

# Self-study: Reproducing Kernel Hilbert Space

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# 1 Hilbert Space and Functional Analysis Basis

## 1.1 Complete Metric Space

- **Definition** A *metric space* is a set  $M$  and a real-valued function  $d(\cdot, \cdot) : M \times M \rightarrow \mathbb{R}$  which satisfies:

1. (**Non-Negativity**)  $d(x, y) \geq 0$
2. (**Definiteness**)  $d(x, y) = 0$  if and only if  $x = y$
3. (**Symmetric**)  $d(x, y) = d(y, x)$
4. (**Triangle Inequality**)  $d(x, z) \leq d(x, y) + d(y, z)$

The function  $d$  is called a **metric** on  $M$ . The metric space  $M$  equipped with metric  $d$  is denoted as  $(M, d)$ .

- **Definition** (**Cauchy Sequence**)  
A sequence of elements  $\{x_n\}$  of a metric space  $(M, d)$  is called a **Cauchy sequence** if  $\forall \epsilon > 0$ , there exists  $N \in \mathbb{N}$ , for all  $n, m \geq N$ ,  $d(x_n, x_m) < \epsilon$ .
- **Proposition 1.1** *Any convergent sequence is a Cauchy sequence.*

Note that this is the direct result of *triangle inequality property of a metric*.

- **Definition** (**Complete Metric Space**)  
A metric space in which *all Cauchy sequences converge* is called **complete**.
- **Definition** (**Denseness**)  
A set  $B$  in a metric space  $M$  is called **dense** if every  $m \in M$  is a limit of elements in  $B$ .
- **Definition** (**Continuity**)  
A function  $f : (X, d) \rightarrow (Y, p)$  is called **continuous** at  $x$  if  $f(x_n) \xrightarrow{p} f(x)$  whenever  $x_n \xrightarrow{d} x$ .
- **Definition** (**Isometry**)  
A **bijection**  $h : (X, d) \rightarrow (Y, p)$  which **preserves the metric**, that is,

$$p(h(x), h(y)) = d(x, y)$$

is called an **isometry**. It is automatically *continuous*.  $(X, d)$  and  $(Y, p)$  are said to be **isometric** if such an isometry exists.

- **Definition** (**Normed Linear Space**)  
A **normed linear space** is a vector space,  $V$ , over  $\mathbb{R}$  (or  $\mathbb{C}$ ) and a function,  $\|\cdot\| : V \rightarrow \mathbb{R}$  which satisfies:

1. (**Non-Negativity**):  $\|v\| \geq 0$  for all  $v$  in  $V$ ;
2. (**Positive Definiteness**):  $\|v\| = 0$  if and only if  $v = 0$ ;
3. (**Absolute Homogeneity**)  $\|\alpha v\| = |\alpha| \|v\|$  for all  $v$  in  $V$  and  $\alpha$  in  $\mathbb{R}$  (or  $\mathbb{C}$ )
4. (**Subadditivity / Triangle Inequality**)  $\|v + w\| \leq \|v\| + \|w\|$  for all  $v$  and  $w$  in  $V$

We denote the normed linear space as  $(V, \|\cdot\|)$ .

## 1.2 Hilbert Space

- **Definition** An *inner product space* (*pre-Hilbert space*)  $X$  is an abstract vector space possessing the structure of an inner product that allows length and angle to be measured. An inner product on  $X$  is a mapping on  $X \times X$  to a scale field  $E$  of  $X$ ; that is, for every pair  $\mathbf{x}, \mathbf{y} \in X$ , the associated scalar in  $E$  as the inner product, denoted as  $\langle \mathbf{x}, \mathbf{y} \rangle$  satisfies the following properties

1. Addition  $\langle \mathbf{x} + \mathbf{y}, \mathbf{z} \rangle = \langle \mathbf{x}, \mathbf{z} \rangle + \langle \mathbf{y}, \mathbf{z} \rangle$  for all  $\mathbf{x}, \mathbf{y}, \mathbf{z} \in X$ ;
2. Scalar product  $\langle a\mathbf{x}, \mathbf{y} \rangle = a \langle \mathbf{x}, \mathbf{y} \rangle$ , for all  $\mathbf{x}, \mathbf{y} \in X, a \in E$ ;
3. Hermitian  $\langle \mathbf{x}, \mathbf{y} \rangle = \overline{\langle \mathbf{y}, \mathbf{x} \rangle}$ ;
4. Nonnegative  $\langle \mathbf{x}, \mathbf{x} \rangle \geq 0$  with equality holds iff  $\mathbf{x} = \mathbf{0}$ .

- **Remark** A *norm* is induced by inner product via

$$\|\mathbf{x}\| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}$$

and a *metric* is defined via

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{\langle \mathbf{x} - \mathbf{y}, \mathbf{x} - \mathbf{y} \rangle} = \|\mathbf{x} - \mathbf{y}\|.$$

- **Definition** A *complete* inner product space is called a Hilbert space.

Inner product spaces are sometimes called *pre-Hilbert spaces*.

- **Remark** Consider a *complex* Hilbert space  $F_c$ , where a function  $f_1 + i f_2 \in F_c$  for every  $f_1, f_2 \in F$ , a Hilbert space of real valued functions. Note that  $\|f_1 + i f_2\|_2^2 = \|f_1\|_2^2 + \|f_2\|_2^2$ . The following property holds:

1. If  $f \in F_c$ , then  $\bar{f} \in F_c$ ;
2.  $\|f\| = \|\bar{f}\|$ .

- **Definition** (*Complete Orthonormal Basis*)

If  $S$  is an orthonormal set in a Hilbert space  $\mathcal{H}$  and no other orthonormal set contains  $S$  as a proper subset, then  $S$  is called an orthonormal basis (or a *complete orthonormal system*) for  $\mathcal{H}$ .

- **Theorem 1.2** (*Existence of Orthonormal Basis*)

Every Hilbert space  $\mathcal{H}$  has an *orthonormal basis*.

- **Proposition 1.3** (*Orthogonal Representation of Element in Hilbert Space*)

Let  $\mathcal{H}$  be a Hilbert space and  $S = (x_\alpha)_{\alpha \in A}$  an *orthonormal basis*. Then for each  $y \in \mathcal{H}$ ,

$$y = \sum_{\alpha \in A} \langle y, x_\alpha \rangle x_\alpha \tag{1}$$

and

$$\|y\|_{\mathcal{H}}^2 = \sum_{\alpha \in A} |\langle y, x_\alpha \rangle|^2 \tag{2}$$

The equality in (1) means that the sum on the right-hand side converges (independent of order) to  $y$  in  $\mathcal{H}$ . **Conversely**, if  $\sum_{\alpha \in A} |c_\alpha|^2 < \infty$ ,  $c_\alpha \in \mathbb{C}$ , then  $\sum_{\alpha \in A} c_\alpha x_\alpha$  converges to an element of  $\mathcal{H}$ .

- **Remark Orthogonality** is the central concept of Hilbert space. In the presence of closed subspaces, the orthogonality allows us to decompose the Hilbert space into the direct sum of the *subspace* and its *orthogonal complement*.

- **Definition (Direct Sum)**

Suppose that  $\mathcal{H}_1$  and  $\mathcal{H}_2$  are Hilbert spaces. Then the set of pairs  $(x, y)$  with  $x \in \mathcal{H}_1, y \in \mathcal{H}_2$  is a *Hilbert space* with *inner product*

$$\langle (x_1, y_1), (x_2, y_2) \rangle := \langle x_1, x_2 \rangle_{\mathcal{H}_1} + \langle y_1, y_2 \rangle_{\mathcal{H}_2}$$

This space is called **the direct sum** of the spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$  and is denoted by  $\mathcal{H}_1 \oplus \mathcal{H}_2$ .

- **Definition (Orthogonal Complement)**

Let  $\mathcal{M} \subseteq \mathcal{H}$  is a **closed** linear subspace of Hilbert space  $\mathcal{H}$  with induced inner product  $\langle \cdot, \cdot \rangle$  (i.e.  $\langle x, y \rangle_{\mathcal{M}} = \langle x, y \rangle_{\mathcal{H}}$  for all  $x, y \in \mathcal{M}$ ).  $\mathcal{M}$  is also a *Hilbert space*.

We denote by  $\mathcal{M}^\perp$  the set of vectors in  $\mathcal{H}$  which are *orthogonal* to  $\mathcal{M}$ ;  $\mathcal{M}^\perp$  is called **the orthogonal complement of  $\mathcal{M}$** . It follows from the linearity of the inner product that  $\mathcal{M}^\perp$  is a *linear subspace* of  $\mathcal{H}$  and an elementary argument shows that  $\mathcal{M}^\perp$  is *closed*. So  $\mathcal{M}^\perp$  is also a *Hilbert space*.

- **Lemma 1.4** Let  $\mathcal{H}$  be a Hilbert space,  $\mathcal{M}$  a closed subspace of  $\mathcal{H}$ , and suppose  $x \in \mathcal{H}$ . Then there exists in  $\mathcal{M}$  a **unique** element  $z$  **closest** to  $x$ .
- **Theorem 1.5 (The Projection Theorem)**  
Let  $\mathcal{H}$  be a Hilbert space,  $\mathcal{M}$  a closed subspace. Then every  $x \in \mathcal{H}$  can be **uniquely** written  $x = z + w$  where  $z \in \mathcal{M}$  and  $w \in \mathcal{M}^\perp$ .
- **Remark** The projection theorem sets up a natural *isomorphism*  $\mathcal{M} \oplus \mathcal{M}^\perp \rightarrow \mathcal{H}$  given by

$$(z, w) \mapsto z + w$$

We will often suppress the isomorphism and simply write  $\mathcal{H} = \mathcal{M} \oplus \mathcal{M}^\perp$ .

- **Definition (Separability)**

A metric space which has a **countable dense subset** is said to be **separable**.

- **Remark** Most Hilbert space we have seen is separable.

- **Proposition 1.6 (Canonical Hilbert Space)**

A Hilbert space  $\mathcal{H}$  is **separable** if and only if it has a **countable orthonormal basis**  $S$ . If there are  $N < \infty$  elements in  $S$ , then  $\mathcal{H}$  is **isomorphic** to  $\mathbb{C}^N$ , If there are **countably many** elements in  $S$ , then  $\mathcal{H}$  is **isomorphic** to  $\ell^2$ .

### 1.3 Bounded Linear Operator and Dual Space

- **Definition (Bounded Linear Operator)**

A **bounded linear transformation** (or **bounded operator**) is a mapping  $T : (X, \|\cdot\|_X) \rightarrow (Y, \|\cdot\|_Y)$  from a normed linear space  $X$  to a normed linear space  $Y$  that satisfies

1. (**Linearity**)  $T(\alpha x + \beta y) = \alpha T(x) + \beta T(y)$  for all  $x, y \in X$ ,  $\alpha, \beta \in \mathbb{R}$  or  $\mathbb{C}$
2. (**Boundedness**)  $\|Tx\|_Y \leq C \|x\|_X$  for small  $C \geq 0$ .

The smallest such  $C$  is called the norm of  $T$ , written  $\|T\|$  or  $\|T\|_{X,Y}$ . Thus

$$\|T\| := \sup_{\|x\|_X=1} \|Tx\|_Y$$

- **Remark** Denote the space of **all bounded linear operator** between Hilbert space  $\mathcal{H}_1$  and  $\mathcal{H}_2$  as  $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$ . The space  $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$  is linear space with norm

$$\|T\| := \sup_{\|x\|_{\mathcal{H}_1}=1} \|Tx\|_{\mathcal{H}_2}, \quad \forall T \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2).$$

It can be shown that  $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$  is a *complete normed space* (i.e. a *Banach space*).

- **Definition (Dual Space)**

The space  $\mathcal{L}(\mathcal{H}, \mathbb{C})$  is called the dual space of  $\mathcal{H}$  and is denoted by  $\mathcal{H}^*$ . The elements of  $\mathcal{H}^*$  are called continuous linear functionals. That is, the dual space  $\mathcal{H}^*$  is the space of *continuous linear functionals* on  $\mathcal{H}$ .

