Kernel Method: Data Analysis with Positive Definite Kernels

2. Positive Definite Kernel and Reproducing Kernel Hilbert Space

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Definition of Positive Definite Kernel

Definition. Let $\mathcal{X}$ be a set. $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a positive definite kernel if $k(x,y) = k(y,x)$ and for every $x_1, \ldots, x_n \in \mathcal{X}$ and $c_1, \ldots, c_n \in \mathbb{R}$

$$\sum_{i,j=1}^{n} c_i c_j k(x_i, x_j) \geq 0,$$

i.e. the symmetric matrix

$$(k(x_i,x_j))_{i,j=1}^{n} = \begin{pmatrix} k(x_1,x_1) & \cdots & k(x_1,x_n) \\ \vdots & \ddots & \vdots \\ k(x_n,x_1) & \cdots & k(x_n,x_) \end{pmatrix}$$

is positive semidefinite.

- The symmetric matrix $(k(x_i,x_j))_{i,j=1}^{n}$ is often called a Gram matrix.

Definition: Complex-valued Case

Definition. Let $\mathcal{X}$ be a set. $k : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ is a positive definite kernel if for every $x_1, \ldots, x_n \in \mathcal{X}$ and $c_1, \ldots, c_n \in \mathbb{C}$

$$\sum_{i,j=1}^{n} c_i \overline{c_j} k(x_i, x_j) \geq 0.$$

Remark. The Hermitian property $k(y, x) = \overline{k(x, y)}$ is derived from the positive-definiteness. [Exercise]

Some Basic Properties

Facts. Assume $k : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ is positive definite. Then, for any x, y in $\mathcal{X}$,

1. $k(x, x) \geq 0$.
2. $|k(x, y)|^2 \leq k(x, x)k(y, y)$.

Proof. (1) is obvious. For (2), with the fact $k(y, x) = \overline{k(x, y)}$, the definition of positive definiteness implies that the eigenvalues of the hermitian matrix

$$\begin{pmatrix} k(x,x) & \overline{k(x,y)} \\ k(x,y) & k(y,y) \end{pmatrix}$$

is non-negative, thus, its determinant $k(x, x)k(y, y) - |k(x, y)|^2$ is non-negative. □

Examples

Real valued positive definite kernels on $\mathbb{R}^n$:

- Linear kernel[1]

$$k_0(x, y) = x^T y$$

- Exponential

$$k_E(x, y) = \exp(\beta x^T y) \qquad (\beta > 0)$$

- Gaussian RBF (radial basis function) kernel

$$k_G(x, y) = \exp\left(-\frac{1}{2\sigma^2}\|x - y\|^2\right) \qquad (\sigma > 0)$$

- Laplacian kernel

$$k_L(x, y) = \exp\left(-\alpha \textstyle\sum_{i=1}^n |x_i - y_i|\right) \qquad (\alpha > 0)$$

- Polynomial kernel

$$k_P(x, y) = (x^T y + c)^d \qquad (c \geq 0, d \in \mathbb{N})$$

[1] [Exercise] prove that the linear kernel is positive definite.

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Reproducing kernel Hilbert space

Definition. Let $\mathcal{X}$ be a set. A reproducing kernel Hilbert space (RKHS) (over $\mathcal{X}$) is a Hilbert space $\mathcal{H}$ consisting of functions on $\mathcal{X}$ such that for each $x \in \mathcal{X}$ there is a function $k_x \in \mathcal{H}$ with the property

$$\langle f, k_x \rangle_{\mathcal{H}} = f(x) \qquad (\forall f \in \mathcal{H}) \qquad \text{(reproducing property).}$$

$k(\cdot, x) := k_x(\cdot)$ is called a reproducing kernel of $\mathcal{H}$.

Fact 1. A reproducing kernel is Hermitian (or symmetric).

Proof.

$$k(y,x) = \langle k(\cdot,x), k_y \rangle = \langle k_x, k_y \rangle = \overline{\langle k_y, k_x \rangle} = \overline{\langle k(\cdot,y), k_x \rangle} = \overline{k(x,y)}.$$

Fact 2. The reproducing kernel is unique, if exists. [Exercise]

Positive Definite Kernel and RKHS I

Proposition 1 (RKHS ⇒ positive definite kernel)

The reproducing kernel of a RKHS is positive definite.

