Note for RKHS

October 2024

In summary, an RKHS is a space of functions with a special inner product structure that allows evaluating functions using kernel functions. The key concept is that evaluation of any function in this space can be done using the inner product with a kernel, demonstrating the ”reproducing” property.

1 Introduction

1.1 Extrinsic Geometry

consider f that project a point $p = (p_1, p_2)$ to a line L:

- $L(\theta) = \{(t\cos\theta, t\sin\theta) \mid t \in \mathbb{R}\} \subset \mathbb{R}^2$
- $f(\theta) = (r(\theta)\cos\theta, r(\theta)\sin\theta), \quad r(\theta) = p_1\cos\theta + p_2\sin\theta$
- $k_1(\theta) = \cos\theta \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}, \quad k_2(\theta) = \sin\theta \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}$
- $K(\theta) = \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix} \begin{bmatrix} \cos\theta & \sin\theta \end{bmatrix} = \begin{bmatrix} \cos^2\theta & \sin\theta\cos\theta \\ \sin\theta\cos\theta & \sin^2\theta \end{bmatrix}$
- the relationship of f and L can be represented as $f(L) = p_1k_1(L) + p_2k_2(L)$.

1.2 Canonical Coordinates and Pointwise Coordinates

Hilbert space: An arbitrary element of $\mathcal{H}$ can be written as the limit of a linear combination of a manageable set of fixed vectors.
RKHS:An arbitrary element of RKHS $\mathcal{H}$ can be written as the limit of a linear combination of $K(\cdot, t)$ that ,for brevity, we refer to as the presence of a canonical coordinate system.

- canonical coordinate: $\{K(\cdot, t) | t \in T\}$, where $K : T \times T \to \mathbb{R}$
- pointwise coordinate: $v \in \mathcal{H} : T \to \mathbb{R}$, its t th coordinate can be thought of as $v(t)$

The utility of the pointwise coordinate system is that limits in a RKHS can be determined pointwise: if v_k is a Cauchy sequence, $\|v_k - v\| \to 0$, then v is fully determined by $v(t) = \lim_k v_k(t)$ (i.e. convergence can be defined pointwise)

- relationship: $v(t) = \langle v, K(\cdot, t)\rangle$

2 Finite-dimensional RKHS

2.1 The kernel of an inner product subspaces

Motivation of the RKHS theory: How to describe the inner product space V?

Definition 2.1. *Let $V \subset \mathbb{R}^n$ be an inner product space. The kernel of V is the unique matrix $K = \begin{bmatrix} k_1 & k_2 & \cdots & k_n \end{bmatrix} \in \mathbb{R}^{n\times n}$ determined by any of the following three equivalent definitions.*

1. *K is such that each k_i is in V and $\langle v, k_i\rangle = e_i^\top v$ for all $v \in V$.*
2. *$K = u_1 u_1^\top + \cdots + u_r u_r^\top$ where $u_1, \cdots, u_r$ is an orthonormal basis for V .*
3. *K is such that the k_i span V and $\langle k_j, k_i\rangle = K_{ij}$.*

the first definition is saying that taking the inner product with k_i extracts the i th element of a vector.

Lemma 2.1. *Given an inner product space $V \subset \mathbb{R}^n$, there is precisely one $K = [k_1, \cdots, k_n] \in \mathbb{R}^{n\times n}$ for which each k_i is in V and satisfies $\langle v, k_i\rangle = e_i^\top v$ for all $v \in V$.*

Lemma 2.2. *Let $V = \operatorname{span}\{k_1, \cdots, k_n\}$ be the space spanned by the columns $k_1, \cdots, k_n$ of a positive semi-definite matrix $K \in \mathbb{R}^{n\times n}$. There exists an inner product on V satisfying $\langle k_j, k_i\rangle = K_{ij}$.*

Lemma 2.3. *Let $V_1 \subset \mathbb{R}^n$ and $V_2 \subset \mathbb{R}^n$ be two inner product spaces having the same kernel K . Then V_1 and V_2 are identical spaces: $V_1 = V_2$ and their inner products are the same.*

There is a bijective correspondence between inner product spaces $V \subset \mathbb{R}^n$ and positive semi-definite matrices $K \in \mathbb{R}^{n\times n}$.

