathcal{K}(\cdot,\, x_j)$ for some set of points $\{x_j\}_{j=1}^n \subset \mathcal{X}$ with $n \geq 1$, and some weight vector $\alpha \in \mathbb{R}^n$. This set of functions forms a vector space under the usual definitions of function addition and scalar multiplication. Given any $f, \bar{f} \in \widetilde{\mathbb{H}}$—say of the form $f(\cdot) = \sum_{j=1}^n \alpha_j \mathcal{K}(\cdot,\, x_j)$ and $\bar{f}(\cdot) = \sum_{k=1}^{\bar{n}} \bar{\alpha}_k \mathcal{K}(\cdot,\, \bar{x}_k)$—we can define their inner product

$$\langle f,\, \bar{f} \rangle_{\widetilde{\mathbb{H}}} := \sum_{j=1}^{n} \sum_{k=1}^{\bar{n}} \alpha_j \bar{\alpha}_k \mathcal{K}(x_j,\, \bar{x}_k).$$

Clearly, this definition satisfies conditions (12.1a) and (12.1c) of an inner product; it remains to verify the condition (12.1b). The positive semidefiniteness of $\mathcal{K}$ implies that $\|f\|_{\widetilde{\mathbb{H}}^2} = \langle f,\, f \rangle_{\widetilde{\mathbb{H}}} \geq 0$ for all f, so we need only show that $\|f\|_{\widetilde{\mathbb{H}}}^2 = 0$ if and only if $f = 0$. Consider a function of the form $f(\cdot) = \sum_{i=1}^n a_i \mathcal{K}(\cdot,\, x_i)$, and suppose that $\langle f,\, f \rangle_{\widetilde{\mathbb{H}}} = \sum_{i,j=1}^n \alpha_i \alpha_j \mathcal{K}(x_j,\, x_i) = 0$. We must then show that $f = 0$, or equivalently that $f(x) = \sum_{i=1}^n \alpha_i \mathcal{K}(x,\, x_i) = 0$ for all $x \in \mathcal{X}$. Let $(a, x) \in \mathbb{R} \times \mathcal{X}$ be arbitrary, and note that by the positive semidefiniteness of $\mathcal{K}$, we have

$$0 \;\leq\; \|a\mathcal{K}(\cdot,\, x) + \sum_{i=1}^{n} \alpha_i \mathcal{K}(\cdot,\, x_i)\|_{\mathbb{H}}^2 = a^2 \mathcal{K}(x,\, x) + 2a \sum_{i=1}^{n} \alpha_i \mathcal{K}(x,\, x_i)$$

Since $\mathcal{K}(x,\, x) \geq 0$ and $a \in \mathbb{R}$ is arbitrary, we must have $\sum_{i=1}^n \alpha_i \mathcal{K}(x,\, x_i) = 0$, as claimed. Thus, we have shown that the pair $(\widetilde{\mathbb{H}}, \langle \cdot,\, \cdot \rangle_{\widetilde{\mathbb{H}}})$ is an inner product space.

It remains to extend $\widetilde{\mathbb{H}}$ to a complete inner product space—that is, a Hilbert space—with the given reproducing kernel. If $(f_n)_{n=1}^\infty$ is a Cauchy sequence in $\widetilde{\mathbb{H}}$, then for each $x \in \mathcal{X}$, the sequence $\big(f_n(x)\big)_{n=1}^\infty$ is Cauchy in $\mathbb{R}$, and so must converge to some real number. We can thus define the pointwise limit function $f(x) := \lim_{n \to \infty} f_n(x)$, and we let $\mathbb{H}$ be the completion of $\widetilde{\mathbb{H}}$ by these objects. We define the norm of the limit function f as $\|f\|_{\mathbb{H}} := \lim_{n \to \infty} \|f_n\|_{\widetilde{\mathbb{H}}}$.

To verify that this definition is sensible, we need to show that for any Cauchy sequence $(g_n)_{n=1}^\infty$ in $\widetilde{\mathbb{H}}$ such that $\lim\limits_{n \to \infty} g_n(x) = 0$ for all $x \in \mathcal{X}$, we also have $\lim\limits_{n \to \infty} \|g_n\|_{\widetilde{\mathbb{H}}} = 0$. Taking subsequences as necessary, suppose that $\lim_{n \to \infty} \|g_n\|_{\widetilde{\mathbb{H}}}^2 = 2\epsilon > 0$, so that for n, m sufficiently large, we have $\|g_n\|_{\widetilde{\mathbb{H}}}^2 \geq \epsilon$ and $\|g_m\|_{\widetilde{\mathbb{H}}}^2 > \epsilon$. Since the sequence $(g_n)_{n=1}^\infty$ is Cauchy, we also have $\|g_n - g_m\|_{\widetilde{\mathbb{H}}} < \epsilon/2$ for n, m sufficiently large. Now since $g_m \in \widetilde{\mathbb{H}}$, we can write $g_m = \sum_{i=1}^{N_m} \alpha_i R_{x_i}$, for some finite positive integer N_m and vector $\alpha \in \mathbb{R}^{N_m}$. By the reproducing property, we have

$$\langle g_m,\, g_n \rangle_{\widetilde{\mathbb{H}}} = \sum_{i=1}^{N_m} \alpha_i g_n(x_i) \to 0 \quad \text{as } n \to +\infty,$$

since $g_n(x) \to 0$ for each fixed x. Hence for n sufficiently large, we can ensure that $|\langle g_m,\, g_n \rangle_{\widetilde{\mathbb{H}}}| \leq \epsilon/2$. Putting together the pieces, we have

$$\|g_n - g_m\|_{\widetilde{\mathbb{H}}} = \|g_n\|^2_{\widetilde{\mathbb{H}}} + \|g_m\|^2_{\widetilde{\mathbb{H}}} - 2\langle g_n,\, g_m \rangle_{\widetilde{\mathbb{H}}} \;\geq\; \epsilon + \epsilon - \epsilon \;=\; \epsilon$$

But this contradicts the fact that $\|g_n - g_m\|_{\widetilde{\mathbb{H}}} \leq \epsilon/2$.

Thus, the norm that we have defined is sensible, and it can be used to define an inner product on $\mathbb{H}$ via the polarization identity

$$\langle f,\, g \rangle_{\mathbb{H}} := \frac{1}{2}\big\{\|f + g\|^2_{\mathbb{H}} - \|f\|^2_{\mathbb{H}} + \|g\|^2_{\mathbb{H}}\big\}.$$

With this definition, it can be verified that $\langle \mathcal{K}(\cdot,\, x),\, f \rangle_{\mathbb{H}} = f(x)$ for all $f \in \mathbb{H}$, so that $\mathcal{K}(\cdot,\, x)$ is again reproducing over $\mathbb{H}$.

Finally, let us verify uniqueness. Suppose that $\mathbb{G}$ is some other Hilbert space with $\mathcal{K}$ as its reproducing kernel, so that $\mathcal{K}(\cdot,\, x) \in \mathbb{G}$ for all $x \in \mathcal{X}$. Since $\mathbb{G}$ is complete and closed under linear operations, we must have $\mathbb{H} \subseteq \mathbb{G}$. Consequently, $\mathbb{H}$ is a closed linear subspace of $\mathbb{G}$, so that we can write $\mathbb{G} = \mathbb{H} \oplus \mathbb{H}^\perp$. Let $g \in \mathbb{H}^\perp$ be arbitrary, and note that $\mathcal{K}(\cdot,\, x) \in \mathbb{H}$. By orthogonality, we must have $0 = \langle \mathcal{K}(\cdot,\, x),\, g \rangle_{\mathbb{G}} = g(x)$, from which we conclude that $\mathbb{H}^\perp = \{0\}$, and hence that $\mathbb{H} = \mathbb{G}$ as claimed.

□

Example 12.11 (First-order Sobolev space, or linear splines)**.** In this example, we show that the kernel $\mathcal{K} : [0,1] \times [0,1] \to \mathbb{R}$ given by $\mathcal{K}(x,\, z) = \min\{x, z\}$ is positive semi-definite, and establish a link to the first-order Sobolev space from Example 12.5. In particular, recalling the indicator function $R'_x(z) = \mathbb{I}_{[0,x]}(z)$, observe that

$$\langle \mathbb{I}_{[0,x]},\, \mathbb{I}_{[0,z]} \rangle_{L^2[0,1]} \;=\; \int_0^1 \mathbb{I}_{[0,x]}(u)\; \mathbb{I}_{[0,z]}(u)\, du = \int_0^{\min\{x,z\}} (1)\, du \;=\; \mathcal{K}(x,\, z).$$

Consequently, we have demonstrated a Gram representation for the kernel, based on the representers of evaluation for the first-order Sobolev space $\mathbb{H}^1[0,1]$. We conclude that $\mathcal{K}(x,\, z) = \min\{x, z\}$ is the unique positive semidefinite kernel function associated with this first-order Sobolev space. ♣

Example 12.12 (Sinusoidal basis expansion)**.** Recall the RKHS based on an orthogonal sinusoidal basis expansion, previously introduced in Example 12.6. We claim that the associated kernel takes the form

$$\mathcal{K}(x,\, z) = \sum_{j=1}^{\infty} \mu_j \phi_j(x) \phi_j(z).$$

Recall that we previously showed that the representer of evaluation has the form $R_x = \sum_{j=1}^{\infty} \widetilde{\alpha}_j \phi_j$, where $\widetilde{\alpha}_j = \mu_j \phi_j(x)$. Similarly, we write $R_z = \sum_{j=1}^{\infty} \widetilde{\beta}_j \phi_j$, where $\widetilde{\beta}_j = \mu_j \phi_j(z)$. Using our previous definition of the Hilbert inner product, we compute

$$\langle R_x,\, R_z \rangle_{\mathbb{H}} = \sum_{j=1}^{\infty} \frac{\widetilde{\alpha}_j \, \widetilde{\beta}_j}{\mu_j} \; = \; \sum_{j=1}^{\infty} \frac{\mu_j^2 \phi_j(x) \phi_j(z)}{\mu_j} \; = \; \sum_{j=1}^{\infty} \mu_j \phi_j(x) \phi_j(z),$$

so that the claim follows as a special case of the construction of Example 12.10.

♣

■ 12.4 Mercer's theorem and its consequences

We now turn to a useful representation of a broad class of positive semidefinite kernel functions, namely in terms of their eigenfunctions. Recall from classical linear algebra that any positive semidefinite matrix has an orthonormal basis of eigenvectors, and the associated eigenvalues are non-negative. The abstract version of Mercer's theorem generalizes this decomposition to positive semidefinite kernel functions.