Proof.

$$\sum_{i,j=1}^{n} c_i \overline{c_j} k(x_i, x_j) = \sum_{i,j=1}^{n} c_i \overline{c_j} \langle k(\cdot, x_i), k(\cdot, x_j) \rangle$$

$$= \Big\langle \sum_{i=1}^{n} c_i k(\cdot, x_i), \sum_{j=1}^{n} c_j k(\cdot, x_j) \Big\rangle = \Big\| \sum_{i=1}^{n} c_i k(\cdot, x_i) \Big\|^2 \geq 0.$$

□

Positive Definite Kernel and RKHS II

Theorem 2 (positive definite kernel $\Rightarrow$ RKHS. Moore-Aronszajn)

Let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ (or $\mathbb{R}$) be a positive definite kernel on a set $\mathcal{X}$. Then, there uniquely exists a RKHS $\mathcal{H}_k$ on $\mathcal{X}$ such that

1. $k(\cdot, x) \in \mathcal{H}_k$ *for every* $x \in \mathcal{X}$,
2. $\mathrm{Span}\{k(\cdot, x) \mid x \in \mathcal{X}\}$ *is dense in* $\mathcal{H}_k$,
3. k *is the reproducing kernel on* $\mathcal{H}_k$, i.e.,

$$\langle f, k(\cdot, x)_{\mathcal{H}} \rangle = f(x) \qquad (\forall x \in \mathcal{X}, \forall f \in \mathcal{H}_k).$$

Proof omitted.

Positive Definite Kernel and RKHS III

One-to-one correspondence between positive definite kernels and RKHS.

$$k \qquad \longleftrightarrow \qquad \mathcal{H}_k$$

- Proposition 1: RKHS $\mapsto$ positive definite kernel k.
- Theorem 2: $k \mapsto \mathcal{H}_k$ (injective).

RKHS as Feature Space

If we define

$$\Phi : \mathcal{X} \to \mathcal{H}_k, \quad x \mapsto k(\cdot, x),$$

then,

$$\langle \Phi(x), \Phi(y) \rangle = \langle k(\cdot, x), k(\cdot, y) \rangle = k(x, y).$$

RKHS associated with a positive definite kernel k gives a desired feature space!!

In kernel methods, the above feature map and feature space are always used.

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Operations that Preserve Positive Definiteness I

Proposition 3

If $k_i : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ *(*$i = 1, 2, \ldots$*) are positive definite kernels, then so are the following:*

1. *(positive combination)* $ak_1 + bk_2 \quad (a, b \geq 0)$.
2. *(product)* $k_1 k_2 \quad (k_1(x, y) k_2(x, y))$.
3. *(limit)* $lim_{i \to \infty} k_i(x, y)$, *assuming the limit exists.*

Remark. From Proposition 3, the set of all positive definite kernels is a closed (w.r.t. pointwise convergence) convex cone stable under multiplication.

Operations that Preserve Positive Definiteness II

Proof.

(1): Obvious.

(3): The non-negativity in the definition holds also for the limit.

(2): It suffices to show that two Hermitian matrices A and B are positive semidefinite, so is their component-wise product. This is done by the following lemma. □

Definition. For two matrices A and B of the same size, the matrix C with $C_{ij} = A_{ij}B_{ij}$ is called the Hadamard product of A and B.

The Hadamard product of A and B is denoted by $A \odot B$.

Lemma 4

Let A and B be non-negative Hermitian matrices of the same size. Then, $A \odot B$ is also non-negative.

Operations that Preserve Positive Definiteness III

Proof.

Let

$$A = U \Lambda U^*$$

be the eigendecomposition of A, where

$U = (u^1, \ldots, u^p)$: a unitary matrix, *i.e.*, $\quad U^* = \overline{U}^T$

Λ: diagonal matrix with non-negative entries $(\lambda_1, \ldots, \lambda_p)$.