- **Remark** The *dual space*  $\mathcal{H}^*$  is also called **covector space** with respect to a vector space  $\mathcal{H}$  and the linear functionals are called **covectors**. This terms are mostly used in *differential geometry* when the vector space is *the tangent space*.
- **Theorem 1.7 (The Riesz Representation Theorem)** [Reed and Simon, 1980, Kreyszig, 1989, Conway, 2019]  
For each  $T \in \mathcal{H}^*$ , there is a **unique**  $y_T \in \mathcal{H}$  such that

$$T(x) = \langle x, y_T \rangle$$

for all  $x \in \mathcal{H}$ . In addition  $\|y_T\|_{\mathcal{H}} = \|T\|_{\mathcal{H}^*}$ .

- **Remark** The *the Riesz representation theorem* together with *the Cauchy-Schwarz inequality* defines an isomorphism  $\mathcal{H}^* \rightarrow \mathcal{H}$  between a Hilbert space  $\mathcal{H}$  and its dual  $\mathcal{H}^*$ . In other words, the bounded linear functional on Hilbert space has a simple form.
- **Corollary 1.8 (The Riesz Representation for Sesquilinear Form)**  
Let  $B(\cdot, \cdot)$  be a function from  $\mathcal{H} \times \mathcal{H}$  to  $\mathbb{C}$  which satisfies:

1. (**Linearity**)  $B(\alpha x + \beta y, z) = \alpha B(x, z) + \beta B(y, z)$
2. (**Conjugate Linearity**)  $B(x, \alpha y + \beta z) = \bar{\alpha} B(x, y) + \bar{\beta} B(x, z)$
3. (**Boundedness**)  $|B(x, y)| \leq C \|x\|_{\mathcal{H}} \|y\|_{\mathcal{H}}$

for all  $x, y, z \in \mathcal{H}$ ,  $\alpha, \beta \in \mathbb{C}$ . Then there is a **unique bounded linear transformation**  $A: \mathcal{H} \rightarrow \mathcal{H}$  so that

$$B(x, y) = \langle Ax, y \rangle$$

for all  $x, y \in \mathcal{H}$ . The **norm** of  $A$  is the smallest constant  $C$  such that (3) holds.

- **Remark** A bilinear function on  $\mathcal{H}$  obeying (1) and (2) is called a sesquilinear form (as a generalization of **blinear form** in complex vector space).

In terms of this, an inner product in complex vector space is **a complex Hermitian form** (also called a **symmetric sesquilinear form**).

## 1.4 Hilbert Adjoints and Self Adjoint Operator

- **Definition (*Hilbert Space Adjoint*)**

Let  $T : \mathcal{H}_1 \rightarrow \mathcal{H}_2$  be a *bounded linear operator*, where  $\mathcal{H}_1$  and  $\mathcal{H}_2$  are *Hilbert spaces*. Then **the Hilbert-adjoint operator  $T^*$**  of  $T$  is the operator

$$T^* : \mathcal{H}_2 \rightarrow \mathcal{H}_1$$

such that for all  $x \in \mathcal{H}_1$  and  $y \in \mathcal{H}_2$ ,

$$\langle Tx, y \rangle_{\mathcal{H}_2} = \langle x, T^*y \rangle_{\mathcal{H}_1} \quad (3)$$

- **Proposition 1.9 (*Existence of Adjoint Operator*)** [Kreyszig, 1989]

The Hilbert-adjoint operator  $T^*$  of  $T$  **exists, is unique and is a bounded linear operator with norm**

$$\|T^*\| = \|T\|.$$

- **Proposition 1.10 (*Properties of Hilbert-adjoint operators*)**. [Reed and Simon, 1980, Kreyszig, 1989]

Let  $\mathcal{H}_1, \mathcal{H}_2$  be Hilbert spaces,  $S : \mathcal{H}_1 \rightarrow \mathcal{H}_2$  and  $T : \mathcal{H}_1 \rightarrow \mathcal{H}_2$  bounded linear operators and  $\alpha$  any scalar. Then we have

1.  $\langle T^*y, x \rangle = \langle y, Tx \rangle, (x \in \mathcal{H}_1, y \in \mathcal{H}_2)$
2.  $(S + T)^* = S^* + T^*$
3.  $(\alpha T)^* = \alpha T^*$
4.  $(T^*)^* = T$
5.  $\|T^*T\| = \|TT^*\| = \|T\|^2$
6.  $T^*T = 0 \Leftrightarrow T = 0$
7.  $(ST)^* = T^*S^*$  (assuming  $\mathcal{H}_2 = \mathcal{H}_1$ )
8. If  $T$  has a **bounded inverse**,  $T^{-1}$ , then  $T^*$  has a **bounded inverse** and  $(T^*)^{-1} = (T^{-1})^*$ .

- **Definition** A **bounded linear operator**  $T : \mathcal{H} \rightarrow \mathcal{H}$  on a Hilbert space  $\mathcal{H}$  is said to be

1. **self-adjoint** or **Hermitian** if

$$T^* = T \quad \Leftrightarrow \quad \langle Tx, y \rangle = \langle x, Ty \rangle$$

2. **unitary** if  $T$  is *bijective* and

$$T^* = T^{-1}$$

3. normal if

$$T^*T = TT^*$$

- **Definition (*Projection Operator*)**

If  $P \in \mathcal{L}(\mathcal{H})$  and  $P^2 = P$ , then  $P$  is called a projection. If in addition  $P = P^*$ , then  $P$  is called an orthogonal projection.

- **Remark** If  $T$  is **self-adjoint** and **unitary**, then  $T$  is **normal**.

- **Proposition 1.11 (*Self-adjointness*)**. [Kreyszig, 1989]

Let  $T : \mathcal{H} \rightarrow \mathcal{H}$  be a bounded linear operator on a Hilbert space  $\mathcal{H}$ . Then:

1. If  $T$  is **self-adjoint**,  $\langle Tx, x \rangle$  is **real** for all  $x \in \mathcal{H}$ .
2. If  $\mathcal{H}$  is complex and  $\langle Tx, x \rangle$  is **real** for all  $x \in \mathcal{H}$ , the operator  $T$  is **self-adjoint**

- **Proposition 1.12 (*Self-adjointness of product*)**. [Kreyszig, 1989]

The product of two bounded **self-adjoint** linear operators  $S$  and  $T$  on a Hilbert space  $\mathcal{H}$  is **self-adjoint** if and only if the operators **commute**,

$$ST = TS.$$

- **Proposition 1.13 (*Sequences of self-adjoint operators*)**. [Kreyszig, 1989]

Let  $(T_n)$  be a sequence of **bounded self-adjoint** linear operators  $T_n : \mathcal{H} \rightarrow \mathcal{H}$  on a Hilbert space  $\mathcal{H}$ . Suppose that  $(T_n)$  converges, say,

$$T_n \rightarrow T, \quad \text{i.e. } \|T_n - T\| \rightarrow 0$$

where  $\|\cdot\|$  is the norm on the space  $\mathcal{L}(\mathcal{H}, \mathcal{H})$ . Then the limit operator  $T$  is a **bounded self-adjoint** linear operator on  $H$ .

- **Proposition 1.14 (*Unitary operator*)**. [Kreyszig, 1989]

Let the operators  $U : \mathcal{H} \rightarrow \mathcal{H}$  and  $V : \mathcal{H} \rightarrow \mathcal{H}$  be **unitary**; here,  $\mathcal{H}$  is a Hilbert space. Then:

1.  $U$  is **isometric**; thus  $\|Ux\| = \|x\|$  for all  $x \in \mathcal{H}$ ;
2.  $\|U\| = 1$ , provided  $\mathcal{H} \neq \{0\}$ ,
3.  $U^{-1} = U^*$  is **unitary**,
4.  $UV$  is **unitary**,
5.  $U$  is **normal**.
6. A bounded linear operator  $T$  on a complex Hilbert space  $\mathcal{H}$  is **unitary** if and only if  $T$  is **isometric** and **surjective**.

## 1.5 Regular Measure and Duality of $\mathcal{C}_0(X)$

- **Definition (*Subspace of Continuous Functions*)**

Let  $\mathcal{C}(X) := \mathcal{C}(X, \mathbb{R})$  be the space of **continuous** real-valued functions on topological space  $X$  and  $\mathcal{B}(X) := \mathcal{B}(X, \mathbb{R})$  be the space of **bounded** real-valued functions on  $X$ .

1. The intersection of  $\mathcal{B}(X)$  and  $\mathcal{C}(X)$  is the space of all **bounded continuous** functions

$$\mathcal{BC}(X) := \mathcal{BC}(X, \mathbb{R}) = \mathcal{B}(X, \mathbb{R}) \cap \mathcal{C}(X, \mathbb{R})$$

Note that  $\mathcal{BC}(X) \subseteq \mathcal{B}(X)$  is a **closed subspace**.

2. Define the **support** of a function  $f$ ,  $\text{supp}(f)$  as the **smallest closed set** outside of which  $f$  vanishes. The subset  $\mathcal{C}_c(X) \subseteq \mathcal{C}(X)$  is the space of all continuous functions with **compact support**

$$\mathcal{C}_c(X) = \{f \in \mathcal{C}(X, \mathbb{R}) : \text{supp}(f) \text{ is compact}\}.$$

Note that by *Tietze Extension Theorem*, the locally compact Hausdorff space  $X$  has a rich supply of continuous functions that vanishes outside a compact set.

3. Recall also that  $\mathcal{C}_0(X)$  is the space of continuous functions on  $X$  that **vanishes at infinity**, i.e. for all  $\epsilon > 0$ ,  $|f(x)| < \epsilon$  if  $x \in X \setminus C$  for some **compact subset**  $C \subseteq X$ .

$$\mathcal{C}_0(X) = \{f \in \mathcal{C}(X, \mathbb{R}) : f \text{ vanishes at infinity}\}.$$

Note that

$$\mathcal{C}_c(X) \subseteq \mathcal{C}_0(X) \subseteq \mathcal{BC}(X) \subseteq \mathcal{C}(X)$$

- **Definition (Radon Measure)** [Folland, 2013]

A **Radon measure**  $\mu$  on  $X$  is a Borel measure that is

1. **finite** on all compact sets; i.e. for any compact subset  $K \subseteq X$ ,

$$\mu(K) < \infty.$$

2. **outer regular** on all Borel sets; i.e. for any Borel set  $E$

$$\mu(E) = \inf \{\mu(U) : E \subseteq U, U \text{ is open}\}.$$

3. **inner regular** on all open sets; i.e. for any open set  $E$

$$\mu(E) = \sup \{\mu(C) : C \subseteq E, C \text{ is compact and Borel}\}.$$

- **Definition (Complex Radon Measure)**

A **signed Radon measure** is a **signed Borel measure** whose **positive** and **negative variations** are **Radon**, and a **complex Radon measure** is a **complex Borel measure** whose real and imaginary parts are signed Radon measures.

- **Definition (Space of Complex Radon Measures)**

On locally compact Hausdorff space  $X$ , We denote the space of complex Radon measures on  $X$  by  $\mathcal{M}(X)$ . For  $\mu \in \mathcal{M}(X)$  we define

$$\|\mu\| = |\mu|(X),$$

where  $|\mu|$  is the **total variation** of  $\mu$ .



- **Theorem 1.15** (*The Riesz-Markov Theorem, Locally Compact Version*) [Reed and Simon, 1980, Folland, 2013]

Let  $X$  be a **locally compact Hausdorff** space. For any continuous linear functional  $I$  on  $\mathcal{C}_0(X)$ , (the space of continuous functions on  $X$  that vanishes at infinity), there is a unique regular countably additive complex Borel measure  $\mu$  on  $X$  such that

$$I(f) = \int_X f d\mu, \quad \text{for all } f \in \mathcal{C}_0(X).$$

The norm of  $I$  as a linear functional is the total variation of  $\mu$ , that is

$$\|I\| = |\mu|(X).$$

Finally,  $I$  is **positive** if and only if the measure  $\mu$  is **non-negative**.