Let $\mathbb{P}$ be a non-negative measure over a compact metric space $\mathcal{X}$, and consider the function class $L^2(\mathcal{X}; \mathbb{P})$ with the usual norm

$$\|f\|_{L^2(\mathcal{X};\mathbb{P})}^2 = \int_{\mathcal{X}} f^2(x) d\mathbb{P}(x).$$

Since the measure $\mathbb{P}$ remains fixed throughout, we frequently adopt the shorthand notation $L^2(\mathcal{X})$, or even just L^2 for this norm. Given a symmetric PSD kernel function $\mathcal{K} : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ that is continuous, we can define a linear operator $T_{\mathcal{K}}$ on $L^2(\mathcal{X})$ via

$$T_{\mathcal{K}}(f)(x) := \int_{\mathcal{X}} \mathcal{K}(x,\, z) f(z) d\mathbb{P}(z). \tag{12.10}$$

We assume that the kernel function satisfies the condition

$$\int_{\mathcal{X} \times \mathcal{X}} \mathcal{K}^2(x,\, z) d\mathbb{P}(x) d\mathbb{P}(z) < \infty, \tag{12.11}$$

which ensures that $T_{\mathcal{K}}$ is a bounded linear operator on $L^2(\mathcal{X})$. Indeed, we have

$$\begin{aligned}\|T_{\mathcal{K}}(f)\|^2_{L^2(\mathcal{X})} &= \int_{\mathcal{X}} \Big(\int_{\mathcal{X}} \mathcal{K}(x,\, y) f(x) d\mathbb{P}(x) \Big)^2 d\mathbb{P}(y) \\ &\leq \|f\|^2_{L^2(\mathcal{X})} \int_{\mathcal{X}\times\mathcal{X}} \mathcal{K}^2(x,y) d\mathbb{P}(x) d\mathbb{P}(y),\end{aligned}$$

where the upper bound follows by the Cauchy-Schwarz inequality. Operators of this type are known as *Hilbert-Schmidt operators.*

Let us illustrate these definitions with some examples.

Example 12.13 (PSD matrices)**.** Let $\mathcal{X} = [d] := \{1, 2, \ldots, d\}$ be equipped with the Hamming metric, and let $\mathbb{P}(\{j\}) = 1$ for all $j \in \{1, 2, \ldots, d\}$ be the counting measure on this discrete space. In this case, any function $f : \mathcal{X} \to \mathbb{R}$ can be identified with the vector $(f(1), \ldots, f(d)) \in \mathbb{R}^d$, and a symmetric kernel function $\mathcal{K} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ can be identified with the symmetric $d \times d$ matrix $\mathbf{K}$ with entries $K_{ij} = \mathcal{K}(i,\, j)$. Consequently, the integral operator (12.10) reduces to ordinary matrix-vector multiplication

$$T_{\mathcal{K}}(f)(x) \;=\; \int_{\mathcal{X}} \mathcal{K}(x,\, z) f(z) d\mathbb{P}(z) = \sum_{z=1}^{d} \mathcal{K}(x,\, z) f(z).$$

Thus, in this special case, the assertion that $T_{\mathcal{K}}$ is a PSD operator is equivalent to asserting that the symmetric matrix $\mathbf{K} \in \mathbb{R}^{d\times d}$ is positive semidefinite. By standard linear algebra, we know that the matrix $\mathbf{K}$ has an orthonormal collection of eigenvectors, say $\{v_1, \ldots, v_d\}$, along with a set of non-negative eigenvalues $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_d$, such that

$$\mathbf{K} = \sum_{j=1}^{d} \mu_j v_j v_j^T. \tag{12.12}$$

Mercer's theorem, to be stated shortly, provides a substantial generalization of this decomposition to a general positive semidefinite kernel function. ♣

Example 12.14 (First-order Sobolev kernel)**.** Now suppose that $\mathcal{X} = [0, 1]$, and that $\mathbb{P}$ is the Lebesgue measure. Recalling the kernel function $\mathcal{K}(x,\, z) = \min\{x, z\}$, we have

$$T_{\mathcal{K}}(f)(x) = \int_0^1 \min\{x, z\} f(z) dz \;=\; \int_0^x z f(z) dz + \int_x^1 x f(z) dz.$$

We return to analyze this particular integral operator in Example 12.17. ♣

Having gained some intuition for the general notion of a kernel integral operator, we are now ready for the statement of the abstract Mercer's theorem.

Theorem 12.3 (Mercer's theorem)**.** Suppose that $\mathcal{X}$ is compact, the kernel function $\mathcal{K}$ is continuous and positive semidefinite, and satisfies condition (12.11). Then there exist a sequence of eigenfunctions $(\phi_j)_{j=1}^{\infty}$ that form an orthonormal basis of $L^2(\mathcal{X}; \mathbb{P})$, and an associated set of non-negative eigenvalues $(\mu_j)_{j=1}^{\infty}$ such that $T_{\mathcal{K}}(\phi_j) = \mu_j \phi_j$ for $j = 1, 2, \ldots$. Moreover, the kernel function can be represented as

$$\mathcal{K}(x,\, z) = \sum_{j=1}^{\infty} \mu_j \phi_j(x) \phi_j(z), \tag{12.13}$$

where the convergence of the infinite series holds uniformly.

Remarks: The original theorem proved by Mercer applied only to operators defined on $L^2([a, b])$ for some finite $a < b$. The more abstract version stated here follows as a consequence of more general results on the eigenvalues of compact operators on Hilbert spaces; we refer the reader to the bibliography section for references.

Among other consequences, Mercer's theorem provides intuition on how reproducing kernel Hilbert spaces can be viewed as providing a particular embedding of the function domain $\mathcal{X}$ into a subset of the sequence space $\ell^2(\mathbb{N})$. In particular, given the eigenfunctions and eigenvalues guaranteed by Mercer's theorem, we may define a mapping $\Phi : \mathcal{X} \rightarrow \ell^2(\mathbb{N})$ via

$$x \mapsto \Phi(x) := \big(\sqrt{\mu_1}\, \phi_1(x), \quad \sqrt{\mu_2}\, \phi_2(x), \quad \sqrt{\mu_3}\, \phi_3(x), \quad \ldots \big). \tag{12.14}$$

By construction, we have

$$\|\Phi(x)\|_{\ell^2(\mathbb{N})}^2 = \sum_{j=1}^{\infty} \mu_j \phi_j^2(x) \; = \; \mathcal{K}(x,\, x) < \infty$$

showing that the map $x \mapsto \Phi(x)$ is a type of (weighted) feature map that embeds the original vector into a subset of $\ell^2(\mathbb{N})$. Moreover, this feature map also provides an explicit inner product representation of the kernel over $\ell^2(\mathbb{N})$—namely

$$\langle \Phi(x),\, \Phi(z) \rangle_{\ell^2(\mathbb{N})} = \sum_{j=1}^{\infty} \mu_j\, \phi_j(x)\, \phi_j(z) \; = \; \mathcal{K}(x,\, z).$$

Let us illustrate Mercer's theorem by considering some examples:

Example 12.15 (Eigenfunctions for a symmetric PSD matrix)**.** As discussed in Example 12.13, a symmetric PSD matrix (of size $d \times d$) can be viewed as a kernel function on the space $[d] \times [d]$, where we recall the shorthand $[d] := \{1, 2, \ldots, d\}$. In this case, the eigenfunction $\phi_j : [d] \rightarrow \mathbb{R}$ can be identified with the d-vector $v_j := (\phi_j(1), \ldots, \phi_j(d))$. Thus, in this special case, the eigenvalue equation $T_{\mathcal{K}}(\phi_j) = \mu_j \phi_j$ is equivalent to asserting that $v_j \in \mathbb{R}^d$ is an eigenvector of the kernel matrix. Consequently, the decomposition (12.13) then reduces to the familiar statement that any symmetric PSD matrix has an orthonormal basis of eigenfunctions, with associated non-negative eigenvalues, as previously stated in equation (12.12). ♣

Example 12.16 (Eigenfunctions of a polynomial kernel)**.** Let us compute the eigenfunctions of the second-order polynomial kernel $\mathcal{K}(x, z) = (1 + xz)^2$ defined over the Cartesian product $[-1, 1] \times [-1, 1]$, where the unit interval is equipped with the Lebesgue measure. For any function $f : [-1, 1] \rightarrow \mathbb{R}$, we have

$$\begin{aligned}
\int_{-1}^{1} \mathcal{K}(x, z) f(z) dz &= \int_{-1}^{1} \big(1 + 2xz + x^2 z^2\big) f(z) dz \\
&= \Big\{ \int_{-1}^{1} f(z) dz \Big\} + \Big\{ 2 \int_{-1}^{1} z f(z) dz \Big\} x + \Big\{ \int_{-1}^{1} z^2 f(z) dz \Big\} x^2,
\end{aligned}$$

showing that any eigenfunction of the kernel integral operator must be a polynomial of degree at most two. Consequently, the eigenfunction problem can be reduced to an ordinary eigenvalue problem in terms of the coefficients in the expansion $f(x) = a_0 + a_1 x + a_2 x^2$. Following some simple algebra, we find that if f is an eigenfunction with eigenvalue μ, then these coefficients must satisfy the linear system

$$\begin{bmatrix} 2 & 0 & 2/3 \\ 0 & 4/3 & 0 \\ 2/3 & 0 & 2/5 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \mu \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix}.$$

Solving this ordinary eigensystem, we find the following eigenfunction/value pairs

$$\begin{aligned}
\phi_1(x) &= -0.9403 - 0.3404 x^2, & \text{with } \mu_1 &= 2.2414, \\
\phi_2(x) &= x, & \text{with } \mu_2 &= 1.3333, \\
\phi_3(x) &= -0.3404 + 0.9403 x^2, & \text{with } \mu_3 &= 0.1586.
\end{aligned}$$

♣

Example 12.17 (Eigenfunctions for a first-order Sobolev space)**.** In Example 12.5, we introduced the first-order Sobolev space $\mathbb{H}^1[0, 1]$. In Examples 12.11 and 12.14, we found that its kernel function takes the form $\mathcal{K}(x, z) = \min\{x, z\}$, and determined the form of the associated integral operator. Using this previous development, if $\phi : [0, 1] \rightarrow \mathbb{R}$ is an eigenfunction of $T_{\mathcal{K}}$ with eigenvalue $\mu \neq 0$, then it must satisfy the relation $T_{\mathcal{K}}(\phi) = \mu\phi$, or equivalently

$$\int_0^x z\phi(z)dz + \int_x^1 x\phi(z)dz \;=\; \mu\phi(x) \quad \text{for all } x \in [0,1].$$

Since this relation must hold for all $x \in [0,1]$, we may take derivatives with respect to x. Doing so twice yields the second-order differential equation $\mu\phi''(x) + \phi(x) = 0$. Combined with the boundary condition $\phi(0) = 0$, we obtain $\phi(x) = \sin(x/\sqrt{\mu})$ as potential eigenfunctions. Since we also have the boundary condition $\int_0^1 z\phi(z)dz = \mu\phi(1)$, we obtain that the eigenfunction/eigenvalue pairs are given by

$$\phi_j(t) = \sin\frac{(2j-1)\pi t}{2} \quad \text{and} \quad \mu_j = \big(\frac{2}{(2j-1)\,\pi}\big)^2 \quad \text{for } j = 1, 2, \ldots.$$

♣

Example 12.18 (Translation invariant kernels)**.** An important class of kernels have a translation-invariant form. In particular, given a function $\psi : [-1,1] \rightarrow \mathbb{R}$ that is even (meaning that $\psi(u) = \psi(-u)$ for all $u \in [-1,1]$), let us extend its domain to the real line by the periodic extension $\psi(u + 2k) = \psi(u)$ for all $u \in [-1,1]$ and integers $k \in \mathbb{Z}$.