Then, for arbitrary $c_1, \ldots, c_p \in \mathbb{C}$,

$$\sum_{i,j=1} c_i \bar{c}_j (A \odot B)_{ij} = \sum_{a=1}^{p} \lambda_a c_i \bar{c}_j u_i^a \bar{u}_j^a B_{ij} = \sum_{a=1}^{p} \lambda_a \xi^{aT} B \overline{\xi^a},$$

where $\xi^a = (c_1 u_1^a, \ldots, c_p u_p^a)^T \in \mathbb{C}^p$.

Since $\xi^{aT} B \overline{\xi^a}$ and λ_a are non-negative for each a, so is the sum. $\square$

Feature Map must be Positive Definite

Proposition 5

Let V be an vector space with an inner product $\langle \cdot, \cdot \rangle$. If we have a map

$$\Phi : \mathcal{X} \to V, \qquad x \mapsto \Phi(x),$$

a positive definite kernel on $\mathcal{X}$ is defined by

$$k(x, y) = \langle \Phi(x), \Phi(y) \rangle.$$

Proof. Let $x_1, \ldots, x_n$ in $\mathcal{X}$ and $c_1, \ldots, c_n \in \mathbb{C}$.

$$\begin{aligned}
\textstyle\sum_{i,j=1}^{n} c_i \overline{c_j} k(x_i, x_j) &= \textstyle\sum_{i,j=1}^{n} c_i \overline{c_j} \langle \Phi(x_i), \Phi(x_j) \rangle \\
&= \left\langle \textstyle\sum_{i=1}^{n} c_i \Phi(x_i), \textstyle\sum_{j=1}^{n} c_j \Phi(x_j) \right\rangle \\
&= \left\| \textstyle\sum_{i=1}^{n} c_i \Phi(x_i) \right\|^2 \quad \geq 0.
\end{aligned}$$

Modification

Proposition 6

Let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ *be a positive definite kernel and* $f : \mathcal{X} \to \mathbb{C}$ *be an arbitrary function. Then,*

$$\tilde{k}(x, y) = f(x)k(x, y)\overline{f(y)}$$

is positive definite. In particular,

$$f(x)\overline{f(y)}$$

and

$$\frac{k(x, y)}{\sqrt{k(x, x)}\sqrt{k(y, y)}} \qquad (\textit{normalized kernel})$$

are positive definite.

Proof is left as an exercise.

Proofs for Positive Definiteness of Examples

- Linear kernel: Proposition 5
- Exponential:

$$\exp(\beta x^T y) = 1 + \beta x^T y + \frac{\beta^2}{2!}(x^T y)^2 + \frac{\beta^3}{3!}(x^T y)^3 + \cdots$$

  Use Proposition 3.
- Gaussian RBF kernel:

$$\exp\left(-\frac{1}{2\sigma^2}\|x-y\|^2\right) = \exp\left(-\frac{\|x\|^2}{2\sigma^2}\right)\exp\left(\frac{x^T y}{\sigma^2}\right)\exp\left(-\frac{\|y\|^2}{2\sigma^2}\right).$$

  Apply Proposition 6.
- Laplacian kernel: The proof is shown later.
- Polynomial kernel: Just sum and product.

□

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Definition by Evaluation Map

Proposition 7

Let $\mathcal{H}$ be a Hilbert space consisting of functions on a set $\mathcal{X}$. Then, $\mathcal{H}$ is a RKHS if and only if the evaluation map

$$e_x : \mathcal{H} \to \mathbb{K}, \qquad e_x(f) = f(x),$$

is a continuous linear functional for each $x \in \mathcal{X}$.

Proof. Assume $\mathcal{H}$ is a RKHS. The boundedness of e_x is obvious from

$$|e_x(f)| = |\langle f, k_x \rangle| \leq \|k_x\| \|f\|.$$

Conversely, assume the evaluation map is continuous. By Riesz lemma, there is $k_x \in \mathcal{H}$ such that

$$\langle f, k_x \rangle = e_x(f) = f(x),$$

which means $\mathcal{H}$ is a RKHS having k_x as a reproducing kernel. $\square$

Continuity

The functions in a RKHS are "nice" functions under some conditions.

Proposition 8

Let k be a positive definite kernel on a topological space $\mathcal{X}$, and $\mathcal{H}_k$ be the associated RKHS. If $\mathrm{Re}[k(y,x)]$ is continuous for every $x, y \in \mathcal{X}$, then all the functions in $\mathcal{H}_k$ are continuous.