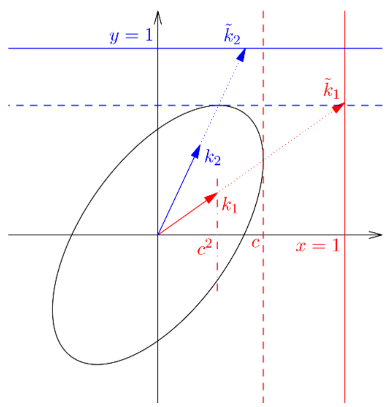
2.2 Sequences of Inner Product Spaces

The kernel representation of an inner product space induces a concept of convergence for the broader situation of a sequence of inner product subspaces, possibly of differing dimensions. The limit $V_\infty \subset \mathbb{R}^n$ of a sequence of inner product spaces $V_1, V_2, \cdots \subset \mathbb{R}^n$ is the space whose kernel is $K_\infty = \lim_{n\to\infty} K_n$, if the limit exists.

2.3 Extrinsic Geometry and Interpolation

Extrinsic Geometry: Sometimes its valuable to use extrinsic coordinates that represent an element of V as a combination of the basis of the space. In finite dimension vector space, this is trivial. But for an abstract vector space, the basis may not be well-defined. RKHS theory replaces an ad-hoc choice of basis for V by the particular choice $k_1, \dots, k_n$ of spanning vectors for V.
Interpolation: The usefulness of extrinsic geometry is exemplified by considering the interpolation problem of finding a vector $x \in V$ of smallest norm and some of whose coordinates $e_i^\top x$ are specified. Soving this motivate us to chose a basis for V, thus we find the relationship between K and the solution x, which leads to another definition of K.

Definition 2.2. *Let $H_i = \left\{ z \in \mathbb{R}^n \mid e_i^\top z = 1 \right\}$ be the hyperplane consisting of all vectors whose i th coordinate is unity. If $V \cap H_i$ is empty then define $k_i = 0$. Otherwise, let $\tilde{k}_i$ be the point in the intersection $V \cap H_i$ that is closest to the origin. Define k_i to be $k_i = c\tilde{k}_i$ where $c = \left\langle \tilde{k}_i, \tilde{k}_i \right\rangle^{-1}$.*



3 Function Spaces

3.1 Function Approximation

Consider finding $g \in V$ that minimises $||f - g||^2$, treating $f - g$ as elements of a function space suggests g can be found by solving the linear equations $\langle f - g, v \rangle = 0$ for all $v \in V$.

3.2 Topological Aspects of Inner Product Spaces

Inner product spaces have two structures: a vector space structure and a norm whose square is “quadratic”. In certain cases, the norm is coarser than the

vector space structure.
Here are the differences between the infinit dimension and the finit dimension:

- In infinite dimensions, different norms can induce different topologies. Whereas in finite dimensions, every norm gives rise to the same topology as every other norm.
- An infinite dimensional subspace need not be topologically closed. Whereas every finite-dimensional subspace $V \subset W$ of an inner product space W is closed.

3.3 Evaluation Functions

Let V be a subspace of $\mathbb{R}^X$ where X is an arbitrary set. An element f of V is therefore a function $f : X \to \mathbb{R}$ and can be evaluated pointwise. This means mathematically that for any $x \in X$, there is a function $l_x : V \to \mathbb{R}$ given by $l_x(f) = f(x)$.
A key requirement for $V \subset \mathbb{R}^X$ to be a RKHS is for the l_x to be bounded for all x . This implies that if $f_n \in V$ is a sequence converging in norm, meaning $\|f_n - f\| \to 0$, then the sequence also converges pointwise, meaning $f_n(x) \to f(x)$.

4 Infinite-dimensional RKHS

Fix an arbitrary set X, endow a subspace V of the function space $\mathbb{R}^X$ with a inner product, $(V, \langle \cdot, \cdot, \rangle, X)$. Then RKHS requires:

- $(V, \langle \cdot, \cdot, \rangle)$ to be a Hilbert space.
  An inner product space that is complete is called a Hilbert space.
- l_x bounded for all $x \in X$

Some extra discussion on the necessities of the space V to be complete:

- A completion is needed for reconstruction V from its kernel K because in general the kernel can describe only a dense subspace of the general space. Any space containing this dense subspace and contained in its completion would have the same kernel.
- A unique correspondence is achieved by insisting V is complete. That is, given K, the space V is the completion of the subspace described by K.