Using this function, we may define a *translation-invariant* kernel on the Cartesian product space $[-1,1] \times [-1,1]$ via $\mathcal{K}(x,\, z) = \psi(x - z)$. Note that the evenness of ψ ensures that this kernel is symmetric. Moreover, the kernel integral operator takes the form

$$T_{\mathcal{K}}(f)(x) = \underbrace{\int_{-1}^{1} \psi(x-z)f(z)dz}_{\big(\psi * f\big)(x)},$$

and thus is a convolution operator.

A classical result from analysis is that the eigenfunctions of convolution operators are given by the Fourier basis; let us verify this fact here. We first show that the cosine functions $\phi_j(x) = \cos(\pi j x)$ for $j = 0, 1, 2, \ldots$ are eigenfunctions of the operator $T_{\mathcal{K}}$. Indeed, we have

$$T_{\mathcal{K}}(\phi_j)(x) \;=\; \int_{-1}^{1} \psi(x-z)\cos(\pi j z)dz = \int_{-1-x}^{1-x} \psi(-u)\cos(2\pi j(x+u))du,$$

where we have made the change of variable $u = z - x$. Note that the interval of integration $[-1-x, 1-x]$ is of length two, and since both $\psi(-u)$ and $\cos(2\pi(x+u))$ have period two, we can shift the interval of integration to $[-1,1]$. Combined with the evenness of ψ, we conclude that $T_{\mathcal{K}}(\phi_j)(x) = \int_{-1}^{1} \psi(u)\cos(2\pi j(x+u))du$. Using the elementary trigonometric identity

$$\cos(\pi j(x+u)) = \cos(\pi j x)\cos(\pi j u) - \sin(\pi j x)\sin(\pi j u),$$

we find that

$$\begin{aligned} T_{\mathcal{K}}(\phi_j)(x) &= \Big\{ \int_{-1}^{1} \psi(u)\cos(\pi j u) du \Big\} \cos(\pi j x) - \Big\{ \int_{-1}^{1} \psi(u)\sin(\pi j u) du \Big\} \sin(\pi j x) \\ &= c_j \cos(\pi j x) \end{aligned}$$

where $c_j = \int_{-1}^{1} \psi(u)\cos(\pi j u)du$ is the j^{th} cosine coefficient of ψ. In this calculation, we have used the evenness of ψ to argue that the integral with the sine function vanishes.

A similar argument shows that each of the sinusoids

$$\widetilde{\phi}_j(x) = \sin(j\pi x) \quad \text{for } j = 1, 2, \ldots$$

are also eigenfunctions with eigenvalue c_j. Since the functions $\{\phi_j,\ j = 0, 1, 2, \ldots\} \cup \{\widetilde{\phi}_j,\ j = 1, 2, \ldots\}$ form a complete orthogonal basis of $L^2[-1, 1]$, there are no other eigenfunctions that are not linear combinations of these functions. Consequently, by Mercer's theorem, the kernel function has the eigenexpansion

$$\mathcal{K}(x,\, z) = \sum_{j=0}^{\infty} c_j \big\{ \cos(\pi j x)\cos(\pi j z) + \sin(\pi j x)\sin(\pi j z) \big\} \;=\; \sum_{j=0}^{\infty} c_j \cos(\pi j(x - z)).$$

Noting that c_j are the (cosine) Fourier coefficients of ψ, we see that $\mathcal{K}$ is positive semidefinite if and only if $c_j \geq 0$ for $j = 0, 1, 2, \ldots$.

♣

Example 12.19 (Gaussian kernel)**.** Given a subset $\mathcal{X} \subseteq \mathbb{R}^d$, a popular kernel on the Cartesian product space $\mathcal{X} \times \mathcal{X}$ is the Gaussian kernel $\mathcal{K}(x,\, z) = \exp(-\frac{\|x-z\|_2^2}{2\sigma^2})$, where $\sigma > 0$ is a bandwidth parameter. To keep our calculations relatively simple, let us focus here on the univariate case $d = 1$, and let $\mathcal{X}$ be some compact interval of the real line. By a rescaling argument, we can restrict ourselves to the case $\mathcal{X} = [-1, 1]$, so that we are considering solutions to the integral equation

$$\int_{-1}^{1} e^{-\frac{(x-z)^2}{2\sigma^2}}\, \phi_j(z) dz = \mu_j \phi_j(x). \tag{12.15}$$

Note that this problem cannot be tackled by the methods of the previous example, since we are *not* performing the periodic extension of our function.[1] Nonetheless, the

[1] If we were to consider the periodically extended version, then the eigenvalues would be given by the cosine coefficients $c_j = \int_{-1}^{1} \exp(-\frac{u^2}{2\sigma^2})\, \cos(\pi j u)du$, with the cosine functions as eigenfunctions.

eigenvalues of the Gaussian integral operator are very closely related to the Fourier transform.

In the remainder of our development, let us consider a slightly more general integral equation. Given a bounded, continuous and even function $\Psi : \mathbb{R} \rightarrow [0, \infty)$, we may define its (real-valued) Fourier transform $\psi(u) = \int_{-\infty}^{\infty} \Psi(\omega) e^{-i\omega u} d\omega$, and use it to define a translation-invariant kernel via $\mathcal{K}(x, z) := \psi(x - z)$. We are then led to the integral equation

$$\int_{-1}^{1} \psi(x - z) \phi_j(z) dz = \mu_j \phi_j(x). \tag{12.16}$$

Classical theory on integral operators can be used to characterize the spectrum of this integral operator: more precisely, for any operator such that $\log \Psi(\omega) \asymp -\omega^{\alpha}$ for some $\alpha > 1$, then there is a constant c such that the eigenvalues $(\mu_j)_{j=1}^{\infty}$ associated with the integral equation (12.16) scale as $\mu_j \asymp e^{-cj \log j}$ as $j \rightarrow +\infty$. See the bibliographic section for further discussion of results of this type.

The Gaussian kernel is a special case of this set-up with $\Psi(\omega) = \exp(-\frac{\sigma^2 \omega^2}{2})$ and $\psi(u) = \exp(-\frac{u^2}{2\sigma^2})$. Applying the previous reasoning guarantees that the eigenvalues of the Gaussian kernel over a compact interval scale as $\mu_j \asymp \exp(-cj \log j)$ as $j \rightarrow +\infty$. We thus see that the Gaussian kernel class is relatively small, since its eigenvalues decay at exponential rate. (The reader should contrast this fast decay with the significantly slower $\mu_j \asymp j^{-2}$ decay rate of the first-order Sobolev class from Example 12.17.)

♣

An interesting consequence of Mercer's theorem is in showing how any RKHS with an eigendecomposition of the given form is isomorphic to a subset of $\ell^2(\mathbb{N})$, with its unit ball corresponding to an ellipse within this same sequence space.

Corollary 12.1. Consider an RKHS $\mathbb{H}$ satisfying the conditions of Mercer's theorem with associated eigenfunctions $(\phi_j)_{j=1}^{\infty}$ and non-negative eigenvalues $(\mu_j)_{j=1}^{\infty}$. Then any function $f \in \mathbb{H}$ can be written in the form $f = \sum_{j=1}^{\infty} \alpha_j \phi_j$ for a sequence of coefficients $(\alpha_j)_{j=1}^{\infty}$ such that

$$\|f\|_{L^2(\mathcal{X};\mathbb{P})}^2 = \sum_{j=1}^{\infty} \mu_j \alpha_j^2, \quad \text{and} \quad \|f\|_{\mathbb{H}}^2 = \sum_{j=1}^{\infty} \alpha_j^2.$$

Remarks: Equivalently, if we define $\beta_j := \sqrt{\mu_j}\alpha_j$, then we can write $f = \sum_{j=1}^\infty \beta_j \phi_j$ with

$$\|f\|^2_{L^2(\mathcal{X};\mathbb{P})} = \sum_{j=1}^\infty \beta_j^2, \quad \text{and} \quad \|f\|^2_{\mathbb{H}} = \sum_{j=1}^\infty \frac{\beta_j^2}{\mu_j},$$

where we interpret $\beta_j^2/\mu_j = 0$ as implying $\beta_j = 0$ for any index such that $\mu_j = 0$.

Proof. Without loss of generality, we assume that $\mu_j > 0$ for all $j \in \mathbb{N}$. (Otherwise, the same argument will apply with relevant summations truncated to the positive eigenvalues of the kernel function.) Since $(\phi_j)_{j=1}^\infty$ is an orthonormal basis of $L^2 \equiv L^2(\mathcal{X}; \mathbb{P})$ by assumption, any function $f \in \mathbb{H} \subset L^2$ can be expanded as $f = \sum_{j=1}^\infty a_j \phi_j$ where $\beta_j = \langle f,\, \phi_j \rangle_{L^2}$. By Parseval's theorem, we then have $\|f\|^2_{L^2} = \sum_{j=1}^\infty \beta_j^2$.

It remains to show that $\|f\|^2_{\mathbb{H}} = \sum_{j=1}^\infty \beta_j^2/\mu_j$. Since each ϕ_j is an eigenfunction of the kernel operator, it belongs to the image of the kernel operator, which is contained within the Hilbert space. Thus, each function ϕ_j belongs to the Hilbert space $\mathbb{H}$, and hence the reproducing property implies that $\phi_j(x) = \langle \phi_j,\, \mathcal{K}(\cdot,\, x)\rangle_{\mathbb{H}}$ for each $x \in \mathcal{X}$. Applying the expansion of the kernel function guaranteed by Mercer's theorem, we have

$$\phi_j(x) = \langle \phi_j,\, \sum_{j=1}^\infty \mu_j \phi_j \phi_j(x) \rangle_{\mathbb{H}} = \sum_{j=1}^\infty \mu_j \phi_j(x)\; \langle \phi_j,\, \phi_j \rangle_{\mathbb{H}}.$$

Now this relation holds for each $x \in \mathcal{X}$, and hence the linear independence of the eigenfunctions guarantees that

$$\langle \phi_j,\, \phi_j \rangle_{\mathbb{H}} = \frac{1}{\mu_j}, \quad \text{and} \quad \langle \phi_j,\, \phi_j \rangle_{\mathbb{H}} = 0 \quad \text{for all } j \neq j.$$

Combining these relations with linearity of the Hilbert inner product, we have

$$\|f\|^2_{\mathbb{H}} = \|\sum_{j=1}^\infty \beta_j \phi_j\|^2_{\mathbb{H}} = \sum_{j,k=1}^\infty \beta_j \beta_k \langle \phi_j,\, \phi_k \rangle_{\mathbb{H}} = \sum_{j=1}^\infty \frac{\beta_j^2}{\mu_j},$$

as claimed. □

An important consequence of Corollary 12.1 is that any separable RKHS satisfying the conditions of Mercer's theorem has a unit ball that is isomorphic to an *ellipsoid* in $\ell^2(\mathbb{N})$—in particular, any function f in the unit ball $\mathbb{B}_{\mathbb{H}}(1) = \big\{f \in \mathbb{H} \mid \|f\|^2_{\mathbb{H}} \leq 1\big\}$ can be identified with the sequence $\{\beta_j\}_{j=1}^n$ with elements $\beta_j := \langle f,\, \phi_j \rangle_{L^2(\mathcal{X};\mathbb{P})}$. As shown in the preceding proof, this sequence is guaranteed to belong to the infinite-dimensional ellipsoid

$$\mathcal{E} \;=\; \Big\{(\beta_j)_{j=1}^{\infty} \in \ell^2(\mathbb{N}) \mid \sum_{j=1}^{\infty} \frac{\beta_j^2}{\mu_j} \leq 1\Big\}. \tag{12.17}$$

We study the properties of such ellipsoids at more length in Chapters 13 and 14.