Proof. Let f be an arbitrary function in $\mathcal{H}_k$.

$$|f(x) - f(y)| = |\langle f, k(\cdot,x) - k(\cdot,y)\rangle| \le \|f\|\|k(\cdot,x) - k(\cdot,y)\|.$$

The assertion is easy from

$$\|k(\cdot,x) - k(\cdot,y)\|^2 = k(x,x) + k(y,y) - 2\mathrm{Re}[k(x,y)].$$

□

Remark. If $k(x,y)$ is differentiable, then all the functions in $\mathcal{H}_k$ are differentiable.

c.f. L^2 space contains non-continuous functions.

Summary of Sections 1 and 2

- We would like to use a feature map $\Phi : \mathcal{X} \to \mathcal{H}$ to incorporate nonlinearity or high order moments.
- The inner product in the feature space must be computed efficiently. Ideally,

$$\langle \Phi(x), \Phi(y) \rangle = k(x, y).$$

- To satisfy the above relation, the kernel k must be positive definite.
- A positive definite kernel k defines an associated RKHS, where k is the reproducing kernel;

$$\langle k(\cdot, x), k(\cdot, y) \rangle = k(x, y).$$

- Use a RKHS as a feature space, and $\Phi : x \mapsto k(\cdot, x)$ as the feature map.

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Basic properties of Hilbert space

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Vector space with inner product I

Definition. V: vector space over a field $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$.
V is called an inner product space if it has an inner product (or scalar product, dot product) $(\cdot, \cdot) : V \times V \to \mathbb{K}$ such that for every $x, y, z \in V$

1. (Strong positivity) $(x, x) \geq 0$, and $(x, x) = 0$ if and only if $x = 0$,
2. (Addition) $(x + y, z) = (x, z) + (y, z)$,
3. (Scalar multiplication) $(\alpha x, y) = \alpha(x, y)$ ($\forall \alpha \in \mathbb{K}$),
4. (Hermitian) $(y, x) = \overline{(x, y)}$.

Vector space with inner product II

$(V, (\cdot,\cdot))$: inner product space.

Norm of $x \in V$:

$$\|x\| = (x,x)^{1/2}.$$

Metric between x and y:

$$d(x,y) = \|x - y\|.$$

Theorem 9

Cauchy-Schwarz inequality

$$|(x,y)| \leq \|x\|\|y\|.$$

Remark: Cauchy-Schwarz inequality holds without requiring $\|x\| = 0 \Rightarrow x = 0$.

Hilbert space I

Definition. A vector space with inner product $(\mathcal{H}, (\cdot,\cdot))$ is called Hilbert space if the induced metric is complete, *i.e.* every Cauchy sequence[2] converges to an element in $\mathcal{H}$.

Remark 1:
A Hilbert space may be either finite or infinite dimensional.

Example 1.
$\mathbb{R}^n$ and $\mathbb{C}^n$ are finite dimensional Hilbert space with the ordinary inner product

$$(x,y)_{\mathbb{R}^n} = \sum_{i=1}^n x_i y_i \quad \text{or} \quad (x,y)_{\mathbb{C}^n} = \sum_{i=1}^n x_i \overline{y_i}.$$

[2] A sequence $\{x_n\}_{n=1}^{\infty}$ in a metric space (X,d) is called a Cauchy sequence if $d(x_n, x_m) \to 0$ for $n, m \to \infty$.

Hilbert space II

Example 2. $L^2(\Omega, \mu)$.
Let $(\Omega, \mathcal{B}, \mu)$ is a measure space.

$$\mathcal{L} = \left\{ f : \Omega \to \mathbb{C} \;\middle|\; \int |f|^2 d\mu < \infty \right\}.$$

The inner product on $\mathcal{L}$ is define by

$$(f, g) = \int f\overline{g} d\mu.$$

$L^2(\Omega, \mu)$ is defined by the equivalent classes identifying f and g if their values differ only on a measure-zero set.

- $L^2(\Omega, \mu)$ is complete.
- $L^2(\mathbb{R}^n, dx)$ is infinite dimensional.

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Orthogonality

- Orthogonal complement.