- **Remark** In other word, the map  $\mu \mapsto I_\mu$ , is an **isometric isomorphism** from  $\mathcal{M}(X)$  to  $(\mathcal{C}_0(X))^*$ , or

$$\mathcal{M}(X) \simeq (\mathcal{C}_0(X))^*.$$

- **Corollary 1.16** [Reed and Simon, 1980, Folland, 2013]

Let  $X$  be a **compact Hausdorff** space. Then the dual space  $\mathcal{C}(X)^*$  is **isometric isomorphism** to  $\mathcal{M}(X)$ .

- **Definition** Given  $\mathcal{M}(X) \simeq (\mathcal{C}_0(X))^*$ , we define subspaces of  $\mathcal{M}$ :

$$\begin{aligned} \mathcal{M}_+(X) &= \{I \in \mathcal{M}(X) : I \text{ is a positive linear functional}\}, \\ \mathcal{M}_{+,1}(X) &= \{I \in \mathcal{M}(X) : \|I\| = 1\}. \end{aligned}$$

Thus  $\mathcal{M}_+(X)$  is *identified* with **the space of all positive Radon measures on  $X$** .

- **Remark** (**Isometric Embedding of  $L^1(\mu)$  into  $\mathcal{M}(X)$** )

Let  $\mu$  be a fixed positive Radon measure on  $X$ . If  $f \in L^1(\mu)$ , the complex measure

$$d\nu_f = f d\mu$$

is easily seen to be **Radon**, and  $\|\nu\| = \int |f| d\mu = \|f\|_1$ . Thus  $f \mapsto \nu_f$  is an **isometric embedding** of  $L^1(\mu)$  into  $\mathcal{M}(X)$  whose range consists precisely of those  $\nu \in \mathcal{M}(X)$  such that  $\nu \ll \mu$ .

- **Proposition 1.17** ( **$\mathcal{M}(X)$  is Normed Linear Space**) [Folland, 2013]

If  $\mu$  is a **complex Borel measure**, then  $\mu$  is **Radon** if and only if  $|\mu|$  is **Radon**. Moreover,  $\mathcal{M}(X)$  is a vector space and  $\mu \mapsto \|\mu\|$  is a **norm** on it.

- **Remark** (**Two Perspectives of Measures**)

For regular Borel measure  $\mu$  or in general, Radon measures on **locally compact** space  $X$ , there are two perspectives:

1. **Nonegative set function on the  $\sigma$ -algebra  $\mathcal{A}$** : as a **measure of the volume** of a subset in  $X$ ;
2. **Positive linear functional on  $\mathcal{C}_0(X)$** : as a **integral** of compactly supported continuous functions with respect to **given measure**.

In some cases, it is important to think of **measures** not merely as individual objects but instead as *elements of  $(\mathcal{C}_0(X))^*$* , so that we can employ *geometric* ideas.

## 1.6 Spectrum of Bounded Linear Operator

- **Definition (*Resolvent and Spectrum*)**

Let  $T \in \mathcal{L}(X)$ . A complex number  $\lambda$  is said to be in the resolvent set  $\rho(T)$  of  $T$  if

$$\lambda I - T$$

is a bijection with a bounded inverse.

$$R_\lambda(T) := (\lambda I - T)^{-1}$$

is called the resolvent of  $T$  at  $\lambda$ . Note that  $R_\lambda(T)$  is defined on  $\text{Ran}(\lambda I - T)$ .

If  $\lambda \notin \rho(T)$ , then  $\lambda$  is said to be in the spectrum  $\sigma(T)$  of  $T$ .

- **Remark** The name “*resolvent*” is appropriate, since  $R_\lambda(T)$  helps to solve the equation  $(\lambda I - T)x = y$ . Thus,  $x = (\lambda I - T)^{-1}y = R_\lambda(T)y$  provided  $R_\lambda(T)$  exists.

- **Definition (*Point Spectrum, Continuous Spectrum and Residual Spectrum*)**

Let  $T \in \mathcal{L}(X)$

1. **Point Spectrum**: An  $x \neq 0$  which satisfies

$$Tx = \lambda x$$

$$\text{or } (\lambda I - T)x = 0, \quad \text{for some } \lambda \in \mathbb{C}$$

is called an eigenvector of  $T$ ;  $\lambda$  is called the corresponding eigenvalue.

If  $\lambda$  is an *eigenvalue*, then  $(\lambda I - T)$  is **not injective** (i.e.  $\text{Ker}(\lambda I - T) \neq \{0\}$ ) so  $\lambda$  is *in the spectrum of  $T$* . **The set of all eigenvalues** is called the point spectrum of  $T$ . It is denoted as  $\sigma_p(T)$ .

2. **Continuous Spectrum**: If  $\lambda$  is **not an eigenvalue** and if  $\text{Ran}(\lambda I - T)$  is **dense** but the resolvent  $R_\lambda(T)$  is **unbounded**, then  $\lambda$  is said to be in the continuous spectrum. It is denoted as  $\sigma_c(T)$ .

3. **Residual Spectrum**: If  $\lambda$  is **not an eigenvalue** and if  $\text{Ran}(\lambda I - T)$  is **not dense**, then  $\lambda$  is said to be in the residual spectrum. It is denoted as  $\sigma_r(T)$ .

- **Remark (*Pure Point Spectrum for Finite Dimensional Case*)**

If  $X$  is **finite dimensional** normed linear space,  $T \in \mathcal{L}(X)$  then  $\sigma_c(T) = \sigma_r(T) = \emptyset$ .

- **Remark** If  $X$  is a function space, the *eigenvectors* of linear operator  $T$  is called the **eigenfunctions** of  $T$ .

- **Definition (*Eigenspace of Linear Operator*)**

The subspace of domain  $D(T)$  consisting of  $\{0\}$  and **all eigenvectors** of  $T$  corresponding to an *eigenvalue*  $\lambda$  of  $T$  is called the eigenspace of  $T$  corresponding to that eigenvalue  $\lambda$ .

- **Definition (*Spectral Radius of Linear Operator*)**

Let

$$r(T) = \sup_{\lambda \in \sigma(T)} |\lambda|$$

$r(T)$  is called the spectral radius of  $T$ .

- **Proposition 1.18** (*Spectral Radius Calculation*) [Reed and Simon, 1980]  
Let  $X$  be a **Hilbert space**,  $T \in \mathcal{L}(X)$  and  $T$  is **self-adjoint**. Then

$$r(T) = \|T\|$$

- **Theorem 1.19** (*Spectrum and Resolvent of Adjoint*) (Phillips) [Reed and Simon, 1980]  
If  $X$  is a **Hilbert space** and  $T \in \mathcal{L}(X)$ , then

$$\sigma(T) = \sigma(T^*) \quad \text{and} \quad R_\lambda(T^*) = (R_\lambda(T))^*.$$

- **Proposition 1.20** (*Spectrum of Self-Adjoint Operator*) [Reed and Simon, 1980]  
Let  $T$  be a **self-adjoint operator** on a **Hilbert space**  $\mathcal{H}$ . Then,

1.  $T$  has **no residual spectrum**, i.e.  $\sigma_r(T) = \emptyset$ .
2.  $\sigma(T)$  is a subset of  $\mathbb{R}$ .
3. **Eigenvectors** corresponding to **distinct eigenvalues** of  $T$  are **orthogonal**.

- **Definition** (*Positive-Semidefinite Operator*)

Let  $\mathcal{H}$  be a **Hilbert space**. An operator  $B \in \mathcal{L}(\mathcal{H})$  is called **positive-semidefinite** if

$$\langle Bx, x \rangle \geq 0 \text{ for all } x \in \mathcal{H}.$$

We write  $B \succeq 0$  if  $B$  is **positive-semidefinite** and  $B \succeq A$  if  $(B - A) \succeq 0$ .

Similarly,  $B$  is called **positive-definite** if

$$\langle Bx, x \rangle > 0 \text{ for all } x \neq 0 \in \mathcal{H}.$$

The **positive semidefinite operator** is sometimes called **positive operator**.

- **Proposition 1.21** (*Positive Semi-Definiteness  $\Rightarrow$  Self-Adjoint*) [Reed and Simon, 1980]  
Every (bounded) **positive semidefinite operator** on a **complex Hilbert space** is **self-adjoint**.

**Theorem 1.22** (*Square Root Lemma*) [Reed and Simon, 1980]

Let  $A \in \mathcal{L}(\mathcal{H})$  and  $A \succeq 0$ . Then there is a **unique**  $B \in \mathcal{L}(\mathcal{H})$  with  $B \succeq 0$  and  $B^2 = A$ . Furthermore,  $B$  **commutes** with every bounded operator which commutes with  $A$ .

- **Definition** For  $A \in \mathcal{L}(\mathcal{H})$ , we can define **absolute value** of  $A$  as the square root of its normal operation

$$|A| := \sqrt{A^*A}$$

## 1.7 Compact Operator

- **Definition** (*Compact Operator*)

Let  $X$  and  $Y$  be *Banach spaces*. An operator  $T \in \mathcal{L}(X, Y)$  is called **compact** (or **completely continuous**) if  $T$  takes **bounded sets** in  $X$  into **precompact sets** in  $Y$ .

Equivalently,  $T$  is **compact** if and only if for every **bounded sequence**  $\{x_n\} \subseteq X$ ,  $\{Tx_n\}$  has a **subsequence convergent** in  $Y$ .

- **Example (*Finite Rank Operators*)**

Suppose that the **range** of  $T$  is **finite dimensional**. That is, every vector in the range of  $T$  can be written

$$Tx = \sum_{i=1}^n \alpha_i y_i,$$

for some fixed family  $\{y_i\}_{i=1}^n$  in  $Y$ . If  $x_n$  is any *bounded sequence* in  $X$ , the corresponding  $\alpha_i^{(n)}$  are *bounded* since  $T$  is *bounded*. The usual subsequence trick allows one to extract a *convergent subsequence* from  $\{Tx_n\}$  which proves that  $T$  is *compact*. ■

- An important property of the compact operator is

**Theorem 1.23 (*Weakly Convergent + Compact Operator = Uniformly Convergent*)** [Reed and Simon, 1980]

A **compact** operator maps **weakly convergent** sequences into **norm convergent** sequences; i.e. if  $T \in \mathcal{L}(X)$  is compact, then

$$x_n \xrightarrow{w} x \quad \Rightarrow \quad Tx_n \xrightarrow{norm} Tx.$$

The converse holds true if  $X$  is **reflective**.

- **Theorem 1.24 (*Compact Operator Approximated by Finite Rank Operator*)** [Reed and Simon, 1980]

Let  $\mathcal{H}$  be a **separable Hilbert space**. Then every **compact operator** on  $\mathcal{H}$  is the **norm limit** of a sequence of operators of **finite rank**.

- **Theorem 1.25 (*Analytic Fredholm Theorem*)** [Reed and Simon, 1980]

Let  $D$  be an **open connected** subset of  $\mathbb{C}$ . Let  $f : D \rightarrow \mathcal{L}(\mathcal{H})$  be an **analytic operator-valued function** such that  $f(z)$  is **compact** for each  $z \in D$ . Then, either

1.  $(I - f(z))^{-1}$  exists for **no**  $z \in D$ ; or
2.  $(I - f(z))^{-1}$  exists for **all**  $z \in D \setminus S$  where  $S$  is a **discrete** subset of  $D$  (i.e.  $S$  is a set which has no limit points in  $D$ .) In this case,  $(I - f(z))^{-1}$  is **meromorphic** in  $D$ , **analytic** in  $D \setminus S$ , the **residues** at the poles are **finite rank operators**, and if  $z \in S$  then

$$f(z)\varphi = \varphi$$

has a **nonzero solution** in  $\mathcal{H}$

- **Corollary 1.26 (*The Fredholm Alternative*)** [Reed and Simon, 1980]

If  $A$  is a **compact operator** on  $\mathcal{H}$ , then **either**  $(I - A)^{-1}$  exists **or**  $\varphi = \varphi$  has a solution.