12.5 Operations on reproducing kernel Hilbert spaces

In this section, we describe a number of operations on reproducing kernel Hilbert spaces that allow us to build new spaces.

12.5.1 Sums of reproducing kernels

Given two Hilbert space $\mathbb{H}_1$ and $\mathbb{H}_2$ of functions defined on domains $\mathcal{X}_1$ and $\mathcal{X}_2$ respectively, consider the space

$$\mathbb{H}_1 + \mathbb{H}_2 := \big\{f_1 + f_2 \mid f_j \in \mathbb{H}_j,\; j = 1, 2\big\},$$

corresponding to the set of all functions obtained as sums of pairs of functions from the two spaces.

Proposition 12.1. Suppose that $\mathbb{H}_1$ and $\mathbb{H}_2$ are both RKHS's with kernels $\mathcal{K}_1$ and $\mathcal{K}_2$ respectively. Then the space $\mathbb{H} = \mathbb{H}_1 + \mathbb{H}_2$ with norm

$$\|f\|_{\mathbb{H}}^2 := \min_{\substack{f = f_1 + f_2 \\ f_1 \in \mathbb{H}_1, f_2 \in \mathbb{H}_2}} \big\{\|f_1\|_{\mathbb{H}_1}^2 + \|f_2\|_{\mathbb{H}_2}^2\big\} \tag{12.18}$$

is an RKHS with kernel $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2$.

Remark: This construction is particularly simple when $\mathbb{H}_1$ and $\mathbb{H}_2$ share only the 0 function, since any function $f \in \mathbb{H}$ can then be written as $f = f_1 + f_2$ for a unique pair (f_1, f_2), and hence $\|f\|_{\mathbb{H}}^2 = \|f_1\|_{\mathbb{H}_1}^2 + \|f_2\|_{\mathbb{H}_2}^2$. Let us illustrate the use of summation with some examples:

Example 12.20 (First-order Sobolev space and constant functions)**.** Consider the kernel functions on $[0,1] \times [0,1]$ given by $\mathcal{K}_1(x,z) = 1$ and $\mathcal{K}_2(x,z) = \min\{x,z\}$. They generate the reproducing kernel Hilbert spaces

$$\mathbb{H}_1 = \text{span}\{1\}, \quad \text{and} \quad \mathbb{H}_2 = \mathbb{H}^1[0,1],$$

where span$\{1\}$ is the set of all constant functions, and $\mathbb{H}^1[0,1]$ is the first-order Sobolev space from Example 12.5. Note that $\mathbb{H}_1 \cap \mathbb{H}_2 = \{0\}$, since $f(0) = 0$ for any element of $\mathbb{H}_2$. Consequently, the RKHS with kernel $\mathcal{K}(x,\, z) = 1 + \min\{x, z\}$ consists of all functions

$$\bar{\mathbb{H}}^1[0,1] =:= \big\{ f : [0,1] \to \mathbb{R} \mid f \text{ is absolutely continuous with } f' \in L^2[0,1] \big\},$$

equipped with the norm $\|f\|^2_{\bar{\mathbb{H}}^1[0,1]} = f^2(0) + \int_0^1 (f'(z))^2 dz$. ♣

As a continuation of the previous example, let us describe an extension of the higher-order Sobolev spaces from Example 12.7:

Example 12.21 (Extending higher-order Sobolev spaces)**.** For an integer $\alpha \geq 1$, consider the kernel functions on $[0,1] \times [0,1]$ given by

$$\mathcal{K}_1(x,z) = \sum_{\ell=0}^{\alpha-1} \frac{x^\ell}{\ell!} \frac{z^\ell}{\ell!} \quad \text{and} \quad \mathcal{K}_2(x,z) = \int_0^1 \frac{(x-z)_+^{\alpha-1}}{(\alpha-1)!} \frac{(y-z)_+^{\alpha-1}}{(\alpha-1)!} dz.$$

The first kernel generates an RKHS $\mathbb{H}_1$ of polynomials of degree $\alpha - 1$, whereas the second kernel generates the α-order Sobolev space $\mathbb{H}_2 = \mathbb{H}^\alpha[0,1]$ previously defined in Example 12.7.

Recall that any function $f \in \mathbb{H}^\alpha[0,1]$ satisfies the boundary conditions $f^{(\ell)}(0) = 0$ for $\ell = 0, 1, \ldots, \alpha - 1$, where $f^{(\ell)}$ denotes the ℓ^{th} order derivative. Consequently, we have $\mathbb{H}_1 \cap \mathbb{H}_2 = \{0\}$ so that Proposition 12.1 guarantees that the kernel

$$\mathcal{K}(x,\, z) = \sum_{\ell=0}^{\alpha-1} \frac{x^\ell}{\ell!} \frac{z^\ell}{\ell!} + \min \int_0^1 \frac{(x-z)_+^{\alpha-1}}{(\alpha-1)!} \frac{(y-z)_+^{\alpha-1}}{(\alpha-1)!} dz \tag{12.19}$$

generates the Hilbert space $\bar{\mathbb{H}}^\alpha[0,1]$ of all functions that are α-times differentiable almost everywhere, with $f^{(\alpha)}$ Lebesgue integrable. As we verify in Exercise 12.15, the associated RKHS norm takes the form

$$\|f\|^2_{\mathbb{H}} = \sum_{\ell=0}^{\alpha-1} \big(f^{(\ell)}(0)\big)^2 + \int_0^1 \big(f^{(\alpha)}(z)\big)^2 dz. \tag{12.20}$$

♣

Example 12.22 (Additive models)**.** It is often convenient to build up a multivariate function from simpler pieces, and additive models provide one way in which to do so. For $j = 1, 2, \ldots, M$, let $\mathbb{H}_j$ be a reproducing kernel Hilbert space, and let us consider functions that have an additive decomposition of the form $f = \sum_{j=1}^M f_j$, where $f_j \in \mathbb{H}_j$. By Proposition 12.1, the space $\mathbb{H}$ of all such functions is itself an RKHS equipped with the kernel function $\mathcal{K} = \sum_{j=1}^M \mathcal{K}_j$. A commonly used instance of such an additive model is when the individual Hilbert space $\mathbb{H}_j$ correspond to functions of the j^{th} co-ordinate of a d-dimensional vector, so that the space $\mathbb{H}$ consists of functions $f : \mathbb{R}^d \rightarrow \mathbb{R}$ that have the additive decomposition

$$f(x_1, \ldots, x_d) = \sum_{j=1}^{d} f_j(x_j),$$

where $f_j : \mathbb{R} \rightarrow \mathbb{R}$ is a univariate function for the j^{th} co-ordinate. Since $\mathbb{H}_j \cap \mathbb{H}_k = \{0\}$ for all $j \neq k$, the associated Hilbert norm takes the form $\|f\|_{\mathbb{H}}^2 = \sum_{j=1}^{d} \|f_j\|_{\mathbb{H}_j}^2$. We provide some additional discussion of these additive decompositions in Exercise 13.8 and Example 14.6 to follow in later chapters.

More generally, it is natural to consider expansions of the form

$$f(x_1, \ldots, x_d) = \sum_{j=1}^{d} f_j(x_j) + \sum_{j \neq k} f_{jk}(x_j, x_k) + \cdots .$$

When the expansion functions are chosen to be mutually orthogonal, such expansions are known as *functional ANOVA* decompositions. ♣

We now turn to the proof of Proposition 12.1.

Proof. Consider the direct sum $\mathbb{F} := \mathbb{H}_1 \oplus \mathbb{H}_2$ of the two Hilbert spaces; by definition, it is the Hilbert space $\{(f_1, f_2) \mid f_j \in \mathbb{H}_j, j = 1, 2\}$ of all ordered pairs, along with the norm

$$\|(f_1, f_2)\|_{\mathbb{F}}^2 := \|f_1\|_{\mathbb{H}_1}^2 + \|f_2\|_{\mathbb{H}_2}^2. \tag{12.21}$$

Now consider the linear operator $L : \mathbb{F} \rightarrow \mathbb{H}$ defined by $(f_1, f_2) \mapsto f_1 + f_2$, and note that it maps $\mathbb{F}$ onto $\mathbb{H}$. The null space $\mathbb{N}(L)$ of this operator is a subspace of $\mathbb{F}$, and we claim that it is closed. Consider some sequence $\Big((f_n, -f_n)\Big)_{n=1}^{\infty} \subset \mathbb{N}(L)$ that converges to a point $(f, g) \in \mathbb{F}$. By the definition of the norm (12.21), this convergence implies that $f_n \rightarrow f$ in $\mathbb{H}_1$ (and hence pointwise) and $-f_n \rightarrow g$ in $\mathbb{H}_2$ (and hence pointwise). Overall, we conclude that that $f = -g$, meaning $(f, g) \in \mathbb{N}(L)$.

Let $\mathbb{N}^{\perp}$ be the orthogonal complement of $\mathbb{N}(L)$ in $\mathbb{F}$, and let $L_{\perp}$ be the restriction of L to $\mathbb{N}^{\perp}$. Since this map is a bijection between $\mathbb{N}^{\perp}$ and $\mathbb{H}$, we may define an inner product on $\mathbb{H}$ via

$$\langle f,\, g \rangle_{\mathbb{H}} := \langle L_{\perp}^{-1}(f),\, L_{\perp}^{-1}(g) \rangle_{\mathbb{F}}.$$

It can be verified that the space $\mathbb{H}$ with this inner product is a Hilbert space.

It remains to check that $\mathbb{H}$ is a RKHS with kernel $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2$, and that the norm $\| \cdot \|_{\mathbb{H}}^2$ takes the given form (12.18). Since the functions $\mathcal{K}_1(\cdot, x)$ and $\mathcal{K}_2(\cdot, x)$

belong to $\mathbb{H}_1$ and $\mathbb{H}_2$ respectively, the function $\mathcal{K}(\cdot, x) = \mathcal{K}_1(\cdot, x) + \mathcal{K}_2(\cdot, x)$ belongs to $\mathbb{H}$. For a fixed $f \in \mathbb{F}$, let $(f_1, f_2) = L_\perp^{-1}(f) \in \mathbb{F}$, and for a fixed $x \in \mathcal{X}$, let $(g_1, g_2) = L_\perp^{-1}(\mathcal{K}(\cdot, x)) \in \mathbb{F}$. Since $(g_1 - \mathcal{K}_1(\cdot, x), g_2 - \mathcal{K}_2(\cdot, x))$ must belong to $\mathbb{N}(L)$, it must be orthogonal (in $\mathbb{F}$) to the element $(f_1, f_2) \in \mathbb{N}^\perp$. Consequently, we have $\langle (g_1 - \mathcal{K}_1(\cdot, x), g_2 - \mathcal{K}_2(\cdot, x)), \, (f_1, f_2)\rangle_{\mathbb{F}} = 0$, and hence

$$\begin{aligned}\langle f_1, \, \mathcal{K}_1(\cdot, x)\rangle_{\mathbb{H}_1} + \langle f_2, \, \mathcal{K}_2(\cdot, x)\rangle_{\mathbb{H}_2} &= \langle f_1, \, g_1\rangle_{\mathbb{H}_1} + \langle f_2, \, g_2\rangle_{\mathbb{H}_2} \\ &= \langle f, \, \mathcal{K}(\cdot, x)\rangle_{\mathbb{H}}.\end{aligned}$$

Since $\langle f_1, \, \mathcal{K}_1(\cdot, x)\rangle_{\mathbb{H}_1} \langle f_2, \, \mathcal{K}_2(\cdot, x)\rangle_{\mathbb{H}_2} = f_1(x) + f_2(x) = f(x)$, we have established that $\mathcal{K}$ has the reproducing property.

