What's this?

This document consists of a collection of basic results about Reproducing Kernel Hilbert Space useful in machine learning context. Nearly every statement and proof is borrowed mainly from [1] [2]. [3] [4] [5]

Overview

1 Basic Property of RKHS

Definition 1.1 (Reproducing Kernel). Let E be a nonempty set. A function K defined by

$$K: E \times E \ni (x, y) \mapsto K(x, y) \in \mathbb{F}$$

is called a reproducing kernel of a Hilbert space H of functions on E if it satisfies the following conditions:

- (a) $K(\cdot, x) \in H$ for every $x \in E$
- (b) $\langle f, K(\cdot, x) \rangle_H = f(x)$ for every $x \in E$ and every $f \in H$.

Such a Hilbert space, associated with its reproducing kernel, is called a reproducing kernel hilbert space, and is denoted by (H, K).

Theorem 1.2 (Characterization of RKHS). A Hilbert space H of functions on a nonempty set E admits a reproducing kernel K if and only if all evaluation functionals $\{ev_x\}_{x\in E}$ are continuous on H.

Proof. Suppose (H, K) is a RKHS. For $x \in E$ and for $f \in H$ we have

$$|\text{ev}_x(f)| = |f(x)| = |\langle f, K(\cdot, x) \rangle| \le ||f|| \, ||K(\cdot, x)|| \le ||f|| \, K(x, x)^{1/2} \to 0$$

as $||f|| \to 0$. Thus, ev_x is continuous linear functional (with norm $K(x,x)^{1/2}$). Conversely, if $\operatorname{ev}_x : H \ni f \mapsto f(x) \in \mathbb{F}$ is continuous, then, by Riesz's representation theorem, there exists $r_x \in H$ such that

$$\langle f, r_x \rangle = f(x)$$

for every $f \in H$. If this happens for every $x \in E$, then $K(x,y) := r_x(y)$ is a reproducing kernel of H.

Corollary 1.3. Every convergent sequence in RKHS converges pointwise to the same limit.

Proof. $|f_n(x) - f(x)| = |\operatorname{ev}_x(f_n - f)| \to 0$ when $f_n \to f$ in norm by continuity of evaluation functional.

Definition 1.4. (Positive definite function) Let E be a nonempty set. A function $K: E \times E \to \mathbb{C}$ is called positive definite if for any $n \in \mathbb{N}$ and for any $a \in \mathbb{C}^n$ and $x \in E^n$ there holds

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i \overline{a_j} K(x_i, x_j) \ge 0,$$

where \bar{c} is the complex conjugate of c.

Proposition 1.5. Suppose φ is a mapping of a set E into a Hilbert space H. Then the mapping $K: E \times E \ni (x,y) \mapsto \langle \varphi(x), \varphi(y) \rangle \in \mathbb{C}$ is positive definite.

Proof. For a and x taken as in the definition, we have

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i \overline{a_j} K(x_i, x_j) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_i \overline{a_j} \langle \varphi(x_i), \varphi(x_j) \rangle = \left\| \sum_{i=1}^{n} a_i \varphi(x_i) \right\|^2 \ge 0.$$

Proposition 1.6. Every reproducing kernel is positive definite.

Proof.
$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i \overline{a_j} K(x_i, x_j) = \left\| \sum_{i=1}^{n} K(\cdot, x_i) \right\|^2$$
.

Proposition 1.7. Every positive definite function $K: E \times E \to \mathbb{C}$ satisfies

- (a) $K(x,x) \ge 0$ for every $x \in E$
- (b) $K(x,y) = \overline{K(y,x)}$ for every $x,y \in E$
- (c) \overline{K} is also positive definite
- (d) $|K(x,y)| \le K(x,x)K(y,y)$ for every $x,y \in E$.

Proof. (a) and (c) clearly hold. For $\alpha, \beta \in \mathbb{C}$ and $x, y \in E$, we have

$$g(\alpha, \beta) := |\alpha|^2 K(x, x) + \alpha \overline{\beta} K(x, y) + \overline{\alpha} \beta K(y, x) + |\beta|^2 K(y, y) \ge 0.$$

Choose $\alpha = \beta = 1$ and $\alpha = i$, $\beta = 1$ to get

$$K(x,y) + K(y,x) = g(1,1) - K(x,x) - K(y,y) =: A \in \mathbb{R}$$

 $iK(x,y) - iK(y,x) = g(i,1) - K(x,x) - K(y,y) =: B \in \mathbb{R}.$

Therefore,

$$2K(y, x) = A + iB$$
$$2K(x, y) = A - iB,$$

which proves (b). Finally, for $x, y \in E$ with $K(x, y) \neq 0$ and for $r \in \mathbb{R}$, (b) gives

$$0 \ge g(r, K(x, y)) = r^2 K(x, x) + 2r |K(x, y)|^2 + |K(x, y)|^2 K(y, y).$$

As RHS is quadratic in r, it must satisfy

$$|K(x,x)|^4 - |K(x,y)|^2 K(x,x)K(y,y) \le 0,$$

from which (c) follows.