- **Theorem 1.27 (*Riesz-Schauder Theorem*)** [Reed and Simon, 1980]

Let  $A$  be a **compact operator** on  $\mathcal{H}$ , then  $\sigma(A)$  is a **discrete set** having **no limit points except perhaps**  $\lambda = 0$ .

Further, any **nonzero**  $\lambda \in \sigma(A)$  is an **eigenvalue** of **finite multiplicity** (i.e. the corresponding space of eigenvectors is **finite dimensional**).

- **Remark (*Compact Operator has only Nonzero Point Spectrum with Finite Dimensional Eigenspace*)**

*Riesz-Schauder Theorem* states that the **spectrum** for **compact** operator on **Hilbert** space consists of *only* the point spectrum besides  $\lambda = 0$ .

Moreover, the **eigenspace** corresponding to each **nonzero eigenvalue** is *finite dimensional*.

- **Theorem 1.28 (The Hilbert-Schmidt Theorem)** [Reed and Simon, 1980]  
Let  $A$  be a **self-adjoint compact operator** on  $\mathcal{H}$ . Then, there is a **complete orthonormal basis**,  $\{\phi_n\}_{n=1}^{\infty}$ , for  $\mathcal{H}$  so that

$$A\phi_n = \lambda_n \phi_n$$

and  $\lambda_n \rightarrow 0$  as  $n \rightarrow \infty$ .

- **Remark (Eigendecomposition of Hilbert Space based on Self-Adjoint Compact Operator)**  
In other word, given a self-adjoint compact operator  $A$  on  $\mathcal{H}$ , the Hilbert space  $\mathcal{H}$  is the direct sum of eigenspaces of  $A$ .

$$\mathcal{H} = \bigoplus_{\lambda_n \in \sigma(A) \subset \mathbb{R}} \text{Ker}(\lambda_n I - A)$$

A **self-adjoint compact operator** on  $\mathcal{H}$  is the closest counterpart of **Hermitian matrix** / **Symmetric Real matrix** in infinite dimensional space.

- **Theorem 1.29 (Canonical Form for Compact Operators)** [Reed and Simon, 1980]  
Let  $A$  be a **compact** operator on  $\mathcal{H}$ . Then there exist (*not necessarily complete*) **orthonormal sets**  $\{\psi_n\}_{n=1}^N$  and  $\{\phi_n\}_{n=1}^N$  and **positive real numbers**  $\{\lambda_n\}_{n=1}^N$  with  $\lambda_n \rightarrow 0$  so that

$$A = \sum_{n=1}^N \lambda_n \langle \psi_n, \cdot \rangle \phi_n \quad (4)$$

The sum in (4), which may be finite or infinite, **converges in norm**. The numbers,  $\{\lambda_n\}_{n=1}^N$ , are called the **singular values of  $A$** .

## 1.8 Trace Class and Hilbert-Schmidt Operators

- **Definition (Trace of Positive Semi-Definite Operator)**  
Let  $\mathcal{H}$  be a **separable Hilbert space**,  $\{\phi_n\}_{n=1}^{\infty}$  an **orthonormal basis** Then for any **positive semi-definite** operator  $A \in \mathcal{L}(\mathcal{H})$ , we define

$$\text{tr}(A) = \sum_{n=1}^{\infty} \langle A\phi_n, \phi_n \rangle$$

The number  $\text{tr}(A)$  is called **the trace of  $A$** .

- **Remark (Trace of General Linear Operator)**  
Let  $A \in \mathcal{L}(\mathcal{H})$  be a bounded linear operator on separable Hilbert space. Instead of considering the trace of  $A$ , we consider the trace of absolute value of  $A$ ,

$$\text{tr}(|A|) = \text{tr}(\sqrt{A^*A}).$$

• **Definition (*Hilbert-Schmidt Operator*)**

An operator  $T \in \mathcal{L}(\mathcal{H})$  is called **Hilbert-Schmidt** if and only if

$$\text{tr}(T^*T) < \infty.$$

The family of all Hilbert-Schmidt operators is denoted by  $\mathcal{B}_2(\mathcal{H})$  or  $\mathcal{B}_{HS}(\mathcal{H})$ .

• **Proposition 1.30 (*Space of Hilbert-Schmidt Operator*)** [Reed and Simon, 1980]

1. The space of all Hilbert-Schmidt operators  $\mathcal{B}_2(\mathcal{H})$  is a **\*-ideal** in  $\mathcal{L}(\mathcal{H})$ ,
2. (**Inner Product**): If  $A, B \in \mathcal{B}_2(\mathcal{H})$ , then for **any orthonormal basis**  $\{\varphi_n\}_{n=1}^\infty$ ,

$$\sum_{n=1}^{\infty} \langle A^* B \varphi_n, \varphi_n \rangle$$

is **absolutely summable**, and its **limit**, denoted by  $\langle A, B \rangle_{HS}$ , is **independent** of the orthonormal basis chosen, i.e.

$$\langle A, B \rangle_{HS} = \text{tr}(A^* B)$$

3.  $\mathcal{B}_2(\mathcal{H})$  with inner product  $\langle \cdot, \cdot \rangle_{HS}$  is a **Hilbert space**.
4. (**Norm**): Let  $\|\cdot\|_2$  be defined in  $\mathcal{B}_2(\mathcal{H})$  by

$$\|A\|_2 := \sqrt{\langle A, A \rangle_{HS}} = \sqrt{\text{tr}(A^* A)}.$$

Then

$$\|A\| \leq \|A\|_2 \leq \|A\|_1, \quad \text{and} \quad \|A\|_2 = \|A^*\|_2$$

5. (**Compactness**) Every  $A \in \mathcal{B}_2(\mathcal{H})$  is **compact** and a **compact operator**,  $A$ , is in  $\mathcal{B}_2(\mathcal{H})$  **if and only if**

$$\sum_{n=1}^{\infty} \lambda_n^2 < \infty$$

where  $\{\lambda_n\}$  are the **singular values** of  $A$ .

6. (**Finite Rank Approximation**) The **finite rank operators** are  $\|\cdot\|_2$ -dense in  $\mathcal{B}_2(\mathcal{H})$ .
7.  $A \in \mathcal{B}_2(\mathcal{H})$  **if and only if**

$$\{\|A\varphi_n\|\}_{n=1}^\infty \in \ell^2$$

for **some** orthonormal basis  $\{\varphi_n\}_{n=1}^\infty$ .

8.  $A \in \mathcal{B}_1(\mathcal{H})$  if and only if  $A = BC$  with  $B, C \in \mathcal{B}_2(\mathcal{H})$ .
9.  $\mathcal{B}_2(\mathcal{H})$  is not  $\|\cdot\|$ -closed in  $\mathcal{L}(\mathcal{H})$ .

- **Theorem 1.31 (Hilbert-Schmidt Operator of  $L^2$  Space)** [Reed and Simon, 1980]  
Let  $(M, \mu)$  be a **measure space** and  $\mathcal{H} = L^2(M, \mu)$ . Then  $T \in \mathcal{L}(\mathcal{H})$  is **Hilbert-Schmidt** if **and only if** there is a function

$$K \in L^2(M \times M, \mu \otimes \mu)$$

with

$$(Tf)(x) = \int_M K(x, y)f(y)d\mu(y),$$

Moreover,

$$\|T\|_2^2 = \int_{M \times M} |K(x, y)|^2 d\mu(x)d\mu(y).$$

- **Definition (Kernel of Integral Operator)**  
Consider the simple operator  $T_K$ , defined in  $\mathcal{C}[0, 1]$  by

$$(T_K f)(x) = \int_0^1 K(x, y)f(y)dy,$$

where the function  $K(x, y)$  is *continuous* on the square  $0 \leq x, y \leq 1$ .  $T_K$  is called an **integral kernel operator** and  $K(x, y)$  is called **the kernel** of the integral operator  $T_K$ .

- **Remark (Properties of Integral Kernel Operator)**  
We summary some important property of the integral kernel operator  $T_K$ :

1.  $T_K$  is **compact operator** on  $\mathcal{C}[0, 1]$ .
2. For  $K^*(x, y) := \overline{K(y, x)}$ ,

$$(T_K)^* = T_{K^*}$$

3. Let  $B_M$  denote the functions  $f$  in  $\mathcal{C}[0, 1]$  such that  $\|f\|_\infty \leq M$ , i.e. closed  $\|\cdot\|_\infty$ -ball in  $\mathcal{C}[0, 1]$

$$B_M := \{f \in \mathcal{C}[0, 1] : \|f\|_\infty \leq M\}$$

The set of functions  $T_K(B_M) := \{T_K f : f \in B_M\}$  is **equicontinuous**.

4. The **operator norm** of  $T_K$  is **bounded above** by the  $L^2$  **norm** of kernel function  $K$

$$\|T_K\| \leq \|K\|_{L^2}$$

5. The eigenfunctions of  $T_K$ ,  $\{\varphi_n\}_{n=1}^\infty$ , forms a complete orthonormal basis in  $L^2(M, \mu)$ .  
Then

$$K(x, y) = \sum_{n=1}^{\infty} \lambda_n \varphi_n(x) \overline{\varphi_n(y)}$$

where  $\lambda_n$  is the eigenvalue corresponding to eigenfunction  $\varphi_n$ .

- **Theorem 1.32 (Mercer's Theorem)**

Suppose  $\Omega$  is a **compact domain** and  $T$  is a **positive Hilbert-Schmidt operator** on  $L^2(\Omega)$ . If the integral kernel  $K(\cdot, \cdot)$  is **continuous** on  $\Omega \times \Omega$ , then the **eigenfunction**  $\varphi_k$  is **continuous** on  $\Omega$  if  $\lambda_k > 0$ , and the expansion

$$K(x, y) = \sum_{n=1}^{\infty} \lambda_n \varphi_n(x) \overline{\varphi_n(y)}$$

converges **uniformly** on **compact sets**.

## 2 Reproducing Kernel Hilbert Space (RKHS)

### 2.1 Definitions

- **Definition (Evaluation Functional)**

Let  $X$  be a space,  $\mathcal{H}$  be the *Hilbert space* of complex-valued functions on  $X$ , a linear functional  $\delta_x : \mathcal{H} \rightarrow \mathbb{C}$  is called an **evaluation functional** if

$$\delta_x(f) = f(x), \quad \forall f \in \mathcal{H}$$

That is,  $\delta_x$  evaluates each function  $f \in \mathcal{H}$  at a point  $x$ .