Finally, let us the validity of the definition (12.18) as a norm. Consider some pair $(f_1, f_2) \in \mathbb{F}$ with $f = f_1 + f_2 \in \mathbb{H}$. Define $(v_1, v_2) = (f_1, f_2) - L_\perp^{-1}(f)$. Since $(v_1, v_2) \in \mathbb{N}(L)$ and $L_\perp^{-1}(f) \in \mathbb{N}^\perp$, we have

$$\|f_1\|_{\mathbb{H}_1}^2 + \|f_2\|_{\mathbb{H}_2}^2 \; = \; \|(f_1, f_2)\|_{\mathbb{F}}^2 = \|(v_1, v_2)\|_{\mathbb{F}}^2 + \|L_\perp^{-1}(f)\|_{\mathbb{F}}^2$$

Consequently, we have

$$\|f\|_{\mathbb{H}}^2 = \|L_\perp^{-1}(f)\|_{\mathbb{F}}^2 \; \leq \|f_1\|_{\mathbb{H}_1}^2 + \|f_2\|_{\mathbb{H}_2}^2,$$

with equality if and only if $(v_1, v_2) = (0, 0)$, or equivalently $(f_1, f_2) = L_\perp^{-1}(f)$. □

12.5.2 Tensor products

Consider two separable Hilbert spaces $\mathbb{H}_1$ and $\mathbb{H}_2$ of functions, say with domains $\mathcal{X}_1$ and $\mathcal{X}_2$ respectively. We begin by defining a new Hilbert space denoted by $\mathbb{H}_1 \otimes \mathbb{H}_2$, which is known as the tensor product of $\mathbb{H}_1$ and $\mathbb{H}_2$. Consider the set of functions $h : \mathcal{X}_1 \times \mathcal{X}_2 \rightarrow \mathbb{R}$ that have the form

$$\big\{h = \sum_{j=1}^n f_j g_j \; \mid \text{for some } n \in \mathbb{N} \text{ and } \quad f_j \in \mathbb{H}_1, \; g_j \in \mathbb{H}_2 \text{ for all } j \in [n]\big\}.$$

If $h = \sum_{j=1}^n f_j g_j$ and $\widetilde{h} = \sum_{k=1}^m \widetilde{f}_k \widetilde{g}_k$ are two members of this set, we define their inner product

$$\langle h, \, \widetilde{h}\rangle_{\mathbb{H}} := \sum_{j=1}^n \sum_{k=1}^m \langle f_j, \, \widetilde{f}_k\rangle_{\mathbb{H}_1} \, \langle g_j, \, \widetilde{g}_k\rangle_{\mathbb{H}_2}. \tag{12.22}$$

Note the value of the inner product does not depend on the representation of h (or $\widetilde{h}$) that is chosen; indeed, using linearity of the inner product, we have

$$\langle h,\, \widetilde{h}\rangle_{\mathbb{H}} = \sum_{k=1}^{m} \langle\, (h \odot \widetilde{f}_k),\, \widetilde{g}_k \rangle_{\mathbb{H}_2},$$

where $(h \odot \widetilde{f}_k) \in \mathbb{H}_2$ is the function given by $x_2 \mapsto \langle h(\cdot, x_2),\, \widetilde{f}_k\rangle_{\mathbb{H}_1}$. A similar argument shows that the inner product does not depend on the representation of $\widetilde{h}$, so that the inner product (12.22) is well-defined.

It is straightforward to check that the inner product (12.22) is bilinear, symmetric, and that $\langle h,\, h\rangle_{\mathbb{H}}^2 = \|h\|_{\mathbb{H}}^2 \geq 0$ for all $h \in \mathbb{H}$. It remains to check that $\|h\|_{\mathbb{H}} = 0$ if and only if $h = 0$. Consider some $h \in \mathbb{H}$ with the representation $h = \sum_{j=1}^n f_j g_j$. Let $(\phi_j)_{j=1}^{\infty}$ and $(\psi_k)_{k=1}^{\infty}$ be complete orthonormal bases of $\mathbb{H}_1$ and $\mathbb{H}_2$ respectively, ordered such that

$$\operatorname{span}\{f_1, \ldots, f_n\} \subseteq \operatorname{span}\{\phi_1, \ldots, \phi_n\}, \quad \text{and} \quad \operatorname{span}\{g_1, \ldots, g_n\} \subseteq \operatorname{span}\{\psi_1, \ldots, \psi_n\}.$$

Consequently, we can write f equivalently as the double summation $f = \sum\limits_{j,j=1}^{n} \alpha_{j,k}\phi_j\psi_k$ for some set of real numbers $\{\alpha_{j,k}\}_{j,k=1}^n$. Using this representation, we are guaranteed that $\|f\|_{\mathbb{H}}^2 = \sum_{j=1}^n \sum_{k=1}^n \alpha_{j,k}^2$, which shows that $\|f\|_{\mathbb{H}} = 0$ if and only if $\alpha_{j,k} = 0$ for all (j,k), or equivalently $f = 0$.

In this way, we have defined the tensor product $\mathbb{H} = \mathbb{H}_1 \otimes \mathbb{H}_2$ of two Hilbert spaces. The next result asserts that when the two component spaces have reproducing kernels, then the tensor product space is also a reproducing kernel Hilbert space:

Proposition 12.2. Suppose that $\mathbb{H}_1$ and $\mathbb{H}_2$ are reproducing kernel Hilbert spaces of real-valued functions with domains $\mathcal{X}_1$ and $\mathcal{X}_2$, and equipped with kernels $\mathcal{K}_1$ and $\mathcal{K}_2$ respectively. Then the tensor product space $\mathbb{H} = \mathbb{H}_1 \otimes \mathbb{H}_2$ is an RKHS of real-valued functions with domain $\mathcal{X}_1 \times \mathcal{X}_2$, and with kernel function

$$\mathcal{K}((x_1, x_2), (x_1', x_2')) = \mathcal{K}_1(x_1, x_1')\, \mathcal{K}_2(x_2, x_2'). \tag{12.23}$$

Proof. In Exercise 12.16, it is shown that $\mathcal{K}$ defined in equation (12.23) is a positive semidefinite function. By definition of the tensor product space $\mathbb{H} = \mathbb{H}_1 \otimes \mathbb{H}_2$, for each pair $(x_1, x_2) \in \mathcal{X}_1 \times \mathcal{X}_2$, the function $\mathcal{K}((\cdot,\cdot),(x_1,x_2)) = \mathcal{K}_1(\cdot, x_1)\mathcal{K}_2(\cdot, x_2)$ is an element of the tensor product space $\mathbb{H}$. Let $f = \sum_{j,k=1}^n \alpha_{j,k}\phi_j\psi_k$ be an arbitrary element of $\mathbb{H}$.

By definition of the inner product (12.22), we have

$$\begin{aligned}\langle f,\, \mathcal{K}((\cdot,\cdot),(x_1,x_2))\rangle_{\mathbb{H}} &= \sum_{j,k=1}^{n} \alpha_{j,k} \langle \phi_j,\, \mathcal{K}_1(\cdot,x_1)\rangle_{\mathbb{H}_1}\, \langle \psi_k,\, \mathcal{K}_2(\cdot,x_2)\rangle_{\mathbb{H}_2} \\ &= \sum_{j,k=1}^{n} \alpha_{j,k} \phi_j(x_1)\psi_k(x_2) \;=\; f(x_1,x_2),\end{aligned}$$

thereby verifying the reproducing property. □

12.6 Interpolation and fitting

Reproducing kernel Hilbert spaces are useful for the classical problems of interpolating and fitting functions. An especially attractive property is the ease of computation: in particular, the representer theorem allows many optimization problems over the RKHS to be reduced to relatively simple calculations involving the kernel matrix.

12.6.1 Function interpolation

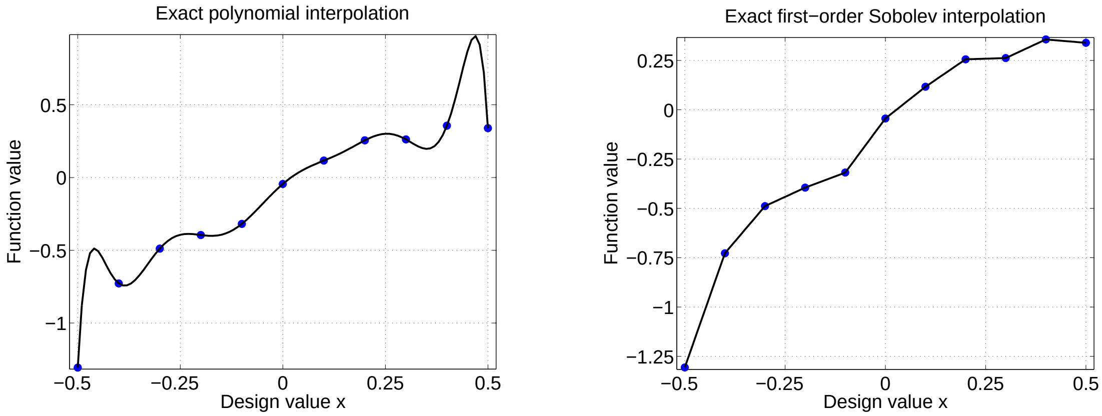
Let us begin with the problem of function interpolation. Suppose that we observe n samples of an unknown function $f^* : \mathcal{X} \rightarrow \mathbb{R}$, say of the form $y_i = f^*(x_i)$ for $i = 1, 2, \ldots, n$, where the design sequence $\{x_i\}_{i=1}^n$ is known to us. Note that we are assuming for the moment that the function values are observed without any noise or corruption. In this context, some questions of interest include:

- For a given function class $\mathscr{F}$, does there exist a function $f \in \mathscr{F}$ that exactly fits the data, meaning that $f(x_i) = y_i$ for all $i = 1, 2, \ldots, n$?
- Of all functions in $\mathscr{F}$ that exactly fit the data, which does the "best" job of interpolating the data?

