

# A Primer on Reproducing Kernel Hilbert Spaces

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## Abstract

Reproducing kernel Hilbert spaces are elucidated without assuming prior familiarity with Hilbert spaces. Compared with extant pedagogic material, greater care is placed on motivating the definition of reproducing kernel Hilbert spaces and explaining when and why these spaces are efficacious. The novel viewpoint is that reproducing kernel Hilbert space theory studies extrinsic geometry, associating with each geometric configuration a canonical overdetermined coordinate system. This coordinate system varies continuously with changing geometric configurations, making it well-suited for studying problems whose solutions also vary continuously with changing geometry. This primer can also serve as an introduction to infinite-dimensional linear algebra because reproducing kernel Hilbert spaces have more properties in common with Euclidean spaces than do more general Hilbert spaces.



# 1

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## Introduction

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Hilbert space theory is a prime example in mathematics of a beautiful synergy between symbolic manipulation and visual reasoning. Two-dimensional and three-dimensional pictures can be used to reason about infinite-dimensional Hilbert spaces, with symbolic manipulations subsequently verifying the soundness of this reasoning, or suggesting modifications and refinements. Visualising a problem is especially beneficial because over half the human brain is involved to some extent with visual processing. Hilbert space theory is an invaluable tool in numerous signal processing and systems theory applications [61, 11, 9].

Hilbert spaces satisfying certain additional properties are known as Reproducing Kernel Hilbert Spaces (RKHSs), and RKHS theory is normally described as a transform theory between Reproducing Kernel Hilbert Spaces and positive semi-definite functions, called kernels: every RKHS has a unique kernel, and certain problems posed in RKHSs are more easily solved by involving the kernel. However, this description hides the crucial aspect that the kernel captures not just intrinsic properties of the Hilbert space but also how the Hilbert space is embedded in a larger function space, which is referred to here as its extrinsic geometry. A novel feature of this primer is drawing attention to this

extrinsic geometry, and using it to explain why certain problems can be solved more efficiently in terms of the kernel than the space itself.

Another novel feature of this primer is that it motivates and develops RKHS theory in finite dimensions before considering infinite dimensions. RKHS theory is ingenious; the underlying definitions are simple but powerful and broadly applicable. These aspects are best brought out in the finite-dimensional case, free from the distraction of infinite-dimensional technicalities. Essentially all of the finite-dimensional results carry over to the infinite-dimensional setting.

This primer ultimately aims to empower readers to recognise when and how RKHS theory can profit them in their own work. The following are three of the known uses of RKHS theory.

1. If a problem involves a subspace of a function space, and if the subspace (or its completion) is a RKHS, then the additional properties enjoyed by RKHSs may help solve the problem. (Explicitly computing limits of sequences in Hilbert spaces can be difficult, but in a RKHS the limit can be found pointwise.)
2. Certain classes of problems involving positive semi-definite functions can be solved by introducing an associated RKHS whose kernel is precisely the positive semi-definite function of interest. A classic example, due to Parzen, is associating a RKHS with a stochastic process, where the kernel of the RKHS is the covariance function of the stochastic process (see §7.2).
3. Given a set of points and a function specifying the desired distances between points, the points can be embedded in a RKHS with the distances between points being precisely as prescribed; see §5. (Support vector machines use this to convert certain non-linear problems into linear problems.)

In several contexts, RKHS methods have been described as providing a unified framework [76, 31, 45, 58]; although a subclass of problems was solved earlier by other techniques, a RKHS approach was found to be more elegant, have broader applicability, or offer new insight for obtaining actual solutions, either in closed form or numerically. Parzen

describes RKHS theory as facilitating a coordinate-free approach [45]. While the underlying Hilbert space certainly allows for coordinate-free expressions, the power of a RKHS beyond that of a Hilbert space is the presence of two coordinate systems: the pointwise coordinate system coming from the RKHS being a function space, and a canonical (but overdetermined) coordinate system coming from the kernel. The pointwise coordinate system facilitates taking limits while a number of geometric problems have solutions conveniently expressed in terms of what we define to be the canonical coordinate system. (Geometers may wish to think of a RKHS as a subspace  $V \subset \mathbb{R}^X$  with pointwise coordinates being the extrinsic coordinates coming from  $\mathbb{R}^X$  while the canonical coordinates are intrinsic coordinates on  $V$  relating directly to the inner product structure on  $V$ .)

The body of the primer elaborates on all of the points mentioned above and provides simple but illuminating examples to ruminate on. Parenthetical remarks are used to provide greater technical detail that some readers may welcome. They may be ignored without compromising the cohesion of the primer. Proofs are there for those wishing to gain experience at working with RKHSs; simple proofs are preferred to short, clever, but otherwise uninformative proofs. Italicised comments appearing in proofs provide intuition or orientation or both.