Completeness is important in that it ensures existence of solutions to certain classes of problems by preventing the solution from having been accidentally or deliberately removed from the space. Here is a standard procedure for the existence proof of a solution:

- Construct a sequence of approximate solutions f_n by mimicking how differential equations are solved numerically , with decreasing step size. The hope is that $f_n \to f$, but as f cannot be exhibited explicitly,it is not possible to prove $f_n \to f$ directly.
- Instead, f_n is shown to be Cauchy and therefore, by **completeness**, has a limit $\tilde{f}$
- $\tilde{f}$ is verified by some limit argument to be the solution, thus proving the existence of $f = \tilde{f}$

4.1 Definition of RKHS

Definition 4.1. *Let X be an arbitrary set and denote by $\mathbb{R}^X$ the vector space of all functions $f : X \to \mathbb{R}$, equipped with pointwise operations. A subspace $V \in \mathbb{R}^X$ endowed with an inner product is a RKHS if V is complete and for every $x \in X$ the evaluation functional $f \to f(x) = l_x(f)$ on V is bounded.*

The kernel of a RKHS exists and is unique.

Definition 4.2. *If $V \subset \mathbb{R}^X$ is a RKHS, then its kernel is the function $K : X \times X \to \mathbb{R}$ satisfying $\rangle f, K(\cdot, y)\langle = f(y)$ for all $f \in V$.Here $K(\cdot, y)$ denotes the function $X \to K(x, y)$ and is an element of V.*

4.2 Basic Properties

- The kernel of a RKHS is positive semi-definite and every positive semi-definite function is the kernel of a unique RKHS.
- K is symmetric
- In RKHS, strong convergence ($||f_n - f|| \to 0$) implies pointwise convergence ($f(x) \to f(x)$ for all $x \in X$)

4.3 Completing a Function Space

Proposition 4.1. *An arbitrary inner product space $V_0 \subset \mathbb{R}^X$ has a RKHS completion V, where $V_0 \subset V \subset \mathbb{R}^X$, if and only if:*
1. the evaluation functions on V_0 are bounded.
2. if $f_n \in V_0$ is a Cauchy sequence converging pointwise to 0 then $||f_n|| \to 0$

Condition (2) ensures different Cauchy sequence converging pointwise to the same limit yield the same norm. This condition is not automatically true because there are examples where $f_n(x) \to f(x) = 0 for x \in X$ but $||f_n|| \to ||f|| \neq 0$. This can be understand as X did not contain enough points to distinguish the strong limit of the Cauchy sequence f_n from the zero function.

4.4 Joint Properties of a RKHS and its Kernel

4.4.1 Continuity

Proposition 4.2. *$V \subset \mathbb{R}^X$ are continuous where X is a metric space, if and only if*
1. $x \to K(x, y)$ is continuous for all $y \in X$
2. for every $x \in X \exists r > 0 s.t. y \to K(y, y)$ is bounded on $B(x, r)$

4.4.2 Invertibility of Matrices

$$A_{ij} = K(x_i, x_j)$$

$$\begin{aligned}\sum_{i=1}^{r}\sum_{j=1}^{r} c_i c_j K\left(x_i, x_j\right) &= \sum_{i=1}^{r}\sum_{j=1}^{r} c_i c_j \left\langle K\left(\cdot, x_j\right), K\left(\cdot, x_i\right)\right\rangle \\ &= \left\langle \sum_{j=1}^{r} c_j K\left(\cdot, x_j\right), \sum_{i=1}^{r} c_i K\left(\cdot, x_i\right)\right\rangle \\ &= \left\| \sum_{i=1}^{r} c_i K\left(\cdot, x_i\right)\right\|^2\end{aligned}$$

A is non-singular iff $\sum_{i=1}^{r} c_i K\left(\cdot, x_i\right) = 0$

4.4.3 Restriction of the index set

If $X' \subset X$ then any $f : X \to \mathbb{R}$ restricts to a function $f|_{X'} : X' \to \mathbb{R}$ given by $f|_{X'}(x) = f(x)$ for $x \in X'$. If $V \subset \mathbb{R}^X$ is a RKHS then a new space $V' \subset \mathbb{R}^{X'}$ results from restricting each element of V to X' . Precisely, $V' = \{ f|_{X'} \mid f \in V\}$. Define on V' the norm

$$\|f\| = \inf_{\substack{g \in V \\ g|_{X'} = f}} \|g\|$$

4.4.4 Sums of Kernels

$K = K_1 + K_2$ is positive semi-definite when K_1 and K_2 are kernels. Thus K is a kernel of a RKHS $V \subset \mathbb{R}^X$. The space itself is $V = V_1 \oplus V_2$, that is,

$$V = \{f_1 + f_2 \mid f_1 \in V_1, f_2 \in V_2\}$$

The norm on V is given by a minimisation:

$$\|f\|^2 = \inf_{\substack{f_1 \in V_1 \\ f_2 \in V_2 \\ f_1 + f_2 = f}} \|f_1\|^2 + \|f_2\|^2$$