  Let $\mathcal{H}$ be a Hilbert space and V be a closed subspace.

  $$V^{\perp} := \{x \in \mathcal{H} \mid (x, y) = 0 \text{ for all } y \in V\}$$

  is a closed subspace, and called the orthogonal complement.

- Orthogonal projection.

  Let $\mathcal{H}$ be a Hilbert space and V be a closed subspace. Every $x \in \mathcal{H}$ can be uniquely decomposed

  $$x = y + z, \qquad y \in V \quad \text{and} \quad z \in V^{\perp},$$

  that is,

  $$\mathcal{H} = V \oplus V^{\perp}.$$

Complete orthonormal system I

- ONS and CONS.

  A subset $\{u_i\}_{i \in I}$ of $\mathcal{H}$ is called an orthonormal system (ONS) if $(u_i, u_j) = \delta_{ij}$ (δ_{ij} is Kronecker's delta).

  A subset $\{u_i\}_{i \in I}$ of $\mathcal{H}$ is called a complete orthonormal system (CONS) if it is ONS and if $(x, u_i) = 0$ ($\forall i \in I$) implies $x = 0$.

  Fact: Any ONS in a Hilbert space can be extended to a CONS.

Complete orthonormal system II

- Separability
  A Hilbert space is separable if it has a countable CONS.

Assumption

In this course, a Hilbert space is always assumed to be separable.

Complete orthonormal system III

Theorem 10 (Fourier series expansion)

Let $\{u_i\}_{i=1}^{\infty}$ *be a CONS of a separable Hilbert space. For each* $x \in \mathcal{H}$*,*

$$x = \sum_{i=1}^{\infty}(x, u_i)u_i, \qquad \textit{(Fourier expansion)}$$

$$\|x\|^2 = \sum_{i=1}^{\infty}|(x, u_i)|^2. \qquad \textit{(Parseval's equality)}$$

Proof omitted.

Example: CONS of $L^2([0\ 2\pi], dx)$

$$u_n(t) = \frac{1}{\sqrt{2\pi}}e^{\sqrt{-1}nt} \qquad (n = 0, 1, 2, \ldots)$$

Then,

$$f(t) = \sum_{n=0}^{\infty}a_n u_n(t)$$

is the (ordinary) Fourier expansion of a periodic function.

Bounded operator I

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces. A linear transform $T : \mathcal{H}_1 \to \mathcal{H}_2$ is often called operator.

Definition. A linear operator $\mathcal{H}_1$ and $\mathcal{H}_2$ is called bounded if

$$\sup_{\|x\|_{\mathcal{H}_1}=1} \|Tx\|_{\mathcal{H}_2} < \infty.$$

The operator norm of a bounded operator T is defined by

$$\|T\| = \sup_{\|x\|_{\mathcal{H}_1}=1} \|Tx\|_{\mathcal{H}_2} = \sup_{x \neq 0} \frac{\|Tx\|_{\mathcal{H}_2}}{\|x\|_{\mathcal{H}_1}}.$$

(Corresponds to the largest singular value of a matrix.)

Fact. If $T : \mathcal{H}_1 \to \mathcal{H}_2$ is bounded,

$$\|Tx\|_{\mathcal{H}_2} \leq \|T\| \|x\|_{\mathcal{H}_1}.$$

Bounded operator II

Proposition 11

A linear operator is bounded if and only if it is continuous.

Proof. Assume $T : \mathcal{H}_1 \to \mathcal{H}_2$ is bounded. Then,

$$\|Tx - Tx_0\| \leq \|T\| \|x - x_0\|$$

means continuity of T.

Assume T is continuous. For any $\varepsilon > 0$, there is $\delta > 0$ such that $\|Tx\| < \varepsilon$ for all $x \in \mathcal{H}_1$ with $\|x\| < 2\delta$.
Then,

$$\sup_{\|x\|=1} \|Tx\| = \sup_{\|x\|=\delta} \frac{1}{\delta} \|Tx\| \leq \frac{\varepsilon}{\delta}.$$

□

Riesz lemma I

Definition. A linear functional is a linear transform from $\mathcal{H}$ to $\mathbb{C}$ (or $\mathbb{R}$).