- **Definition (Reproducing Kernel Hilbert Space)**

A Hilbert space  $\mathcal{H}$  is a **reproducing kernel Hilbert space (RKHS)** if, **for all  $x$  in  $X$** , the evaluation functional  $\delta_x$  is **bounded linear operator** on  $\mathcal{H}$ , i.e. there exists some  $M_x > 0$  such that

$$|\delta_x(f)| := |f(x)| \leq M_x \|f\|_{\mathcal{H}} \quad \forall f \in \mathcal{H}.$$

Equivalently, for every  $x \in X$ ,  $\delta_x$  is **continuous at every  $f$  in  $\mathcal{H}$**

- **Remark**

$$\mathcal{H} \text{ is a RKHS} \Leftrightarrow \delta_x \in \mathcal{H}^*, \forall x \in X$$

- **Remark (Unique Representation of Evaluation Functional at Each Point)**

If  $\mathcal{H}$  is a *reproducing kernel Hilbert space*,  $\delta_x \in \mathcal{H}^*$ , then the *Riesz Representation theorem* implies that for all  $x \in X$ , there exists a **unique function**  $k_x \in \mathcal{H}$  so that

$$\begin{aligned} \delta_x &= \langle \cdot, k_x \rangle \\ \Rightarrow f(x) &= \delta_x(f) = \langle f, k_x \rangle, \forall f \in \mathcal{H} \end{aligned}$$

Note that  $k_x : X \rightarrow \mathbb{C}$  is a complex-valued function on  $X$ , so

$$k_x(y) := \delta_y(k_x) = \langle k_x, k_y \rangle := K(x, y)$$

where the complex-valued function  $K : X \times X \rightarrow \mathbb{C}$  is called a **reproducing kernel**

- **Definition (Reproducing Kernel)**

Let  $\mathcal{H}$  be a class of functions on  $X$  forming a Hilbert space (complex in the latter, but possibly real). A function  $K : X \times X \rightarrow \mathbb{C}$  is called a **reproducing kernel (r.k.)** of  $\mathcal{H}$ , if



1. For every  $x \in X$ , the kernel  $K(x, \cdot)$  as a function belongs to  $\mathcal{H}$ ; i.e.,  $K(x, \cdot) := k_x \in \mathcal{H}$ ;
2. The **reproducing property**: for every  $x \in X$  and every  $f \in \mathcal{H}$ ,

$$f(x) = \delta_x(f) = \langle f, k_x \rangle_{\mathcal{H}} = \langle f, K(x, \cdot) \rangle_{\mathcal{H}} \quad (5)$$

• **Remark (Reproducing Kernel via Inner Product in RKHS)**

We can define *the reproducing kernel*  $K : X \times X \rightarrow \mathbb{C}$  using *the inner product*

$$K(x, y) = \langle k_x, k_y \rangle_{\mathcal{H}}, \quad \forall x, y \in X$$

where  $k_x, k_y \in \mathcal{H}$  correspond to evaluation functionals  $\delta_x$  and  $\delta_y$  in RKHS  $\mathcal{H}$ , respectively.

Equivalently, we can the following equation:

$$K(x, y) = \langle K(x, \cdot), K(y, \cdot) \rangle_{\mathcal{H}}$$

• **Remark** The following properties hold for reproducing kernels:

1. (**Existence**). The existence of reproducing kernel  $K$  is based on the definition of RKHS  $\mathcal{H}$  that  $\delta_x \in \mathcal{H}^*$  for all  $x \in X$ . Then by *the Riesz representation theorem (Riesz Lemma)*, we can find a unique  $k_x$  corresponding to  $\delta_x$  so that  $K(x, y) := \delta_y(k_x) = \langle k_x, k_y \rangle$ .
2. (**Uniqueness**) If a reproducing kernel  $K(x, y)$  exists, it is **unique**. This is due to *the Riesz representation theorem (Riesz Lemma)*.
3. (**Positive Semi-Definite**)  $K(x, y)$  is **positive semidefinite** in  $X$ ; i.e.,

$$\sum_{i,j=1}^n K(x_i, x_j) \xi_i \bar{\xi}_j \geq 0$$

for all  $x_1, \dots, x_n \in X$  and all  $\xi_1, \dots, \xi_n \in \mathbb{C}$ . It follows that

$$\begin{aligned} \sum_{i,j=1}^n K(x_i, x_j) \xi_i \bar{\xi}_j &= \sum_{i,j=1}^n \langle k_{x_i}, k_{x_j} \rangle_{\mathcal{H}} \xi_i \bar{\xi}_j \\ &= \left\langle \sum_{i=1}^n \xi_i k_{x_i}, \sum_{j=1}^n \xi_j k_{x_j} \right\rangle_{\mathcal{H}} \\ &= \left\| \sum_{i=1}^n \xi_i k_{x_i} \right\|_{\mathcal{H}}^2 \geq 0 \quad \blacksquare \end{aligned}$$

4. (**Hermitian**):  $K(x, y)$  is *Hermitian* i.e.

$$K(x, y) = \overline{K(y, x)}$$

This is due to the Hermitian property of inner product.

5. (**Cauchy-Schwartz Inequality**)

$$|K(x, y)|^2 \leq K(x, x)^{1/2} K(y, y)^{1/2}.$$

## 2.2 Properties

- **Proposition 2.1 (Closed Subspace)**

A **closed linear subspace**  $\mathcal{F}$  of reproducing kernel Hilbert space  $\mathcal{H}$  is a reproducing kernel Hilbert space with the reproducing kernel  $K_{\mathcal{F}} = K|_{\mathcal{F}}$ .

- **Proposition 2.2 (Orthogonal Complements)**

If  $\mathcal{H}'$  and  $\mathcal{H}''$  are **complementary** subspaces of  $\mathcal{H}$ , i.e.  $\mathcal{H} = \mathcal{H}' \oplus \mathcal{H}''$ , then their reproducing kernels satisfy the equation  $K' + K'' = K$ .

- **Remark (Projection via Reproducing Kernel)**

If the class  $\mathcal{F}$  with the reproducing kernel  $K$  is a *subspace* of a larger Hilbert space  $\mathcal{H}$ , then the formula

$$f(x) = \langle h, K(x, \cdot) \rangle_{\mathcal{H}},$$

gives the projection  $f$  of  $h \in \mathcal{H}$  in  $\mathcal{F}$ .

- **Proposition 2.3** If  $K$  is the reproducing kernel of the class  $F$  with the norm  $\|\cdot\|$ , and if the linear class  $F_1 \subset F$  forms a Hilbert space with the norm  $\|\cdot\|_1$  such that  $\|f_1\|_1 \geq \|f_1\|$  for every  $f_1 \in F_1$ , then the class  $F_1$  possesses a reproducing kernel  $K_1$  satisfying  $K_1 \preceq K$ ; i.e.,  $K - K_1$  is positive definite.

## 2.3 Convergence Properties

- **Remark** Recall different convergence:

1. **Definition (Pointwise Convergence).** [Kreyszig, 1989]

A sequence  $(f_n)$  in a normed space  $\mathcal{H}$  is said to be **pointwise convergent** (or **convergent in pointwise topology**) if there is an  $f \in \mathcal{H}$  such that for every  $x \in X$

$$\lim_{n \rightarrow \infty} f_n(x) = f(x).$$

2. **Definition (Strong Convergence).** [Kreyszig, 1989]

A sequence  $(f_n)$  in a normed space  $\mathcal{H}$  is said to be **strongly convergent** (or **convergent in the norm**) if there is an  $f \in \mathcal{H}$  such that

$$\lim_{n \rightarrow \infty} \|f_n - f\| = 0.$$

This is written  $\lim_{n \rightarrow \infty} f_n = f$  or simply  $f_n \rightarrow f$  is called *the strong limit* of  $(f_n)$ , and we say that  $(f_n)$  **converges strongly** to  $f$ .

3. **Definition (Weak Convergence).** [Kreyszig, 1989]

A sequence  $(f_n)$  in a normed space  $\mathcal{H}$  is said to be **weakly convergent** if there is an  $f \in \mathcal{H}$  such that for every  $I \in \mathcal{H}^*$ ,

$$\lim_{n \rightarrow \infty} I(f_n) = I(f).$$

This is written  $f_n \xrightarrow{w} f$  or  $f_n \rightharpoonup f$ . The element  $f$  is called *the weak limit* of  $(f_n)$ , and we say that  $(f_n)$  **converges weakly** to  $f$ .

• **Proposition 2.4** (*Convergence in Norm leads to Pointwise Convergence*)

If the class  $\mathcal{H}$  possesses a reproducing kernel  $K(x, y)$ , every sequence of functions  $\{f_n\}$  which converges **strongly** to a function  $f$  in the Hilbert space  $\mathcal{H}$ , converges also **at every point** in the ordinary sense, i.e.

$$\|f_n - f\|_{\mathcal{H}} \rightarrow 0 \Rightarrow f_n(x) \rightarrow f(x), \quad \text{for each } x \in X$$

This convergence becomes **uniform** in every subset of  $E$  in which  $K(x, y)$  is **uniformly bounded**.

**Proof:** This follows from

$$\begin{aligned} |f(x) - f_n(x)| &= |\langle f - f_n, K(x, \cdot) \rangle_{\mathcal{H}}| \\ &\leq \|f - f_n\| \|K(x, \cdot)\| = \|f - f_n\| K(x, x)^{1/2}. \end{aligned} \quad (6)$$

Thus  $\|f - f_n\| \rightarrow 0$  leads to  $|f(x) - f_n(x)| \rightarrow 0$  for every  $x \in X$ .

If  $\{f_n\}$  converges **weakly** to  $f$ ; i.e.,  $\langle f_n, K(x, \cdot) \rangle \rightarrow \langle f, K(x, \cdot) \rangle$  for every  $x \in X$ , we have again  $f_n(x) \rightarrow f(x)$  for every  $x$ . That is, in RKHS,

$$\text{strong convergence} \Rightarrow \text{weak convergence} \Rightarrow \text{pointwise convergence}$$

there exists non-increasing nested sets  $E_1 \supset E_2 \supset \dots$  in which  $f_n$  **uniformly** converges to  $f$ . Let  $E = \lim_{n \rightarrow \infty} E_n = \bigcap_n E_n$ . Moreover, if  $x \mapsto K(x, \cdot)$  is a transformation that is *continuous* from  $X$  to a subset of  $\mathcal{H}$ , then in every **compact**  $E_1 \subset E$ ,  $f_n$  converges **uniformly** to  $f$  and it transforms to a **compact subset** of  $\mathcal{H}$ .

To see that, for every  $\epsilon > 0$ ,  $\exists(x_1, \dots, x_n) \subset E_1$  such that for every  $x \in E_1$ , there exists at least one  $x_k$  such that  $\|K(x, \cdot) - K(x_k, \cdot)\| \leq \epsilon/4 \|f\| \leq \epsilon/4 M$  for  $M = \sup_{x \in E} \|f(x)\|$ . Further if we choose  $n_0$ , so that  $n > n_0$ ,  $|f(x_k) - f_n(x_k)| \leq \epsilon/4$ , then for the selected  $x \in E_1$ , the following holds

$$\begin{aligned} |f(x) - f_n(x)| &\leq |f(x_k) - f_n(x_k)| + |\langle f(x) - f_n(x), K(x, \cdot) - K(x_k, \cdot) \rangle| \\ &\leq \frac{\epsilon}{4} + \|f - f_n\| \|K(x, \cdot) - K(x_k, \cdot)\| \\ &\leq \frac{\epsilon}{4} + 2M \frac{\epsilon}{4M} < \epsilon. \end{aligned}$$

The *continuity* of the correspondence  $x \mapsto K(x, \cdot)$  is equivalent to **equicontinuity** of all functions of  $\mathcal{H}$  with  $\|f(x)\| < M$  for any  $M > 0$ . ■

• **Remark** In reproducing kernel Hilbert space,

$$\text{strong (norm) convergence} \Rightarrow \text{weak convergence} \Rightarrow \text{pointwise convergence}$$

## 2.4 Construction from Hermitian Positive Definite Kernel

• **Definition** Let  $X$  be a nonempty set. A *Hermitian form*  $K : X \times X \rightarrow \mathbb{C}$  is called a **positive-definite (p.d.) kernel** on  $X$  if

$$\sum_{i=1}^n \sum_{j=1}^n c_i \bar{c}_j K(x_i, x_j) \geq 0$$

holds for any  $x_1, \dots, x_n \in X$ , given  $n \in \mathbb{N}$ ,  $c_1, \dots, c_n \in \mathbb{C}$ .

- In this section, we show that a RKHS can be constructed from any positive definite kernels:

**Theorem 2.5 (RKHS from Positive Definite Kernel) (Moore-Aronszajn)**

Suppose  $K$  is a **symmetric, positive definite kernel** on a set  $X$ . Then there is a **unique Hilbert space** of functions on  $X$  for which  $K$  is a **reproducing kernel**.

