Reproducing Kernel Hilbert Space

The Big Picture

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Aims of this Talk

We will be reviewing the basic, but relevant, mathematical tools in order to take the big picture of applying RKHS in applications.

Yes or No

In order to achieve this we will

- *not* go in to details
- *not* prove (almost any) theorems
- define some useful function spaces
- try to see the *big picture* of RKHS

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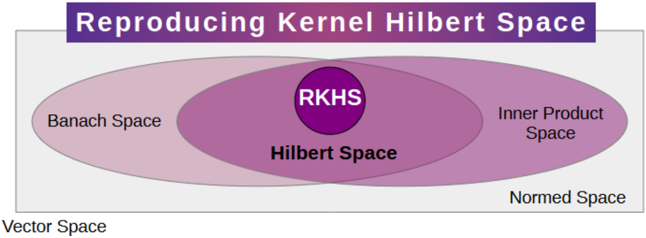
Function Spaces

Apart from the basic definition of a *Vector Space*, we will introduce

- Normed Space
- Banach Space
- Inner Product Space
    - Metric Space
- Hilbert Space (and later *reproducing kernel*)



Normed Space

Definition (Normed Space)

Let V be a vector space over $\mathbb{F}$. A *norm* on V is a function

$$\|\cdot\|_V = \|\cdot\| : V \to \mathbb{R}$$

such that for any two vectors $u, v \in V$ and a scalar $\alpha \in \mathbb{F}$,

1. $\|u\| \geq 0$ with $\|u\| = 0 \iff u = 0$,
2. $\|\alpha u\| = |\alpha| \, \|u\|$, and
3. $\|u + v\| \leq \|u\| + \|v\|$.

The vector space V equipped with the norm $\|\cdot\|$, sometimes written as $(V, \|\cdot\|)$, is called a *normed space*.

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Banach Space

Definition (Banach Space)

Let V be a normed space equipped with a norm $\|\cdot\|$. We say that V is *complete* (with respect to the norm $\|\cdot\|$) if every Cauchy sequence in V converges to a vector in V.
A normed space that is complete with respect to its norm is known as a *Banach space*.

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Inner Product Space

Definition (Inner Product Space)

Let V be a vector space over $\mathbb{F}$. An ($\mathbb{F}$) *inner product* on V is a function

$$\langle \cdot, \cdot \rangle_V = \langle \cdot, \cdot \rangle : V \times V \to \mathbb{F}$$

such that for any vectors $u, v, w \in V$ and scalars $\alpha, \beta \in \mathbb{F}$, the following proporties hold:

1. $\langle u, v \rangle = \overline{\langle v, u \rangle}$, (conjugate symmetry)
2. $\langle \alpha u + \beta v, w \rangle = \alpha \langle u, w \rangle + \beta \langle v, w \rangle$, (linearity in the 1st argument)
3. $\langle u, u \rangle \geq 0$ with $\langle u, u \rangle = 0 \iff u = 0$. (positive semi-definiteness)

The vector space V equipped with the inner product $\langle \cdot, \cdot \rangle$, sometimes written as $(V, \langle \cdot, \cdot \rangle)$, is called an *inner product space*.

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Inner Product Space is a Normed Space

Definition (Norm induced by the Inner Product)

Let $(V, \langle \cdot, \cdot \rangle)$ be an inner product space. For $u \in V$,

$$\|u\| = \sqrt{\langle u, u \rangle}$$

is norm on V referred to as the *norm induced by the inner product*. With this norm, $(V, \|\cdot\|)$ is a *normed space* (as well).

Metric Space

Definition (Metric Space)

A *metric space* is a vector space V that is equipped with a *distance* function (metric), $d : V \times V \to \mathbb{R}$ satisfying the following:

1. $d(u,v) \geq 0$ with $d(u,v) = 0 \iff u = v$,
2. $d(u,v) = d(v,u)$, and (symmetry)
3. $d(u,v) \leq d(u,w) + d(w,v)$. (triangular inequality)

for any $u, v, w \in V$.

Distance, Norm, Inner Product

$$d(u,v) = \|u - v\| = \sqrt{\langle u, v\rangle}$$

Read the equation *from right to left*, rather than *from left to right*!