The vector space of all the bounded (continuous) linear functionals called the dual space of $\mathcal{H}$, and is denoted by $\mathcal{H}^*$.

Theorem 12 (Riesz lemma)

For each $\phi \in \mathcal{H}^*$, there is a unique $y_\phi \in \mathcal{H}$ such that

$$\phi(x) = (x, y_\phi) \qquad (\forall x \in \mathcal{H}).$$

Proof.

Consider the case of $\mathbb{R}$ for simplicity.

$\Leftarrow$) Obvious by Cauchy-Schwartz.

Riesz lemma II

$\Rightarrow$) If $\phi(x) = 0$ for all x, take $y = 0$. Otherwise, let

$$V = \{x \in \mathcal{H} \mid \phi(x) = 0\}.$$

Since ϕ is a bounded linear functional, V is a closed subspace, and $V \neq \mathcal{H}$.
Take $z \in V^\perp$ with $\|z\| = 1$. By orthogonal decomposition, for any $x \in \mathcal{H}$,

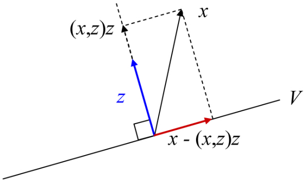
$$x - (x, z)z \in V.$$

Apply ϕ, then

$$\phi(x) - (x, z)\phi(z) = 0, \qquad \text{i.e.,} \quad \phi(x) = (x, \phi(z)z).$$

Take $y_\phi = \phi(z)z$. □

Riesz lemma III



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Proof of Theorem 2 I

Proof. (Described in $\mathbb{R}$ case.)

- Construction of an inner product space:

$$H_0 := \mathrm{Span}\{k(\cdot, x) \mid x \in \mathcal{X}\}.$$

Define an inner product on H_0:
for $f = \sum_{i=1}^n a_i k(\cdot, x_i)$ and $g = \sum_{j=1}^m b_j k(\cdot, y_j)$,

$$\langle f, g \rangle := \sum_{i=1}^n \sum_{j=1}^m a_i b_j k(x_i, y_j).$$

This is independent of the way of representing f and g from the expression

$$\langle f, g \rangle = \sum_{j=1}^m b_j f(y_j) = \sum_{i=1}^n a_i g(x_i).$$

Proof of Theorem 2 II

- Reproducing property on H_0:

$$\langle f, k(\cdot, x)\rangle = \textstyle\sum_{i=1}^{n} a_i k(x_i, x) = f(x).$$

- Well-defined as an inner product:
  It is easy to see $\langle \cdot, \cdot \rangle$ is bilinear form, and

$$\|f\|^2 = \textstyle\sum_{i,j=1}^{n} a_i a_j k(x_i, x_j) \geq 0$$

  by the positive definiteness of f.
  If $\|f\| = 0$, from Cauchy-Schwarz inequality,[3]

$$|f(x)| = |\langle f, k(\cdot, x)\rangle| \leq \|f\| \|k(\cdot, x)\| = 0$$

  for all $x \in \mathcal{X}$; thus $f = 0$.

Proof of Theorem 2 III

- Completion:
  Let $\mathcal{H}$ be the completion of H_0.
  - H_0 is dense in $\mathcal{H}$ by the completion.
  - $\mathcal{H}$ is realized by functions:
    Let $\{f_n\}$ be a Cauchy sequence in $\mathcal{H}$. For each $x \in \mathcal{X}$, $\{f_n(x)\}$ is a Cauchy sequence, because

    $$|f_n(x) - f_m(x)| = |\langle f_n - f_m, k(\cdot, x)\rangle| \leq \|f_n - f_m\|\|k(\cdot, x)\|.$$

    Define $f(x) = \lim_n f_n(x)$.
    This value is the same for equivalent sequences, because $\{f_n\} \sim \{g_n\}$ implies

    $$|f_n(x) - g_n(x)| = |\langle f_n - g_n, k(\cdot, x)\rangle| \leq \|f_n - g_n\|\|k(\cdot, x)\| \to 0.$$

    Thus, any element $[\{f_n\}]$ in $\mathcal{H}$ can be regarded as a function f on $\mathcal{X}$.

[3] Note that Cauchy-Schwarz inequality holds without assuming strong positivity of the inner product.