

Lecture 2: Reproducing Kernel Hilbert Space

Tianpei Xie

Jul. 6th., 2015

Contents

1	Hilbert Space and Functional Analysis Basis	2
1.1	Complete Metric Space	2
1.2	Hilbert Space	3
1.3	Bounded Linear Operator and Dual Space	4
1.4	Hilbert Adjoints and Self Adjoint Operator	6
1.5	Regular Measure and Duality of $\mathcal{C}_0(X)$	7
1.6	Spectrum of Bounded Linear Operator	10
1.7	Compact Operator	11
1.8	Trace Class and Hilbert-Schmidt Operators	13
2	Reproducing Kernel Hilbert Space (RKHS)	16
2.1	Definitions	16
2.2	Properties	18
2.3	Convergence Properties	18
2.4	Construction from Hermitian Positive Definite Kernel	19
2.5	Construction from Integral Kernel Operator on Compact Space	21
2.6	Construction from Feature Map	22
3	Equivalent Definition of Reproducing Kernel Hilbert Space	23
4	Reproducing Kernel Hilbert Space in Machine Learning	25
4.1	Empirical Feature Map	25
4.2	Representer Theorem	25
5	Example and Computation	28

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 α 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 ℓ^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 α 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** μ 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 μ .

- **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 μ 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 μ , that is

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

Finally, I is **positive** if and only if the measure μ 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 μ 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 μ is a **complex Borel measure**, then μ 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 μ or in general, Radon measures on **locally compact** space X , there are two perspectives:

1. **Nonegative set function on the σ -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 λ 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 λ . Note that $R_\lambda(T)$ is defined on $\text{Ran}(\lambda I - T)$.

If $\lambda \notin \rho(T)$, then λ 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 ; λ is called the corresponding eigenvalue.

If λ is an *eigenvalue*, then $(\lambda I - T)$ is **not injective** (i.e. $\text{Ker}(\lambda I - T) \neq \{0\}$) so λ 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 λ is **not an eigenvalue** and if $\text{Ran}(\lambda I - T)$ is **dense** but the resolvent $R_\lambda(T)$ is **unbounded**, then λ is said to be in the continuous spectrum. It is denoted as $\sigma_c(T)$.

3. **Residual Spectrum**: If λ is **not an eigenvalue** and if $\text{Ran}(\lambda I - T)$ is **not dense**, then λ 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* λ of T is called the eigenspace of T corresponding to that eigenvalue λ .

- **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

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

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

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

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, μ) 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 λ_n is the eigenvalue corresponding to eigenfunction φ_n .

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

Suppose Ω 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** φ_k is **continuous** on Ω 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, δ_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 δ_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 $x \in X$, δ_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 δ_x and δ_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 δ_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 $E = \lim_{n \rightarrow \infty} E_n = \bigcap_{n=1}^{\infty} E_n$. 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* μ 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 φ_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 φ_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 Φ , $\mathcal{H} := \Phi(X) \subseteq \mathcal{F}$ 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 Φ 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 Φ via

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

Note that the output dimension of Φ 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, μ) where X is a **compact** space and μ 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 Φ_m maps X to a **m -dimensional space** \mathbb{R}^m as opposed to the original Φ 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 Ω 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 Ω ,

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

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 Ω 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 α_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

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

References

- Nachman Aronszajn. Theory of reproducing kernels. *Transactions of the American mathematical society*, pages 337–404, 1950.
- John B Conway. *A course in functional analysis*, volume 96. Springer, 2019.
- Gerald B Folland. *Real analysis: modern techniques and their applications*. John Wiley & Sons, 2013.
- Loukas Grafakos. *Classical fourier analysis*, volume 2. Springer, 2008.
- Thomas Hofmann, Bernhard Schölkopf, and Alexander J Smola. Kernel methods in machine learning. *The annals of statistics*, pages 1171–1220, 2008.
- Erwin Kreyszig. *Introductory functional analysis with applications*, volume 81. wiley New York, 1989.
- AG Ramm. On the theory of reproducing kernel hilbert spaces. *Journal of Inverse and Ill posed problems*, 6:515–520, 1998.
- Carl Edward Rasmussen and Christopher K. I. Williams. *Gaussian Processes for Machine Learning (Adaptive Computation and Machine Learning)*. The MIT Press, 2005. ISBN 026218253X.
- Michael Reed and Barry Simon. *Methods of modern mathematical physics: Functional analysis*, volume 1. Gulf Professional Publishing, 1980.
- Bernhard Scholkopf and Alexander J Smola. *Learning with kernels: support vector machines, regularization, optimization, and beyond*. MIT press, 2001.