The first question can often be answered in a definitive way—in particular, by producing a function that exactly fits the data. The second question is vaguely posed and can be answered in multiple ways, depending on our notion of "best". In the context of a reproducing kernel Hilbert space, the underlying norm provides a way of ordering functions, and so we are led to the following formalization: of all the functions that exactly fit the data, choose the one with minimal RKHS norm. This approach can be formulated as an optimization problem in Hilbert space—namely,

$$\text{Choose} \quad \widehat{f} \in \arg\min_{f \in \mathbb{H}} \|f\|_{\mathbb{H}} \quad \text{such that } f(x_i) = y_i \text{ for } i = 1, 2, \ldots, n. \tag{12.24}$$

This method is known as *minimal norm interpolation*, and it is feasible whenever there exists at least one function $f \in \mathbb{H}$ that fits the data exactly. We provide necessary and sufficient conditions for such feasibility in the result to follow. Figure 12-1 illustrates this minimal Hilbert norm interpolation method, using either or the polynomial kernel (see Example 12.9), or the first-order Sobolev kernel (see Example 12.11).



(a) (b)

Figure 12-1. Exact interpolation of $n = 11$ equally sampled function values using RKHS methods. (a) Polynomial kernel $\mathcal{K}(x,\, z) = (1 + x\,z)^{12}$. (b) First-order Sobolev kernel $\mathcal{K}(x,\, z) = 1 + \min\{x, z\}$.

For a general Hilbert space, the optimization problem (12.24) may not be well-defined, or may be computationally challenging to solve. Hilbert spaces with reproducing kernels are attractive in this regard, as the computation can be reduced to simple linear algebra involving the kernel matrix $\mathbf{K} \in \mathbb{R}^{n \times n}$ with entries $K_{ij} = \mathcal{K}(x_i,\, x_j)/n$. The following result provides one instance of this general phenomenon:

Proposition 12.3. Let $\mathbf{K} \in \mathbb{R}^{n\times n}$ be the kernel matrix defined by the design points $\{x_i\}_{i=1}^n$. The convex program (12.24) is feasible if and only if $y \in \text{range}(\mathbf{K})$, in which case any optimal solution can be written as

$$\widehat{f}(\cdot) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \widehat{\alpha}_i \mathcal{K}(\cdot,\, x_i), \qquad \text{where } \mathbf{K}\widehat{\alpha} = y/\sqrt{n}.$$

Remark: Our choice of normalization by $1/\sqrt{n}$ is for later theoretical convenience.

Proof. For a given vector $\alpha \in \mathbb{R}^n$, define the function $f_\alpha(\cdot) := \frac{1}{\sqrt{n}} \sum_{i=1}^n \alpha_i \mathcal{K}(\cdot,\, x_i)$, and consider the set $\mathbb{L} := \big\{ f_\alpha \mid \alpha \in \mathbb{R}^n \big\}$. By the reproducing property, for any $f_\alpha \in \mathbb{L}$, we have

$$f_\alpha(x_j) = \langle f_\alpha,\, \mathcal{K}(\cdot,\, x_j)\rangle_{\mathbb{H}} \;=\; \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \alpha_i \langle \mathcal{K}(\cdot,\, x_i),\, \mathcal{K}(\cdot,\, x_j)\rangle_{\mathbb{H}} \;=\; \sqrt{n}(\mathbf{K}\alpha)_j,$$

where $(\mathbf{K}\alpha)_j$ is the j^{th} component of the vector $\mathbf{K}\alpha \in \mathbb{R}^n$. Thus, the function $f_\alpha \in \mathbb{L}$ satisfies the interpolation condition if and only if $\mathbf{K}\alpha = y/\sqrt{n}$. Consequently, the condition $y \in \text{range}(\mathbf{K})$ is sufficient. It remains to show that this range condition is necessary, and that the optimal interpolating function must lie in $\mathbb{L}$.

Note that $\mathbb{L}$ is a finite-dimensional (hence closed) linear subspace of $\mathbb{H}$. Consequently, any function $f \in \mathbb{H}$ can be decomposed uniquely as $f = f_\alpha + f_\perp$, where $f_\alpha \in \mathbb{L}$ and $f_\perp$ is orthogonal to $\mathbb{L}$. (See Exercise 12.3 for details of this direct sum decomposition.) Using this decomposition and the reproducing property, we have

$$f(x_j) = \langle f, \mathcal{K}(\cdot, x_j)\rangle_{\mathbb{H}} \; = \; \langle f_\alpha + f_\perp, \mathcal{K}(\cdot, x_j)\rangle_{\mathbb{H}} \; = \; f_\alpha(x_j)$$

where the final equality follows $\mathcal{K}(\cdot, x_j)$ belongs to $\mathbb{L}$, and hence $\langle f_\perp, \mathcal{K}(\cdot, x_j)\rangle_{\mathbb{H}} = 0$, using the orthogonality of $f_\perp$ and $\mathbb{L}$. Thus, the component $f_\perp$ has no effect on the interpolation property, showing that the condition $y \in \text{range}(\mathbf{K})$ is also a necessary condition. Moreover, the Pythagorean theorem implies that $\|f_\alpha + f_\perp\|_{\mathbb{H}}^2 = \|f_\alpha\|_{\mathbb{H}}^2 + \|f_\perp\|_{\mathbb{H}}^2$, so that any minimal Hilbert norm interpolant must have $f_\perp = 0$. □

■ 12.6.2 Fitting via kernel ridge regression

In a statistical setting, it is usually unrealistic to assume that we observe noiseless observations of function values. Rather, it is more natural to consider a noisy observation model, say of the form

$$y_i = f^*(x_i) + w_i, \qquad \text{for } i = 1, 2, \ldots, n,$$

where the coefficients $\{w_i\}_{i=1}^n$ model noisiness or disturbance in the measurement model. In the presence of noise, the exact constraints in our earlier interpolation method (12.24) are no longer appropriate; instead, it is more sensible to minimize some trade-off between the fit to the data and the Hilbert norm. For instance, we might only require that the mean-squared differences between the observed data and fitted values be small, which then leads to the optimization problem

$$\min_{f \in \mathbb{H}} \|f\|_{\mathbb{H}} \qquad \text{such that } \tfrac{1}{2n} \textstyle\sum_{i=1}^n \big(y_i - f(x_i)\big)^2 \leq \delta^2, \tag{12.25}$$

where $\delta > 0$ is some type of tolerance parameter. Alternatively, we might minimize the mean-squared error subject to a bound on the Hilbert radius of the solution, say

$$\min_{f \in \mathbb{H}} \frac{1}{2n} \sum_{i=1}^n \big(y_i - f(x_i)\big)^2 \qquad \text{such that } \|f\|_{\mathbb{H}} \leq R \tag{12.26}$$

for an appropriately chosen radius $R > 0$. Both of these problems are convex, and so by Lagrangian duality, they can be reformulated in the penalized form

$$\widehat{f} = \arg\min_{f \in \mathbb{H}} \Big\{ \frac{1}{2n} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda_n \|f\|_{\mathbb{H}}^2 \Big\}. \tag{12.27}$$

Here, for a fixed set of observations $\{(x_i, y_i)\}_{i=1}^{n}$, the regularization parameter $\lambda_n \geq 0$ is a function of the tolerance δ or radius R. This form of function estimate is most convenient to implement, and in the case of a reproducing kernel Hilbert space considered here, it is known as the *kernel ridge regression* estimate, or KRR estimate for short. The following result shows how the KRR estimate is easily computed in terms of the kernel matrix $\mathbf{K} \in \mathbb{R}^{n \times n}$ with entries $K_{ij} = \mathcal{K}(x_i,\, x_j)/n$.

Proposition 12.4. For all $\lambda_n > 0$, the kernel ridge regression estimate (12.27) can be written as

$$\widehat{f}(\cdot) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \widehat{\alpha}_i \mathcal{K}(\cdot,\, x_i), \tag{12.28}$$

where the optimal weight vector $\widehat{\alpha} \in \mathbb{R}^n$ is given by

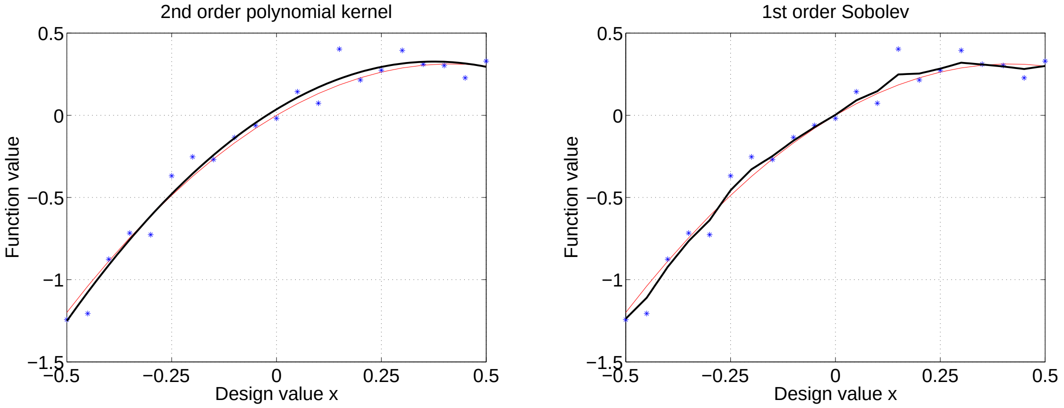
$$\widehat{\alpha} = \big(\mathbf{K} + \lambda_n \mathbf{I}_n\big)^{-1} \frac{y}{\sqrt{n}}. \tag{12.29}$$

Remarks: Note that Proposition 12.4 is a natural generalization of Proposition 12.3, to which it reduces when $\lambda_n = 0$ (and the kernel matrix is invertible). Given the kernel matrix $\mathbf{K}$, computing $\widehat{\alpha}$ via equation (12.29) requires at most $\mathcal{O}(n^3)$ operations, using standard routines in numerical linear algebra (see the bibliography for more details). Assuming that the kernel function can be evaluated in constant time, computing the $n \times n$ matrix requires an additional $\mathcal{O}(n^2)$ operations. See Figure 12-2 for some illustrative examples.

We now turn to the proof of Proposition 12.4.

Proof. Recall the argument of Proposition 12.3, and the decomposition $f = f_\alpha + f_\perp$. Since $f_\perp(x_i) = 0$ for all $i = 1, 2, \ldots, n$, it can have no effect on the least-squares data component of the objective function (12.27). Consquently, following a similar line of reasoning to the proof of Proposition 12.3, we again see that any optimal solution must be of the specified form (12.28).