This primer is neither a review nor a historical survey, and as such, many classic works have not been discussed, including those by leading pioneers such as Wahba [71, 72].

**Contributions** This primer is effectively in two parts. The first part (§1–§7), written by the first author, gives a gentle and novel introduction to RKHS theory. It also presents several classical applications. The second part (§8–§9), with §8 written jointly and §9 written by the second author, focuses on recent developments in the machine learning literature concerning embeddings of random variables.

## 1.1 Assumed Knowledge

Basic familiarity with concepts from finite-dimensional linear algebra is assumed: vector space, norm, inner product, linear independence,

basis, orthonormal basis, matrix manipulations and so forth.

Given an inner product  $\langle \cdot, \cdot \rangle$ , the induced norm is  $\|x\| = \sqrt{\langle x, x \rangle}$ . Not every norm comes from an inner product, meaning some norms cannot be written in this form. If a norm does come from an inner product, the inner product can be uniquely determined from the norm by the polarisation identity  $4\langle x, y \rangle = \|x + y\|^2 - \|x - y\|^2$ . (A corresponding formula exists for complex-valued vector spaces.)

A metric  $d(\cdot, \cdot)$  is a “distance function” describing the distance between two points in a metric space. To be a valid metric, it must satisfy several axioms, including the triangle inequality. A normed space is automatically a metric space by the correspondence  $d(x, y) = \|x - y\|$ .

## 1.2 Extrinsic Geometry and a Motivating Example

Differential geometry groups geometric properties into two kinds: intrinsic and extrinsic. Intrinsic properties depend only on the space itself, while extrinsic properties depend on precisely how the space is embedded in a larger space. A simple example in linear algebra is that the orientation of a straight line passing through the origin in  $\mathbb{R}^2$  describes the *extrinsic* geometry of the line.

The following observation helps motivate the development of finite-dimensional RKHS theory in §2. Let

$$L(\theta) = \{(t \cos \theta, t \sin \theta) \mid t \in \mathbb{R}\} \subset \mathbb{R}^2 \quad (1.1)$$

denote a straight line in  $\mathbb{R}^2$  passing through the origin and intersecting the horizontal axis at an angle of  $\theta$  radians; it is a one-dimensional subspace of  $\mathbb{R}^2$ . Fix an arbitrary point  $p = (p_1, p_2) \in \mathbb{R}^2$  and define  $f(\theta)$  to be the point on  $L(\theta)$  closest to  $p$  with respect to the Euclidean metric. It can be shown that

$$f(\theta) = (r(\theta) \cos \theta, r(\theta) \sin \theta), \quad r(\theta) = p_1 \cos \theta + p_2 \sin \theta. \quad (1.2)$$

Visualising  $f(\theta)$  as the projection of  $p$  onto  $L(\theta)$  shows that  $f(\theta)$  depends *continuously* on the orientation of the line. While (1.2) verifies this continuous dependence, it resorted to introducing an *ad hoc* parametrisation  $\theta$ , and different values of  $\theta$  (e.g.,  $\theta$ ,  $\pi + \theta$  and  $2\pi + \theta$ ) can describe the same line.

Is there a more natural way of representing  $L(\theta)$  and  $f(\theta)$ , using linear algebra?

A first attempt might involve using an orthonormal basis vector to represent  $L(\theta)$ . However, there is no *continuous* map from the line  $L(\theta)$  to an orthonormal basis vector  $v(\theta) \in L(\theta)$ . (This should be self-evident with some thought, and follows rigorously from the Borsuk-Ulam theorem.) Note that  $\theta \mapsto (\cos \theta, \sin \theta)$  is not a well-defined map from  $L(\theta)$  to  $\mathbb{R}^2$  because  $L(0)$  and  $L(\pi)$  represent the same line yet  $(\cos 0, \sin 0) \neq (\cos \pi, \sin \pi)$ .

RKHS theory uses not one but two vectors to represent  $L(\theta)$ . Specifically, it turns out that the kernel of  $L(\theta)$ , in matrix form, is

$$K(\theta) = \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix} \begin{bmatrix} \cos \theta & \sin \theta \end{bmatrix} = \begin{bmatrix} \cos^2 \theta & \sin \theta \cos \theta \\ \sin \theta \cos \theta & \sin^2 \theta \end{bmatrix}. \quad (1.3)$$

The columns of  $K(\theta)$  are

$$k_1(\theta) = \cos \theta \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix}, \quad k_2(\theta) = \sin \theta \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix}. \quad (1.4)$$

Note that  $L(\theta)$  is spanned by  $k_1(\theta)$  and  $k_2(\theta)$ , and moreover, both  $k_1$  and  $k_2$  are well-defined (and continuous) functions of  $L$ ; if  $L(\theta) = L(\phi)$  then  $k_1(\theta) = k_1(\phi)$  and  $k_2(\theta) = k_2(\phi)$ . To emphasise, although  $\theta$  is used here for convenience to describe the construction, RKHS theory defines a map from  $L$  to  $k_1$  and  $k_2$  that does not depend on any *ad hoc* choice of parametrisation. It is valid to write  $k_1(L)$  and  $k_2(L)$  to show they are functions of  $L$  alone.