**Proof:** For all  $x \in X$ , define  $K_x := K(x, \cdot)$ . Let  $\mathcal{H}_0$  be the linear span of  $\{K_x : x \in X\}$ , that is, it is the space of functions of the form

$$\sum_{k=1}^n \xi_k K_{x_k}$$

where  $x_1, x_2, \dots, x_n \in X$  and  $\xi_1, \xi_2, \dots, \xi_n \in \mathbb{C}$ . Define an inner product on  $\mathcal{H}_0$  by

$$\left\langle \sum_{k=1}^n \xi_k K_{x_k}, \sum_{j=1}^m \eta_j K_{y_j} \right\rangle_{\mathcal{H}_0} := \sum_{i=1}^n \sum_{j=1}^m K(x_i, y_j) \xi_i \bar{\eta}_j.$$

which implies  $K(x, y) = \langle K_x, K_y \rangle_{\mathcal{H}_0}$ . It is an inner product due to symmetric and positive definite property of kernel  $K$ .

Let  $\mathcal{H}$  be the completion of  $\mathcal{H}_0$  with respect to this inner product. Then  $\mathcal{H}$  consists of functions of the form

$$f := \sum_{k=1}^{\infty} \xi_k K_{x_k}$$

where

$$\lim_{n \rightarrow \infty} \sup_{p \geq 0} \left\| \sum_{i=n}^{n+p} \xi_i K_{x_i} \right\|_{\mathcal{H}_0}^2 = 0$$

Now we can check the reproducing property

$$\langle f, K_x \rangle_{\mathcal{H}} = \left\langle \sum_{k=1}^{\infty} \xi_k K_{x_k}, K_x \right\rangle_{\mathcal{H}} = \sum_{k=1}^{\infty} \xi_k \langle K_{x_k}, K_x \rangle_{\mathcal{H}} = \sum_{k=1}^{\infty} \xi_k K(x_k, x) = f(x)$$

To prove **uniqueness**, let  $\mathcal{G}$  be *another Hilbert space* of functions for which  $K$  is a reproducing kernel. For every  $x$  and  $y$  in  $X$ , the reproducing property implies that

$$\langle K_x, K_y \rangle_{\mathcal{H}} = K(x, y) = \langle K_x, K_y \rangle_{\mathcal{G}}.$$

By linearity,  $\langle \cdot, \cdot \rangle_{\mathcal{H}} = \langle \cdot, \cdot \rangle_{\mathcal{G}}$  on the span of  $\{K_x : x \in X\}$ . Then  $\mathcal{H} \subseteq \mathcal{G}$  because  $\mathcal{G}$  is complete and contains  $\mathcal{H}_0$  and hence contains its completion.

Now we need to prove that every element of  $\mathcal{G}$  is in  $\mathcal{H}$ . Let  $f$  be an element of  $\mathcal{G}$ . Since  $\mathcal{H}$  is a *closed subspace* of  $\mathcal{G}$ , we can write  $f = f_{\mathcal{H}} + f_{\mathcal{H}^\perp}$  where  $f_{\mathcal{H}} \in \mathcal{H}$  and  $f_{\mathcal{H}^\perp} \in \mathcal{H}^\perp$ . Now if  $x \in X$  then, since  $K$  is a reproducing kernel of  $\mathcal{G}$  and  $\mathcal{H}$ :

$$\begin{aligned} f(x) &= \langle K_x, f \rangle_{\mathcal{G}} = \langle K_x, f_{\mathcal{H}} \rangle_{\mathcal{G}} + \langle K_x, f_{\mathcal{H}^\perp} \rangle_{\mathcal{G}} \\ &= \langle K_x, f_{\mathcal{H}} \rangle_{\mathcal{G}} \\ &= \langle K_x, f_{\mathcal{H}} \rangle_{\mathcal{H}} = f_{\mathcal{H}}(x) \end{aligned}$$

where we have used the fact that  $K_x$  belongs to  $\mathcal{H}$  so that its inner product with  $f_{\mathcal{H}^\perp}$  in  $\mathcal{G}$  is zero. This shows that  $f = f_{\mathcal{H}}$  in  $\mathcal{G}$ . ■

## 2.5 Construction from Integral Kernel Operator on Compact Space

- **Remark (*Integral Operator*)**

Let  $X$  be a **compact** space equipped with a *strictly positive finite Borel measure*  $\mu$  and  $K : X \times X \rightarrow \mathbb{R}$  a **continuous, symmetric, and positive definite function**. We can define a linear operator  $T_K$  on  $L^2(X, \mu)$  by

$$(T_K f)(x) := \int_X K(x, y) f(y) d\mu(y),$$

i.e.  $T_K$  is a **integral kernel operator** on  $L^2(X, \mu)$ .

- **Remark (*RKHS from Integral Kernel Operator*)**

We see that

1.  $T_K \in \mathcal{B}_2(L^2(X, \mu))$  is a *Hilbert-Schmidt operator*, thus
2.  $T_K$  is a **compact operator**.
3.  $T_K$  is a **self-adjoint, positive semi-definite** operator on  $L^2(X, \mu)$  since  $K$  is a symmetric and positive definite kernel.
4. By *Hilbert-Schmidt theorem*, since  $T_K$  is *self-adjoint and compact*, the Hilbert space  $L^2(X, \mu)$  has a **complete orthonormal basis**  $\{\varphi_n\}_{n=1}^\infty$  where each  $\varphi_n$  is the **eigenfunction** of  $T_K$  corresponding to **eigenvalue**  $\lambda_n \geq 0$  with  $\lambda_n \rightarrow 0$ .
5.  $T_K$  maps **continuously** into the space of *continuous functions*  $\mathcal{C}(X)$ .
6. By *Mercer's Theorem*, there exists an orthonormal basis  $\{\varphi_n\}_{n=1}^\infty$  on  $L^2(X, \mu)$  where each  $\varphi_n$  is a **continuous eigenfunction** of  $T_K$  corresponding to the **eigenvalue**  $\lambda_n \geq 0$  so that the kernel  $K$  has an expansion

$$K(x, y) = \sum_{n=1}^{\infty} \lambda_n \varphi_n(x) \overline{\varphi_n(y)}$$

that converges **uniformly** on **compact** set  $X$ . This above series representation is referred to as a **Mercer kernel** or **Mercer representation** of  $K$ . Thus any function  $f$  in  $L^2(X, \mu)$  can be represented as

$$f(x) = \sum_{n=1}^{\infty} \alpha_n \varphi_n(x).$$

7. Finally, a **reproducing kernel Hilbert space**  $\mathcal{H} \subseteq L^2(X, \mu)$  based on spectral decomposition of  $T_K$  is given by

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

where the inner product of  $\mathcal{H}$  given by

$$\langle f, g \rangle_{\mathcal{H}} = \sum_{n=1}^{\infty} \frac{\langle f, \varphi_n \rangle_{L^2} \langle g, \varphi_n \rangle_{L^2}}{\lambda_n}.$$

The kernel  $K$  is the reproducing kernel of  $\mathcal{H}$ .

## 2.6 Construction from Feature Map

- **Definition (*Feature Map*)** [Scholkopf and Smola, 2001]

A **feature map** is a map  $\Phi : X \rightarrow \mathcal{F}$ , where  $\mathcal{F}$  is a *Hilbert space* such that the image of  $X$  under  $\Phi$ ,  $\mathcal{H} := \Phi(X) \subseteq \mathcal{F}$  is a **reproducing kernel Hilbert space** with kernel function

$$K(x, y) := \langle \Phi(x), \Phi(y) \rangle_{\mathcal{F}}.$$

- **Remark (*Feature Map via Kernel Function*)**

We can think of  $\Phi$  as a vector-valued function with possibly *infinite-dimensional* output. Moreover, given kernel function  $K$ , let  $K_x := K(x, \cdot) \in \mathcal{H}$ , we can define the feature map as

$$\Phi : x \rightarrow K_x = K(x, \cdot)$$

- **Remark (*Feature Map via Eigenfunction of Integral Operator*)** [Scholkopf and Smola, 2001, Rasmussen and Williams, 2005]

Any *symmetric positive definite kernel*  $K$  induces a **integral kernel operator**  $T_K$  that is *self-adjoint* and *compact*.  $T_K$  has discrete real spectrum  $\sigma(T_K) \subset \mathbb{R}$  with eigenfunctions  $\{\varphi_n\}$  that spans the entire space  $\mathcal{F}$ .

Use the *Mercer's theorem*. Given the kernel function  $K : X \times X \rightarrow \mathbb{C}$ , the *eigenfunction*  $\varphi_n : X \rightarrow \mathbb{C}$  associated with the *eigenvalue*  $\lambda_n \geq 0$  is defined by the integral equation

$$\begin{aligned} \lambda_n \varphi_n(x) &= \int_X K(x, y) \varphi_n(y) d\mu(y). \\ \text{where } K(x, y) &= \sum_{n=1}^{\infty} \lambda_n \varphi_n(x) \overline{\varphi_n(y)} \end{aligned}$$

And we can define the feature map  $\Phi$  via

$$\Phi : x \mapsto \left( \sqrt{\lambda_n} \varphi_n(x) \right)_{n=1}^{\infty}.$$

Note that the output dimension of  $\Phi$  is determined by the Mercer representation of  $K$ . It can be finite dimensional if the kernel  $K$  is simple. In this way, we have

$$K(x, y) := \langle \Phi(x), \Phi(y) \rangle_{\mathcal{F}}.$$

- **Remark (*Equivalence of Two Representations*)**

The kernel map and the Mercer's feature map are equivalent in that there exists an **isometric isomorphism** between them so that the inner product is preserved. In specific,  $\Phi : x \mapsto K(x, \cdot)$  maps a feature to a function in  $\mathcal{F}$  and the Mercer's kernel  $\Phi : X \mapsto (\sqrt{\lambda_n} \varphi_n(x))_{j=1}^{\infty}$  maps a feature vector to a **vector representation** of  $K(x, \cdot)$  under a set of orthonormal basis  $\{\sqrt{\lambda_n} \varphi_n(\cdot)\}_{n=1}^{\infty} \subset \mathcal{F}$ .

Note, however,  $\{K(x, \cdot)\}_{n \in S}$  for a set of features  $\{x_n\}_{n \in S}$  are not orthonormal.  $\{K(x, \cdot)\}_{n \in S} \not\subset \{\sqrt{\lambda_n} \varphi_n(\cdot)\}_{n=1}^{\infty}$ .

### 3 Equivalent Definition of Reproducing Kernel Hilbert Space

We summarize four different ways to construct a reproducing kernel Hilbert space (RKHS):

1. (**Bounded Evaluation Functional**)

A RKHS  $\mathcal{H}$  is a *Hilbert space* of functions on  $X$  such that *the evaluation functional*  $\delta_x \in \mathcal{H}^*$  is **bounded linear functional** for all  $x \in X$ .

- This implies that

$$f(x) := \delta_x(f) = \langle f, K_x \rangle$$

for some unique  $K_x \in \mathcal{H}$  for each  $x \in X$ ;

- Define *the reproducing kernel* as function  $K : X \times X \rightarrow \mathbb{C}$  such that

$$K(x, y) = \langle K_x, K_y \rangle = K_x(y).$$

Thus  $K(x, y)$  satisfies the reproducing property:

$$f(x) = \langle f, K(x, \cdot) \rangle$$

2. (**Hermitian Positive Definite Kernel**)

Given a **Hermitian positive definite kernel**,  $K : X \times X \rightarrow \mathbb{C}$ , there exists a **unique RKHS**  $\mathcal{H}$  that admits  $K$  as its *reproducing kernel*.