It remains to prove the specific form (12.29) of the optimal $\widehat{\alpha}$. Given a function f



(a)

(b)

Figure 12-2. Illustration of kernel ridge regression estimates of function $f^*(x) = \frac{3x}{2} - \frac{9}{5}x^2$ based on $n = 21$ samples, located at design points $x_i = -0.5 + 0.05\,(i-1)$ over the interval $[-0.5, 0.5]$. (a) Kernel ridge regression estimate using the second-order polynomial kernel $\mathcal{K}(x,\, z) = (1 + xz)^2$ and regularization parameter $\lambda_n = 0.01$. (b) Kernel ridge regression estimate using the first-order Sobolev kernel $\mathcal{K}(x,\, z) = 1 + \min\{x, z\}$ and regularization parameter $\lambda_n = 0.08$.

of the form (12.28), for each $j = 1, 2, \ldots, n$, we have

$$f(x_j) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \alpha_i \mathcal{K}(x_j,\, x_i) \;=\; \sqrt{n} e_j^T \mathbf{K} \alpha,$$

where $e_j \in \mathbb{R}^n$ is the canonical basis vector with 1 in position j, and we have recalled that $K_{ji} = \mathcal{K}(x_j,\, x_i)/n$. Similarly, we have the representation

$$\|f\|_{\mathbb{H}}^2 = \frac{1}{n} \langle \sum_{i=1}^{n} \alpha_i \mathcal{K}(\cdot,\, x_i), \sum_{j=1}^{n} \alpha_j \mathcal{K}(\cdot,\, x_j) \rangle_{\mathbb{H}} \;=\; \alpha^T \mathbf{K} \alpha.$$

Substituting these relations into the cost function, we find that it is a quadratic in the vector α, given by

$$\frac{1}{n} \|y - \sqrt{n}\mathbf{K}\alpha\|_2^2 + \lambda\, \alpha^T \mathbf{K} \alpha \;=\; \frac{1}{n}\|y\|_2^2 + \alpha^T \big(\mathbf{K}^2 + \lambda \mathbf{K}\big)\alpha - \frac{2}{\sqrt{n}} y^T \mathbf{K} \alpha$$

In order to find the minimum of this quadratic function, we compute the gradient and set it equal to zero, thereby obtaining the stationary condition

$$\mathbf{K}\,\big(\mathbf{K} + \lambda \mathbf{I}_n\big)\alpha = \mathbf{K}\frac{y}{\sqrt{n}}.$$

Thus, we see that the vector $\widehat{\alpha}$ previously defined in equation (12.29) is optimal. Note 6031 that any vector $\beta \in \mathbb{R}^n$ such that $\mathbf{K}\beta = 0$ has no effect on the optimal solution. □

We return in Chapter 13 to study the statistical properties of the kernel ridge regression estimate.

■ 12.7 Distances between probability measures

There are various settings in which it is important to construct distances between probability measures, and one way in which to do so is via measuring mean discrepancies over a given function class. More precisely, let $\mathbb{P}$ and $\mathbb{Q}$ be a pair of probability measures on a space $\mathcal{X}$, and let $\mathscr{F}$ be a class of functions $f : \mathcal{X} \rightarrow \mathbb{R}$ that are integrable with respect to $\mathbb{P}$ and $\mathbb{Q}$. We can then define the quantity

$$\rho_{\mathscr{F}}(\mathbb{P}, \mathbb{Q}) := \sup_{f \in \mathscr{F}} \Big| \int f (d\mathbb{P} - d\mathbb{Q}) \Big| \; = \; \sup_{f \in \mathscr{F}} \big| \mathbb{E}_{\mathbb{P}}[f(X)] - \mathbb{E}_{\mathbb{Q}}[f(Z)] \big|. \tag{12.30}$$

It can be verified that for any choice of function class $\mathscr{F}$, this always defines a pseudometric, meaning that $\rho_{\mathscr{F}}$ satisfies all the metric properties, except that there may exist pairs $\mathbb{P} \neq \mathbb{Q}$ such that $\rho_{\mathscr{F}}(\mathbb{P}, \mathbb{Q}) = 0$. When $\mathscr{F}$ is sufficiently rich, then $\rho_{\mathscr{F}}$ becomes a metric, known as an *integral probability metric*. Let us provide some classical examples to illustrate:

Example 12.23 (Kolmogorov metric)**.** Suppose that $\mathbb{P}$ and $\mathbb{Q}$ are measures on the real line. For each $t \in \mathbb{R}$, let $\mathbb{I}_{(-\infty, t]}$ denote the 0-1 valued indicator function for the event $\{x \leq t\}$, and consider the function class $\mathscr{F} = \big\{ \mathbb{I}_{(-\infty, t]} \mid t \in \mathbb{R} \big\}$. We then have

$$\rho_{\mathscr{F}}(\mathbb{P}, \mathbb{Q}) \; = \; \sup_{t \in \mathbb{R}} \big| \mathbb{P}(X \leq t) - \mathbb{Q}(X \leq t) \big| \; = \; \|F_{\mathbb{P}} - F_{\mathbb{Q}}\|_\infty,$$

where $F_{\mathbb{P}}$ and $F_{\mathbb{Q}}$ are the cumulative distribution functions of $\mathbb{P}$ and $\mathbb{Q}$, respectively. Thus, this choice leads to the *Kolmogorov distance* between $\mathbb{P}$ and $\mathbb{Q}$. ♣

Example 12.24 (Total variation distance)**.** Consider the class $\mathscr{F} = \{f : \mathcal{X} \rightarrow \mathbb{R} \mid \|f\|_\infty \leq 1\}$ of real-valued functions bounded by one in the supremum norm. With this choice, we have

$$\rho_{\mathscr{F}}(\mathbb{P}, \mathbb{Q}) = \sup_{\|f\|_\infty \leq 1} \Big| \int f (d\mathbb{P} - d\mathbb{Q}) \Big|.$$

As we show in Exercise 12.17, this metric corresponds to (two times) the total variation distance

$$\|\mathbb{P} - \mathbb{Q}\|_1 = \sup_{A \subset \mathcal{X}} |\mathbb{P}(A) - \mathbb{Q}(A)|,$$

where the supremum ranges over all measurable subsets of $\mathcal{X}$. ♣

When we choose $\mathscr{F}$ to be the unit ball of a RKHS, we obtain a mean discrepancy pseudometric that is easy to compute. In particular, given an RKHS with kernel function $\mathcal{K}$, consider the associated pseudometric

$$\rho_{\mathbb{H}}(\mathbb{P}, \mathbb{Q}) := \sup_{\|f\|_{\mathbb{H}} \leq 1} \big|\mathbb{E}_{\mathbb{P}}[f(X)] - \mathbb{E}_{\mathbb{Q}}[f(Z)]\big|.$$

As verified in Exercise 12.18, the reproducing property allows us to obtain a simple closed-form expression for this pseudometric–namely,

$$\rho^2_{\mathbb{H}}(\mathbb{P}, \mathbb{Q}) = \mathbb{E}\big[\mathcal{K}(X,\, X') + \mathcal{K}(Z,\, Z') - 2\mathcal{K}(X,\, Z)\big], \tag{12.31}$$

where $X, X' \sim \mathbb{P}$ and $Z, Z' \sim \mathbb{Q}$ are all mutually independent random vectors. We refer to this pseudometric as a *kernel means discrepancy*, or KMD for short.

Example 12.25 (KMD for linear and polynomial kernels)**.** Let us compute the KMD for the linear kernel $\mathcal{K}(x,\, z) = \langle x,\, z\rangle$ on $\mathbb{R}^d$. Letting $\mathbb{P}$ and $\mathbb{Q}$ be two distributions on $\mathbb{R}^d$ with mean vectors $\mu_p = \mathbb{E}_{\mathbb{P}}[X]$ and $\mu_q = \mathbb{E}_{\mathbb{Q}}[Z]$ respectively, we have

$$\begin{aligned}
\rho^2_{\mathbb{H}}(\mathbb{P}, \mathbb{Q}) &= \mathbb{E}[\langle X,\, X'\rangle + \langle Z,\, Z'\rangle - 2\langle X,\, Z\rangle] \\
&= \|\mu_p\|_2^2 + \|\mu_q\|_2^2 - 2\langle \mu_p,\, \mu_q\rangle \\
&= \|\mu_p - \mu_q\|_2^2
\end{aligned}$$

Thus, we see that the KMD pseudometric for the linear kernel simply computes the Euclidean distance of the associated mean vectors. This is illustrates that KMD in this case is not actually a metric (but rather just a pseudometric), since $\rho_{\mathbb{H}}(\mathbb{P}, \mathbb{Q}) = 0$ for any pair of distributions (possibly distinct) with $\mu_p = \mu_q$.

Moving onto polynomial kernels, let us consider the homogeneous polynomial kernel of degree two, namely $\mathcal{K}(x,\, z) = \langle x,\, z\rangle^2$. For this choice of kernel, we have

$$\mathbb{E}[\mathcal{K}(X,\, X')] = \mathbb{E}\big(\sum_{j=1}^d X_j X_j'\big)^2 \;=\; \sum_{i,j=1}^d \mathbb{E}[X_i X_j]\mathbb{E}[X_i' X_j'] \;=\; |\!|\!|\mathbf{\Gamma}_p|\!|\!|_F^2,$$

where $\mathbf{\Gamma}_p \in \mathbb{R}^{d\times d}$ is the second-order moment matrix with entries $[\mathbf{\Gamma}_p]_{ij} = \mathbb{E}[X_i X_j]$, and the squared Frobenius norm corresponds to the sum of the squared matrix entries. Similarly, we have $\mathbb{E}[\mathcal{K}(Z,\, Z')] = |\!|\!|\mathbf{\Gamma}_q|\!|\!|_F^2$ where $\mathbf{\Gamma}_q$ is the second-order moment matrix for $\mathbb{Q}$. Finally, similar calculations yield that

$$\mathbb{E}[\mathcal{K}(X,\, Z)] = \sum_{i,j=1}^d [\mathbf{\Gamma}_p]_{ij}[\mathbf{\Gamma}_q]_{ij} \;=\; \langle\!\langle \mathbf{\Gamma}_p,\, \mathbf{\Gamma}_q\rangle\!\rangle,$$

where $\langle\!\langle \cdot,\ \cdot \rangle\!\rangle$ denotes the trace inner product between symmetric matrices. Putting together the pieces, we conclude that for the homogeneous second-order polynomial kernel, we have

$$\rho^2_{\mathbb{H}}(\mathbb{P}, \mathbb{Q}) = |\!|\!| \mathbf{\Gamma}_p - \mathbf{\Gamma}_q |\!|\!|_F^2.$$

♣

Example 12.26 (KMD for a first-order Sobolev kernel)**.** Consider the kernel function $\mathcal{K}(x,\, z) = \min\{x, z\}$, defined on the Cartesian product $[0,1] \times [0,1]$. As seen previously in Example 12.11, this kernel function generates the first-order Sobolev space

$$\mathbb{H}^1[0,1] = \big\{ f : \mathbb{R}[0,1] \to \mathbb{R} \mid f(0) = 0, \quad \text{and} \quad \int_0^1 (f'(x))^2 dx < \infty \big\},$$

with Hilbert norm $\|f\|^2_{\mathbb{H}^1[0,1]} = \int_0^1 (f'(x))^2 dx$. With this choice, we have

$$\rho^2_{\mathbb{H}}(\mathbb{P}, \mathbb{Q}) = \mathbb{E}\big[\min\{X, X'\} + \min\{Z, Z'\} - 2\min\{X, Z\}\big].$$

♣

■ 12.8 Bibliographic details and background

The notion of a reproducing kernel Hilbert space emerged from the study of positive semidefinite kernels and their links to Hilbert space structure. The seminal paper by Aronszajn [Aro50] develops a number of the basic properties from first principles, including Propositions 12.1 and 12.2, as well as Theorem 12.2 from this chapter. The book by Wahba [Wah90] contains a wealth of information on RKHSs, as well as the connections between splines and penalized methods for regression. See also the books by Berlinet and Thomas-Agnan [BTA04] as well as Gu [Gu02]. The book by Schölkopf and Smola [SS02] provides a number of applications of kernels in the setting of machine learning, including the support vector machine and other methods for classification. The book by Steinwart and Christmann [SC08] also contains a variety of theoretical results on kernels and reproducing kernel Hilbert spaces.