Interestingly,  $f$  has a simple representation in terms of the kernel:

$$f(L) = p_1 k_1(L) + p_2 k_2(L). \quad (1.5)$$

Compared with (1.2), this is both simple and natural, and does not depend on any *ad hoc* parametrisation  $\theta$  of the line  $L$ . In summary,

- the kernel represents a vector subspace by a possibly overdetermined (i.e., linearly dependent) ordered set of vectors, and the correspondence from a subspace to this ordered set is continuous;

- this *continuous* correspondence cannot be achieved with an ordered set of basis (i.e., linearly independent) vectors;
- certain problems have solutions that depend continuously on the subspace and can be written elegantly in terms of the kernel:

$$\text{subspace} \rightarrow \text{kernel} \rightarrow \text{solution}. \quad (1.6)$$

The above will be described in greater detail in §2.

**Remark** The above example was chosen for its simplicity. Ironically, the general problem of projecting a point onto a subspace is not well-suited to the RKHS framework for several reasons, including that RKHS theory assumes there is a norm only on the subspace; if there is a norm on the larger space in which the subspace sits then it is ignored. A more typical optimisation problem benefitting from RKHS theory is finding the minimum-norm function passing through a finite number of given points; minimising the norm acts to regularise this interpolation problem; see §6.1.

### 1.3 Pointwise Coordinates and Canonical Coordinates

Aimed at readers already familiar with Hilbert space theory, this section motivates and defines two coordinate systems on a RKHS.

A separable Hilbert space  $\mathcal{H}$  possesses an orthonormal basis  $e_1, e_2, \dots \in \mathcal{H}$ . An arbitrary element  $v \in \mathcal{H}$  can be expressed as an infinite series  $v = \sum_{i=0}^{\infty} \alpha_i e_i$  where the “coordinates”  $\alpha_i$  are given by  $\alpha_i = \langle v, e_i \rangle$ . A classic example is using a Fourier series to represent a periodic function. The utility of such a construction is that an arbitrary element of  $\mathcal{H}$  can be written as the limit of a linear combination of a manageable set of fixed vectors.

RKHS theory generalises this ability of writing an arbitrary element of a Hilbert space as the limit of a linear combination of a manageable set of fixed vectors. If  $\mathcal{H} \subset \mathbb{R}^T$  is a (not necessarily separable) RKHS then an arbitrary element  $v \in \mathcal{H}$  can be expressed as the limit of a sequence  $v_1, v_2, \dots \in \mathcal{H}$  of vectors, each of which is a finite linear combination of the vectors  $\{K(\cdot, t) \mid t \in T\}$ , where  $K: T \times T \rightarrow \mathbb{R}$  is

the kernel of  $\mathcal{H}$ . It is this ability to represent an arbitrary element of a RKHS  $\mathcal{H}$  as the limit of a linear combination of the  $K(\cdot, t)$  that, for brevity, we refer to as the presence of a canonical coordinate system. The utility of this canonical coordinate system was hinted at in §1.2.

There is another natural coordinate system: since an element  $v$  of a RKHS  $\mathcal{H} \subset \mathbb{R}^T$  is a function from  $T$  to  $\mathbb{R}$ , its  $t$ th coordinate can be thought of as  $v(t)$ . The relationship between this pointwise coordinate system and the aforementioned canonical coordinates is that  $v(t) = \langle v, K(\cdot, t) \rangle$ . Note though that whereas an arbitrary linear combination of the  $K(\cdot, t)$  is guaranteed to be an element of  $\mathcal{H}$ , assigning values arbitrarily to the  $v(t)$ , i.e., writing down an arbitrary function  $v$ , may not yield an element of  $\mathcal{H}$ ; canonical coordinates are intrinsic whereas pointwise coordinates are extrinsic. The utility of the pointwise coordinate system is that limits in a RKHS can be determined pointwise: if  $v_k$  is a Cauchy sequence, implying there exists a  $v$  satisfying  $\|v_k - v\| \rightarrow 0$ , then  $v$  is fully determined by  $v(t) = \lim_k v_k(t)$ .

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