- From the subspace  $\mathcal{H}_0 = \text{span} \{K_x : x \in X\}$  where  $K_x := K(x, \cdot)$ :

$$f \in \mathcal{H}_0 \Rightarrow f = \sum_{k=1}^n \xi_k K_{x_k}, \quad \exists n \in \mathbb{N}, \{x_i\}_{i=1}^n \subset X, \{\xi_i\} \subset \mathbb{C}$$

- Define the inner product on  $\mathcal{H}_0$  as

$$\left\langle \sum_{k=1}^n \xi_k K_{x_k}, \sum_{j=1}^m \eta_j K_{y_j} \right\rangle_{\mathcal{H}_0} := \sum_{i=1}^n \sum_{j=1}^m K(x_i, y_j) \xi_i \bar{\eta}_j.$$

Due to Hermitian and positive definite property of  $K$ , the inner product above is well-defined.

- $K(x, y) = \langle K_x, K_y \rangle_{\mathcal{H}_0}$  by definition. The reproducing property holds as well.
- Construct the RKHS  $\mathcal{H}$  by the **completion** of  $\mathcal{H}_0$ .

3. (**Integral Kernel Operator**)

Consider a measure space  $(X, \mu)$  where  $X$  is a **compact** space and  $\mu$  is a *Borel measure*. Given  $K : X \times X \rightarrow \mathbb{C}$  as a **continuous Hermitian positive definite kernel** on  $X$ , we can define a **integral kernel operator**  $T_K$  on  $L^2(X, \mu)$  by

$$(T_K f)(x) := \int_X K(x, y) f(y) d\mu(y).$$

- $T_K$  is a **self-adjoint, positive** and **compact operator** on *separable Hilbert space*.

- The *spectrum* of  $T_K$  is *discrete* and is of *real nonnegative value*  $\lambda_n \geq 0$  such that  $\lambda_n \rightarrow 0$ .
- There exists a *complete orthonormal basis* in  $L^2(X, \mu)$  that are *eigenfunctions*  $\{\varphi_n(x)\}$  of  $T_K$ .
- There exists a *orthonormal basis* formed by continuous eigenfunctions  $\{\varphi_n(x)\}$  and their eigenvalues  $\{\lambda_n\}$  so that the expansion

$$K(x, y) = \sum_{n=1}^{\infty} \lambda_n \varphi_n(x) \overline{\varphi_n(y)}$$

converges *uniformly* on compact set  $X$ .

- The RKHS  $\mathcal{H} \subseteq L^2(X, \mu)$  based on spectral decomposition of  $T_K$  is given by

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

where the inner product of  $\mathcal{H}$  given by

$$\langle f, g \rangle_{\mathcal{H}} = \sum_{n=1}^{\infty} \frac{\langle f, \varphi_n \rangle_{L^2} \langle g, \varphi_n \rangle_{L^2}}{\lambda_n}.$$

The kernel  $K$  is the reproducing kernel of  $\mathcal{H}$ .

#### 4. (**Feature Map**)

Define **feature map**  $\Phi : X \rightarrow \mathcal{F}$  from  $X$  to a Hilbert space  $\mathcal{F}$  so that  $\mathcal{H} := \Phi(X)$  is a RKHS with the reproducing kernel

$$K(x, y) := \langle \Phi(x), \Phi(y) \rangle_{\mathcal{F}}, \quad \forall x, y \in X$$

- We can define

$$\Phi : x \mapsto K_x = K(x, \cdot)$$

- We can also define

$$\Phi : x \mapsto \left( \sqrt{\lambda_n} \varphi_n(x) \right)_{n=1}^{\infty}$$

where the eigenfunctions  $\{\varphi_n(x)\}$  and their eigenvalues  $\{\lambda_n\}$  form expansion of kernel  $K$

$$K(x, y) = \sum_{n=1}^{\infty} \lambda_n \varphi_n(x) \overline{\varphi_n(y)}$$

- These two definitions are equivalent based on Mercer's theorem.



## 4 Reproducing Kernel Hilbert Space in Machine Learning

### 4.1 Empirical Feature Map

- **Definition (*Empirical Feature Map*)** [Scholkopf and Smola, 2001]

Given a set of samples  $S := (z_1, \dots, z_m) \subset X$ , the **empirical feature map**  $\Phi_m : X \rightarrow \mathbb{R}^m$  is the empirical estimate of the feature map  $\Phi : x \mapsto K(x, \cdot) \in \mathcal{H}$  under  $S$ . That is

$$\Phi_m : x \mapsto K(x, \cdot)|_{(z_1, \dots, z_m)} \equiv (K(x, z_n))_{n=1}^m.$$

- **Remark** Note that the image of empirical feature map  $\Phi_m(X) \subset \mathbb{R}^m$  does *not necessarily* form a *closed linear subspace*. Also the inner product defined in the linear span of  $\{\Phi_m(z_i), 1 \leq i \leq m\}$  is *not canonical*, since  $\Phi_m(x_i)$  are *not orthogonal* in  $\mathbb{R}^m$  in general.
- **Remark (*Induced Inner Product on  $\mathbb{R}^m$  from Empirical Feature Map*)**  
The empirical feature map that is associated with kernel  $K$  should be defined by inducing an *inner product* of  $\mathbb{R}^m$  into  $\Phi_m(X)$  as

$$\langle \Phi_m(x), \Phi_m(y) \rangle_m = K(x, y),$$

where  $\langle \cdot, \cdot \rangle_m \equiv \langle M \cdot, \cdot \rangle_{\mathbb{R}^m}$  for **positive definite matrix**  $M$ . Enforcing  $x, y \in S := (z_1, \dots, z_m)$  be in training set, we can obtain the equation

$$\begin{aligned} K &= K M K, \\ \Rightarrow M &= K^\dagger = K^{-1}. \end{aligned}$$

where  $K = [K(z_i, z_j)]_{i,j=1}^m \in \mathbb{R}^{m \times m}$  is **the matrix representation** of  $T_K$  in  $\mathbb{R}^m$ .

- **Remark (*Explicit Form of Empirical Feature Map*)** [Scholkopf and Smola, 2001]  
Therefore, we could define empirical feature map that is associated with kernel  $K$  as

$$\Phi_m : x \mapsto K^{-\frac{1}{2}}(K(x, z_n))_{n=1}^m.$$

The above is equivalent to the **Kernel PCA whitening**.

- **Remark (*Empirical Feature Map as Finite Dimensional Approximation*)**  
This  $\Phi_m$  maps  $X$  to a  **$m$ -dimensional space**  $\mathbb{R}^m$  as opposed to the original  $\Phi$  that maps to  $\mathcal{H}$ , a **Hilbert space of functions** with *high or infinite dimensionality*. Moreover, the induced inner product on  $\mathbb{R}^m$  has representation

$$\langle \Phi_m(x), \Phi_m(y) \rangle_m \equiv \mathbf{k}_x^T K^{-1} \mathbf{k}_y$$

where  $K = [K(z_i, z_j)]_{i,j=1}^m$ , and  $\mathbf{k}_x = ((K(x, z_i))_{i=1}^m)^T$ .

### 4.2 Representer Theorem

- **Definition (*Loss Function*)**

Denote by  $(x, y, f(x)) \in \mathcal{X} \times \mathcal{Y} \times \mathcal{Y}$  the triplet consisting of a **pattern**  $x$ , an **observation**  $y$  and a **prediction**  $f(x)$ . Then the map

$$c : \mathcal{X} \times \mathcal{Y} \times \mathcal{Y} \rightarrow [0, \infty)$$

with the property  $c(x, y, y) = 0$  for all  $x \in \mathcal{X}$  and  $y \in \mathcal{Y}$  will be called a loss function.

- **Definition (*Expected Risk*)**

Let  $((\mathcal{X}, \mathcal{Y}), \mathcal{F}, \mathcal{P})$  be a probability space on domain  $(\mathcal{X}, \mathcal{Y})$  and  $f : \mathcal{X} \rightarrow \mathcal{Y}$  be a measurable function on  $\mathcal{X}$ . The expected risk of  $f$  with respect to  $\mathcal{P}$  and  $c$  is defined as

$$\mathcal{R}(f) = \mathbb{E}_{\mathcal{P}} [c(x, y, f(x))] = \int_{\mathcal{X} \times \mathcal{Y}} c(x, y, f(x)) d\mathcal{P}(x, y)$$

- **Definition (*Empirical Risk*)**

Since  $\mathcal{P}$  is unknown, given a set of samples  $\mathcal{D} := \{(x_n, y_n)\}_{n=1}^m \subset \mathcal{X} \times \mathcal{Y}$ , we replace  $\mathcal{P}$  by *the empirical probability measure*

$$\hat{\mathcal{P}}_m = \frac{1}{m} \sum_{n=1}^m \delta_{(x_n, y_n)}.$$

Then we define the empirical risk of  $f$  with respect to  $\hat{\mathcal{P}}_m$  and  $c$  as

$$\mathcal{R}_{emp}(f) = \mathbb{E}_{\hat{\mathcal{P}}_m} [c(x, y, f(x))] = \frac{1}{m} \sum_{n=1}^m c(x_n, y_n, f(x_n))$$

- **Remark** We assume the *empirical risk functional*  $\mathcal{R}_{emp}(f)$  is **continuous** with respect to  $f$ .

- **Remark (*Regularization*)**

The key idea in **regularization** is to restrict the class of possible minimizers  $\mathcal{F}$  (with  $f \in \mathcal{F}$ ) of the empirical risk functional  $\mathcal{R}_{emp}(f)$  such that  $\mathcal{F}$  becomes a **compact set**.

We do not directly specify a compact set  $\mathcal{F}$ , since this leads to a *constrained optimization problem*, which can be cumbersome in practice. Instead, we add a **stabilization (regularization) term**  $\Omega(f)$  to the original objective function; the latter could be  $\mathcal{R}_{emp}(f)$ , for instance. This, too, leads to **better conditioning** of the problem. We consider *the following class of regularized risk functionals*:

$$\mathcal{R}_{reg}(f) := \mathcal{R}_{emp}(f) + \lambda \Omega(f)$$

Here  $\lambda > 0$  is the so-called **regularization parameter** which specifies the **tradeoff** between minimization of  $\mathcal{R}_{emp}(f)$  and *the smoothness or simplicity* which is enforced by small  $\Omega(f)$ . Usually one chooses  $\Omega(f)$  to be **convex**, since this ensures that there exists *only one global minimum*, provided  $\mathcal{R}_{emp}(f)$  is also *convex*.

- **Definition (*Regularized Risk in Reproducing Kernel Hilbert Space*)**

Suppose that  $f \in \mathcal{H}$  where  $\mathcal{H}$  is a **reproducing kernel Hilbert space** on  $X$ .  $\mathcal{R}_{emp}(f)$  is the empirical risk functional. The regularized risk functionals on  $\mathcal{H}$  is defined as

$$\mathcal{R}_{reg}(f) := \mathcal{R}_{emp}(f) + \frac{\lambda}{2} \|f\|_{\mathcal{H}}^2$$

- **Lemma 4.1 (*Operator Inversion Lemma*)** [Scholkopf and Smola, 2001]

Let  $X$  be a **compact** set and let the map  $f : X \rightarrow Y$  be **continuous**. Then there exists an *inverse map*  $f^{-1} : f(X) \rightarrow X$  that is also **continuous**.

• **Theorem 4.2 (Representer Theorem)** [Scholkopf and Smola, 2001]

Let  $\mathcal{X}$  be a set, and  $c : (\mathcal{X} \times \mathbb{R} \times \mathbb{R})^m \rightarrow \mathbb{R} \cup \{\infty\}$  be an arbitrary loss function,  $\mathcal{H}$  be the reproducing kernel Hilbert space associated with kernel  $K$  on  $X$ . Denote  $\Omega : [0, \infty) \rightarrow \mathbb{R}$  as a **strictly monotonic increasing** function. Then each minimizer  $f \in \mathcal{H}$  of the regularized risk

$$c((x_1, y_1, f(x_1)), \dots, (x_m, y_m, f(x_m))) + \Omega(\|f\|_{\mathcal{H}}) \quad (7)$$

admits a **representation** of the form

$$f(x) = \sum_{n=1}^m \alpha_n K(x_n, x).$$

**Proof:** For convenience we will assume that we are dealing with  $\bar{\Omega}(\|f\|_{\mathcal{H}}^2) := \Omega(\|f\|_{\mathcal{H}})$  rather than  $\Omega(\|f\|_{\mathcal{H}})$ . This is no restriction at all, since the quadratic function is strictly monotonic on  $[0, \infty)$ , and therefore  $\bar{\Omega}$  is strictly monotonic on  $[0, \infty)$  if and only if  $\Omega$  also satisfies this requirement.