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Hilbert Space

Definition (Hilbert Space)

A *Hilbert space* is an inner product space that is complete with respect to the norm (or, metric) induced by the inner product.

Distance, Norm, Inner Product

$$d(u, v) = \|u - v\| = \sqrt{\langle u, v \rangle}$$

- A *Hilbert space* is a vector space equipped with an *inner product* that induces a *metric* so that the space is a *complete metric space*.
- Note that not all complete metric spaces are Hilbert spaces!

What Left: for Future Lectures

Reading the equation,

$$d(u,v) = \|u - v\| = \sqrt{\langle u, v \rangle},$$

from left to right!

To do so, we might need the following (mainly the first one):

1. polarisation (form norms)
2. translation invariant (for metrics)
3. absolute homogenity (for metrics)
4. the notion of angle (between vectors); this is easy

$$\cos\theta = \frac{\langle u, v \rangle}{\|u\| \, \|v\|},$$

where θ is the angle between the vectors u and v in an inner product space.

Thus, a Hilbert space covers the geometric notions of **length**, **distance**, and **angle**.

Continue with . . .

Reproducing Kernel Hilbert Space

Definition (RKHS)

Let Ω be an arbitrary set, and $\mathcal{H}$ a Hilbert space of functions $f : \Omega \to \mathbb{F}$.
For each element $x \in \Omega$, the *evaluation functional* that evaluates each $f \in \mathcal{H}$ at the point x is written as

$$\mathcal{L}_x : \mathcal{H} \to \mathbb{F} \quad \text{or} \quad \mathcal{L}_x : f \mapsto f(x),$$

with $\mathcal{L}_x f = f(x)$ for all $f \in \mathcal{H}$.
We say that $\mathcal{H}$ is a **reproducing kernel Hilbert space** (RKHS) if, for all $x \in \Omega$, $\mathcal{L}_x$ is *continuous* at every $f \in \mathcal{H}$.

Reproducing Property

Corollary (Reproducing Property)

Let $\Omega, f, \mathcal{H}$ *and* $\mathcal{L}_x$ *be defined as in the definition above. If every* $\mathcal{L}_x$ *is continuous at every* $f \in \mathcal{H}$*, then for each* $\mathcal{L}_x$*, there is a unique function* $K_x \in \mathcal{H}$ *such that for every* $f \in \mathcal{H}$*,*

$$\mathcal{L}_x f = f(x) = \langle f, K_x \rangle_{\mathcal{H}} .$$

This equation is know as the reproducing property.

This basically follows from *Riesz* representation theorem.

Reproducing Kernel Hilbert Space

Definition (RKHS)

Let Ω be an arbitrary set, and $\mathcal{H}$ a Hilbert space of functions $f : \Omega \to \mathbb{F}$. If, for each $x \in \Omega$, the *evaluation functional* $\mathcal{L}_x : \mathcal{H} \to \mathbb{F}$ is continuous at every $f \in \mathcal{H}$, we can construct the *reproducing kernel*, which is a bivariate function $K : \Omega \times \Omega \to \mathbb{F}$ defined by

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

The Hilbert space $\mathcal{H}$ is called a *reproducing kernel Hilbert space* (RKHS).

This basically follows by replacing x with y and f by K_x:

$$\mathcal{L}_y f = f(y) = \langle f, K_y \rangle_{\mathcal{H}}$$

and, if $f = K_x$,

$$\mathcal{L}_y(K_x) = K_x(y) = \langle K_x, K_y \rangle_{\mathcal{H}} .$$

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Continue with ...

The Kernel Trick

Let $\mathcal{H}$ be a given RKHS, we can then find a function $\varphi : \Omega \to \mathcal{H}$: a straighforward one is

$$\varphi(x) = K_x, \quad \text{for all} \quad x \in \Omega,$$

which is possible by the *reproducing kernel* property.
In machine learning:

- the function φ is the *feature map*,
- the set Ω is the *attributes*,
- the RKHS $\mathcal{H}$ is the *feature space*.

Therefore, the *kernel trick* used in machine learning (mostly) is the identity:

$$K(x, y) = \langle \varphi(x), \varphi(y) \rangle_{\mathcal{H}} . \qquad \text{(Kernel Trick)}$$

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