The argument underlying the proofs of Propositions 12.3 and 12.4 is known as the *representer theorem*, and is due to Kimeldorf and Wahba [KW71]. From the computational point of view, it is extremely important, since it allows the infinite-dimensional problem of optimizing over an RKHS to be reduced to an n-dimensional convex program. Bochner's theorem relates the positive semidefiniteness of kernel functions to the non-negativity of Fourier coefficients. In its classical formulation, it applies to the Fourier transform over the real line, but it can be generalized to all locally compact Abelian groups [Rud90]. The results used to compute the asymptotic scaling of the eigenvalues of the Gaussian kernel in Example 12.19 are due to Widom [Wid63, Wid64].

There are a number of papers that study the approximation-theoretic properties of various types of reproducing kernel Hilbert spaces. For a given Hilbert space $\mathbb{H}$ and norm $\|\cdot\|$, such results are often phrased in terms of the function

$$A(f^*; R) := \inf_{\|f\|_{\mathbb{H}} \leq R} \|f - f^*\|_p, \tag{12.32}$$

where $\|g\|_p = (\int_{\mathcal{X}} g^p(x)dx)^{1/p}$ is the usual L^p norm on a compact space $\mathcal{X}$. This function measures how quickly the $L^p(\mathcal{X})$-error in approximating some function f^* decays as the Hilbert radius R is increased. See the papers [SZ03, Zho13] for results on this form of the approximation error. A reproducing kernel Hilbert space is said to be $L^p(\mathcal{X})$-*universal* if $\lim_{R\to\infty} A(f^*; R) = 0$ for any $f^* \in L^p(\mathcal{X})$. There are also various other forms of universality; see the book by Steinwart and Christmann [SC08] for further details.

Probability metrics of the form (12.30) have been studied extensively [M9̈7, RKSF13]. The particular case of RKHS-based distances are computationally convenient, and have been studied in the context of proper scoring rules [Daw07, GR07] and two-sample testing [BGR+06, GBR+12].

■ 12.9 Exercises

Exercise 12.1 (Closedness of null space)**.** Let L be a bounded linear functional on a Hilbert space. Show that its null space $\text{null}(L) = \{f \in \mathbb{H} \mid L(f) = 0\}$ is closed.

Exercise 12.2. Let $\mathbb{G}$ be a closed convex subset of a Hilbert space $\mathbb{H}$. In this exercise, we show that for any $f \in \mathbb{H}$, there exists a unique $\widehat{g} \in \mathbb{G}$ such that

$$\|\widehat{g} - f\|_{\mathbb{H}} = \underbrace{\inf_{g \in \mathbb{G}} \|\widehat{g} - f\|_{\mathbb{H}}}_{p^*}$$

This element $\widehat{g}$ is known as the projection of f onto $\mathbb{G}$.

(a) By the definition of infimum, there exists a sequence $(g_n)_{n=1}^{\infty}$ contained in $\mathbb{G}$ such that $\|g_n - f\|_{\mathbb{H}} \to p^*$. Show that this sequence is a Cauchy sequence. (*Hint:* First show that $\|f - \frac{g_n + g_m}{2}\|_{\mathbb{H}}$ converges to p^*.)

(b) Use this Cauchy sequence to establish the existence of $\widehat{g}$.

(c) Show that the projection must be unique.

(d) Does the same claim hold for an arbitrary convex set $\mathbb{G}$?

Exercise 12.3. Let $\mathbb{H}$ be a Hilbert space, and let $\mathbb{G}$ be a closed linear subspace of $\mathbb{H}$. Show that any $f \in \mathbb{H}$ can be decomposed uniquely as $g + g^{\perp}$, where $g \in \mathbb{G}$ and $g^{\perp} \in \mathbb{G}^{\perp}$. In brief, we say that $\mathbb{H}$ has the direct sum decomposition $\mathbb{G} \oplus \mathbb{G}^{\perp}$. (*Hint:* The notion of a projection onto a closed convex set from Exercise 12.2 could be helpful to you.)

Exercise 12.4. Show that the kernel function associated with any reproducing kernel Hilbert space must be unique.

Exercise 12.5. (a) Show that for any positive semidefinite kernel $\mathcal{K} : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ and $x, z \in \mathcal{X}$, we have

$$\mathcal{K}(x,\, z) \leq \sqrt{\mathcal{K}(x,\, x)\, \mathcal{K}(z,\, z)}.$$

(b) Show how the classical Cauchy-Schwarz inequality is a special case.

Exercise 12.6. For an integer $m \geq 1$, consider the kernel functions $\mathcal{K}_1(x, z) = (1 + xz)^m$ and $\mathcal{K}_2(x, z) = \sum_{\ell=0}^{m} \frac{x^\ell}{\ell!} \frac{z^\ell}{\ell!}$.

(a) Show that they are both PSD, and generate RKHSs of polynomial functions of degree at most m.

(b) Why does this not contradict the result of Exercise 12.4?

Exercise 12.7. True or false? If true, provide a short proof; if false, give an explicit counterexample.

(a) Given two PSD kernels $\mathcal{K}_1$ and $\mathcal{K}_2$, the bivariate function $\mathcal{K}(x,\, z) = \min_{j=1,2} \mathcal{K}_j(x, z)$ is also a PSD kernel.

(b) Let $f : \mathcal{X} \rightarrow \mathbb{H}$ be a function from an arbitrary space $\mathcal{X}$ to a Hilbert space $\mathbb{H}$. The bivariate function

$$\mathcal{K}(x,\, z) = \frac{\langle f(x),\, f(z) \rangle_{\mathbb{H}}}{\|f(x)\|_{\mathbb{H}}\, \|f(z)\|_{\mathbb{H}}}$$

defines a PSD kernel on $\mathcal{X} \times \mathcal{X}$.

Exercise 12.8. Let $\mathcal{K} : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be a positive semidefinite kernel, and let $f : \mathcal{X} \rightarrow [0, \infty)$ be an arbitrary function. Show that $\widetilde{\mathcal{K}}(x, y) = f(x) \mathcal{K}(x,\, y) f(y)$ is also a positive semidefinite kernel.

Exercise 12.9. Given a finite set S, its power set $\mathcal{P}(S)$ is the set of all the subsets of S. Show that the function $\mathcal{K} : \mathcal{P}(S) \times \mathcal{P}(S) \rightarrow \mathbb{R}$ given by $\mathcal{K}(A, B) = 2^{|A \cap B|}$ is a positive semidefinite kernel function.

Exercise 12.10. Recall from equation (12.14) the notion of a feature map. Show that the polynomial kernel $\mathcal{K}(x,\, z) = \big(1 + \langle x,\, z\rangle\big)^m$ over $\mathbb{R}^d \times \mathbb{R}^d$ can be realized by a feature map $x \mapsto \Phi(x) \in \mathbb{R}^D$, where $D = \binom{d+m}{m}$.

Exercise 12.11. Consider a probability space with events $\mathcal{E}$ and probability law $\mathbb{P}$. Show that the real-valued function $\mathcal{K}(A, B) = \mathbb{P}[A, B] - \mathbb{P}[A]\mathbb{P}[B]$ is a positive semidefinite kernel function on $\mathcal{E} \times \mathcal{E}$.

Exercise 12.12. Suppose that $\mathcal{K} : S \times S \to \mathbb{R}$ is a symmetric PSD kernel function on a finite set S. Show that

$$\mathcal{K}'(A, B) = \sum_{x \in A, z \in B} \mathcal{K}(x, z)$$

is a symmetric PSD kernel on the power set $\mathcal{P}(S)$.

Exercise 12.13. Consider a PSD kernel $\mathcal{K} : \mathcal{X} \times \mathcal{X} \to [0, \infty)$ such that $\mathcal{K}(x,\, x') \leq b^2$ for all $x, x \in \mathcal{X}$. Show that $\|f\|_\infty \leq b$ for any function f in the unit ball of the associated RKHS.

Exercise 12.14. Let $\mathcal{X}$ be a compact subset of $\mathbb{R}^d$. In this exercise, we work through a proof of the fact that the Gaussian kernel $\mathcal{K}(x,\, z) = e^{-\frac{\|x-z\|_2^2}{2\sigma^2}}$ on $\mathcal{X} \times \mathcal{X}$ is positive semidefinite.

(a) Let $\widetilde{\mathcal{K}}$ be a a PSD kernel, and let p be a polynomial with non-negative coefficients. Show that $\mathcal{K}(x,\, z) = p\big(\widetilde{\mathcal{K}}(x, z)\big)$ is a PSD kernel.

(b) Show that the kernel $\mathcal{K}_1(x, z) = e^{\langle x,\, z\rangle / \sigma^2}$ is positive semidefinite. (*Hint:* Part (a) and the fact that a pointwise limit of PSD kernels is also PSD could be useful.)

(c) Show that the Gaussian kernel is PSD. (*Hint:* The result of Exercise 12.8 could be useful.)

Exercise 12.15. Show that the Sobolev kernel defined in equation (12.19) generates the norm given in equation (12.20).

Exercise 12.16. (a) Given two $n \times n$ matrices $\mathbf{\Gamma}$ and $\mathbf{\Sigma}$ that are symmetric and positive semidefinite, show that the Hadamard product matrix $\mathbf{\Sigma} \odot \mathbf{\Gamma} \in \mathbb{R}^{n \times n}$ is also positive semidefinite. (The Hadamard product is simply the elementwise product—that is, $(\mathbf{\Sigma} \odot \mathbf{\Gamma})_{ij} = \Sigma_{ij}\Gamma_{ij}$ for all $i, j = 1, 2, \ldots, n$.)

(b) Suppose that $\mathcal{K}_1$ and $\mathcal{K}_2$ are positive semidefinite kernel functions on $\mathcal{X} \times \mathcal{X}$. Show that the function $\mathcal{K}(x,\, z) := \mathcal{K}_1(x, z)\, \mathcal{K}_2(x, z)$ is a positive semidefinite kernel function. *Hint:* The result of part (a) could be helpful.

Exercise 12.17. Given two probability measures $\mathbb{P}$ and $\mathbb{Q}$ on $\mathcal{X}$, show that

$$\sup_{\|f\|_\infty \leq 1} |\int f(d\mathbb{P} - d\mathbb{Q})| = 2 \sup_{A \subset \mathcal{X}} |\mathbb{P}(A) - \mathbb{Q}(A)|,$$

where the left supremum ranges over all measurable functions $f : \mathcal{X} \rightarrow \mathbb{R}$, and the right supremum ranges over all measurable subsets A of $\mathcal{X}$.

Exercise 12.18. Let $\mathbb{H}$ be a reproducing kernel Hilbert space of functions with domain $\mathcal{X}$, and let $\mathbb{P}$ and $\mathbb{Q}$ be two probability distributions on $\mathcal{X}$. Show that

$$\sup_{\|f\|_{\mathbb{H}} \leq 1} \big|\mathbb{E}_{\mathbb{P}}[f(X)] - \mathbb{E}_{\mathbb{Q}}[f(Z)]\big|^2 = \mathbb{E}[\mathcal{K}(X,\, X') + \mathcal{K}(Z,\, Z') - 2\mathcal{K}(X,\, Z)],$$

where $X, X' \sim \mathbb{P}$ and $Z, Z' \sim \mathbb{Q}$ are jointly independent.