We may decompose any  $f \in \mathcal{H}$  into a part contained  $\mathcal{H}_0 = \text{span}\{K(x_i, \cdot), i = 1, \dots, m\}$  and one in the **orthogonal complement**  $\mathcal{H}_0^\perp$ ;

$$f(x) = f_{\mathcal{H}_0}(x) + f_{\mathcal{H}_0^\perp}(x) = \sum_{n=1}^m \alpha_n K(x_n, x) + f_{\mathcal{H}_0^\perp}(x)$$

Here  $\alpha_n \in \mathbb{R}$  and  $f_{\mathcal{H}_0^\perp} \in \mathcal{H}$  with  $\langle f_{\mathcal{H}_0^\perp}, K(x_n, \cdot) \rangle_{\mathcal{H}} = 0$  for all  $n \in [m] := \{1, \dots, m\}$ . By reproducing property of  $K$  we may write  $f(x_i)$  (for all  $i \in [m]$ ) as

$$\begin{aligned} f(x_i) &= \langle f, K(x_i, \cdot) \rangle_{\mathcal{H}} \\ &= \sum_{n=1}^m \alpha_n K(x_n, x_i) + \langle f_{\mathcal{H}_0^\perp}, K(x_i, \cdot) \rangle_{\mathcal{H}} \\ &= \sum_{n=1}^m \alpha_n K(x_n, x_i) \end{aligned}$$

Second, for all  $f_{\mathcal{H}_0^\perp}$ , by *Pythagorean theorem* and the *monotonicity* of  $\Omega$ ,

$$\Omega(\|f\|_{\mathcal{H}}) := \bar{\Omega} \left( \left\| \sum_{n=1}^m \alpha_n K(x_n, \cdot) \right\|_{\mathcal{H}}^2 + \|f_{\mathcal{H}_0^\perp}\|_{\mathcal{H}}^2 \right) \geq \bar{\Omega} \left( \left\| \sum_{n=1}^m \alpha_n K(x_n, \cdot) \right\|_{\mathcal{H}}^2 \right)$$

Thus for any fixed  $\alpha_n \in \mathbb{R}$  the risk functional (7) is minimized for  $f_{\mathcal{H}_0^\perp} = 0$ . Since this also has to hold for the solution, the theorem holds. ■

• **Remark (Monotonicity of Regularizer Functional  $\Omega(\cdot)$  is Required)**

**Monotonicity** of  $\Omega$  is **necessary** to ensure that the theorem holds. It does not prevent the **regularized risk functional** from having **multiple local minima**. To ensure a single minimum, we would need to require **convexity**. If we discard the **strictness of the monotonicity**, then it no longer follows that *each minimizer of the regularized risk admits an expansion*; it still follows, however, that *there is always another solution that is as good*, and that does *admit the expansion*.

- **Remark (*Function Space Minimizer Lies in Finite Dimensional Subspace*)**

The *significance* of the *Representer Theorem* is that although we might be trying to solve an *optimization problem in an infinite-dimensional space*  $\mathcal{H}$ , containing *linear combinations of kernels centered on arbitrary points* of  $X$ , it states that the solution lies *in the span of  $m$  particular kernels* – those centered on the *training points*.

In the *Support Vector* community,

$$f(x) = \sum_{n=1}^m \alpha_n K(x_n, x)$$

is called *the Support Vector expansion*. For suitable choices of loss functions, it has empirically been found that many of the  $\alpha_n$  often equal 0.

## 5 Example and Computation

- $K$  as an operator is self-adjoint, i.e.

$$\langle f, Kg \rangle = \langle Kf, g \rangle.$$

- The inner product in Reproducing Kernel Hilbert Space (RKHS)  $\mathcal{H}$  is given by [Ramm, 1998]:

$$\langle f, g \rangle_{\mathcal{H}} \equiv \langle K^{-1}f, g \rangle_x \quad (8)$$

where  $K^{-1}$  is inverse to the linear operator  $K : \mathcal{H} \rightarrow \mathcal{H}$  given by

$$(Kf)(z) = \int_E K(z, x) f(x) dx.$$

Note that the reproducing property holds

$$\begin{aligned} \langle f, K(\cdot, \mathbf{y}) \rangle_{\mathcal{H}} &= \langle K^{-1}f, K(\cdot, \mathbf{y}) \rangle_x = \langle f, K^{-1}K(\cdot, \mathbf{y}) \rangle_x = \langle f, \delta_{\mathbf{y}} \rangle_x \\ &= f(\mathbf{y}). \end{aligned}$$

- The *Gaussian kernel*

$$K(\mathbf{x}, \mathbf{x}') = \exp \left( -\frac{\|\mathbf{x} - \mathbf{x}'\|_2^2}{2\lambda} \right), \lambda > 0 \quad (9)$$

The Gaussian kernel has universally bounded norm  $|K(\mathbf{x}, \mathbf{x})|^{1/2} = \|\Phi(\mathbf{x})\| = 1$ . Moreover,  $K(\mathbf{x}, \mathbf{x}') > 0$  for  $\mathbf{x} \neq \mathbf{x}'$ ; i.e., all points lie in the same orthant

$$\cos(\angle \mathbf{x}, \mathbf{x}') = \langle \Phi(\mathbf{x}), \Phi(\mathbf{x}') \rangle = K(\mathbf{x}, \mathbf{x}') > 0.$$

This indicates that in the Gaussian case, the mapped data lie in a fairly restricted area of feature space. *However*, in another sense, they occupy a space which is as large as possible: given distinct points  $(\mathbf{x}_1, \dots, \mathbf{x}_m) \subset E$ ,  $\{\Phi(\mathbf{x}_1), \dots, \Phi(\mathbf{x}_m)\}$  are linearly independent and  $[K_{i,j}] = [K(\mathbf{x}_i, \mathbf{x}_j)]$  has full rank.

$\{\Phi(\mathbf{x}_1), \dots, \Phi(\mathbf{x}_m)\}$  span an  $m$ -dimensional subspace of  $F$ . Therefore a Gaussian kernel defined on a domain of infinite cardinality, with no a priori restriction on the number of training examples, produces a feature space of *infinite*-dimension.

The eigenfunction of Gaussian kernel can be found using Fourier transformation; i.e.,  $K(\mathbf{x}, \mathbf{x}') = f(\|\mathbf{x} - \mathbf{x}'\|) \equiv G(\mathbf{x} - \mathbf{x}')$

$$\begin{aligned}\lambda\psi(\mathbf{x}) &= \int G(\mathbf{x} - \mathbf{x}')\psi(\mathbf{x}')d\mu(\mathbf{x}') = G \otimes \psi \\ \Rightarrow \lambda\mathcal{F}\{\psi\}(\mathbf{s}) &= \mathcal{F}\{G\} \mathcal{F}\{\psi\} = G(\mathbf{s}) \mathcal{F}\{\psi\}(\mathbf{s}) \\ \psi &\in \mathcal{F}^{-1}\{N(\lambda I - G(\mathbf{s}))\}, \\ \text{where } N(\lambda I - G(\mathbf{s})) &= \{F(\mathbf{s}) : (\lambda I - G(\mathbf{s}))F(\mathbf{s}) = 0\}\end{aligned}$$

Note that  $\mathcal{F}\{G\}$  of Gaussian is also Gaussian which is rescaled in mass and variance from the original one by some constants. Since the spheres centered at 0 are the sets on which the multiplier equality  $\lambda = G(\mathbf{s})$  can hold,  $\psi \equiv 0$  for  $\mathbf{s} \in$  the complementary of a sphere centered at 0.

Thus, the eigenfunctions will be inverse Fourier transforms of *tempered distributions* [Grafakos, 2008] supported in spheres centered at the origin. There are a lot of them, for example, the most familiar ones are the *Bessel functions*, which correspond to uniform surface measure on a nondegenerate sphere.

- The *homogeneous polynomial kernel*

$$K(\mathbf{x}, \mathbf{x}') = \langle \mathbf{x}, \mathbf{x}' \rangle^d, d > 0 \quad (10)$$

and *inhomogeneous polynomial kernel*

$$K(\mathbf{x}, \mathbf{x}') = (\langle \mathbf{x}, \mathbf{x}' \rangle + c)^d, d > 0 \quad (11)$$

- The  *$B_n$ -spline kernel*

$$K(\mathbf{x}, \mathbf{x}') = B_{2p+1}(\|\mathbf{x} - \mathbf{x}'\|), p > 0 \quad (12)$$

where  $B_n = \otimes_{i=1}^n I[-\frac{1}{2}, \frac{1}{2}]$  and  $f \otimes g = \int f(t)g(\tau - t)dt$ .

- All the kernel above (w/o inhomogeneous one) is invariant under the unitary transformation  $U$ , i.e.

$$\begin{aligned}K(U\mathbf{x}, U\mathbf{x}') &= \langle \Phi(U\mathbf{x}), \Phi(U\mathbf{x}') \rangle \\ &= \langle \Phi(\mathbf{x}), \Phi(\mathbf{x}') \rangle = K(\mathbf{x}, \mathbf{x}')\end{aligned}$$

- The *Radial basis function (RBF)* kernels are kernels that can be written in the form

$$K(\mathbf{x}, \mathbf{x}') = f(d(\mathbf{x}, \mathbf{x}')) \quad (13)$$

for  $d(\mathbf{x}, \mathbf{x}')$  is the metric on  $E$ .

The RBF kernels are *unitary invariant*, too. In addition, they are *translation invariant*.

By Bochner's theorem, if a kernel  $K$  can be written in terms of  $\|x - y\|$ , i.e.  $K(x, y) = f(\|x - y\|)$  for some  $f$ , then  $K$  is a kernel iff the Fourier transform of  $f$  is non-negative.

$$K(\mathbf{x}, \mathbf{x}') = \int_{\mathbb{R}^D} S(\mathbf{s}) \exp(-i \mathbf{s}^T (\mathbf{x} - \mathbf{x}')) d\mathbf{s}$$

In terms of this, for RBF kernel, the eigenfunctions can be obtained by Fourier analysis; in particular, it could be Bessel functions etc.

The RBF kernel is sometimes called a convolutional kernel, with the feature map

$$\begin{aligned} \Phi_{\mathbf{u}} : E &\mapsto L^2 \\ \mathbf{x} &\mapsto \frac{1}{(2\pi)^{n/2}} \mathcal{F}^{-1}(\sqrt{S})(\mathbf{x} - \mathbf{u}) \end{aligned}$$

So that

$$K(\mathbf{x}, \mathbf{x}') = \int_{\mathbb{R}^D} \Phi_{\mathbf{u}}(\mathbf{x}) \Phi_{\mathbf{u}}(\mathbf{x}') d\mathbf{u}$$

For example, for Gaussian kernel

$$\exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{\sigma^2}\right) = \left(\frac{4}{\sigma^2\pi}\right)^{n/2} \int_{\mathbb{R}^D} \exp\left(-\frac{2\|\mathbf{x} - \mathbf{u}\|^2}{\sigma^2}\right) \exp\left(-\frac{2\|\mathbf{x}' - \mathbf{u}\|^2}{\sigma^2}\right) d\mathbf{u}$$

with the convolutional feature map

$$\Phi_{\mathbf{u}}(\mathbf{x}) = \left(\frac{2}{\sigma\sqrt{\pi}}\right)^{n/2} \exp\left(-\frac{2\|\mathbf{x} - \mathbf{u}\|^2}{\sigma^2}\right).$$

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