Theorem 1.8. Let H_0 be the subspace of \mathbb{F}^E , equipped with an inner product $\langle \cdot, \cdot \rangle_{H_0}$ with norm $\| \cdot \|_{H_0}$. Then there exists unique RKHS (H, K) that extends H_0 in the sense that

(a) $H_0 \subset H \subset \mathbb{F}^E$ and the subspace topology of H_0 in H coincides with the topology of $(H_0, \|\cdot\|_{H_0})$

if and only if H_0 satisfies the following conditions:

- (b) every evaluation functional ev_x is continuous in $(H_0, \|\cdot\|_{H_0})$
- (c) any Cauchy sequence $\{f_n\} \subset H_0$ converging pointwise to 0 converges to 0 also in H_0 -norm.

Proof. Suppose such an extension H exists. H satisfies (b) by Theorem1.2. Since H is complete, a Cauchy sequence $\{f_n\} \subset H_0$ tends to some f, for which we have

$$f(x) = \operatorname{ev}_x(f) = \lim_{n \to \infty} \operatorname{ev}_x(f_n) = \lim_{n \to \infty} f_n(x) = 0$$

for every $x \in E$. Therefore, f is identically 0.

Conversely, suppose (b)(c) hold. Let H be the set of all functions $f \in \mathbb{F}^E$ for which there exists a Cauchy sequence $\{f_n\} \subset H_0$ converging pointwise to f. Clearly, $H_0 \subset H \subset \mathbb{F}^E$. The rest of proof consists of the following Lemmas.

Lemma 1.9. Let $f, g \in H$ and let $\{f_n\}$ and $\{g_n\}$ be two Cauchy sequences in H_0 that converge pointwise to f and g respectively.

(A) The sequence $\langle f_n, g_n \rangle_{H_0}$ is convergent.

- (B) The limit $\lim_{n\to\infty} \langle f_n, g_n \rangle_{H_0}$ depends solely on f and g, independent of the choice of f_n and g_n .
- (C) $\langle f, g \rangle_H := \lim_{n \to \infty} \langle f_n, g_n \rangle_{H_0}$ is an inner product on H.

Proof. It follows from the definition of f_n and g_n that

$$\begin{aligned} \left| \langle f_n, g_n \rangle_{H_0} - \langle f_m, g_m \rangle_{H_0} \right| &= \left| \langle f_n - f_m, g_n \rangle - \langle f_m, g_n - g_m \rangle \right| \\ &\geq \|g_n\| \|f_n - f_m\| + \|f_m\| \|g_n - g_m\| \to 0, \end{aligned}$$

which proves (A). In order to verify (B), suppose $\{f'_n\}$ and $\{g'_n\}$ are also such approximating sequences. We then similarly deduce that

$$|\langle f_n, g_n \rangle - \langle f'_n, g'_n \rangle| \le ||g_n|| ||f_n - f'_n|| + ||f'_n|| ||g_n - g'_n||.$$

 $\{f_n - f_n'\}$ and $\{g_n - g_n'\}$ are Cauchy sequences tending pointwise to 0. Thus, assumption (c) gives $||f_n - f_n'|| \to 0$ and $||g_n - g_n'|| \to 0$. So, (A) and (B) show that $\langle f, g \rangle_H$ is well-defined. Note that if $\langle f, f \rangle_H = 0$, then for every $x \in E$

$$f(x) = \operatorname{ev}_x(f) = \lim_{n \to \infty} \operatorname{ev}_x(f_n) = \lim_{n \to \infty} f_n(x) = 0$$

and hence $f \equiv 0$. As the symmetry, positivity, linearity are quite obvious, we conclude that (C) is true.

Lemma 1.10. (A) Let $f \in H$ and let $\{f_n\} \subset H_0$ be a Cauchy sequence converging pointwise to f. Then $f_n \to f$ also in H-norm.

(B) H_0 is dense in H.

Proof. (A): Fix $\epsilon > 0$. Choose $N \in \mathbb{N}$ large enough so that

$$||f_n - f_m||_{H_0} < \epsilon$$

for all n, m > N. For fixed n, $\{f_n - f_m\}_{m \in \mathbb{N}}$ is a Cauchy sequence converging pointwise to $f_n - f$. Therefore, by definition of $\langle \cdot, \cdot \rangle_H$,

$$||f - f_n||_H = \lim_{n \to \infty} ||f_n - f_m||_{H_0} \le \epsilon.$$

(B) is obvious from (A).

Lemma 1.11. Every evaluation functional ev_x is continuous on H.

Proof. Fix $x \in E$. As a linear functional ev_x is assumed to be continuous on H_0 , it admits unique continuous extension T_x onto the closure of H_0 in H, that is, onto whole H, where we use the assumption (a) and Lemma2(B). T_x is also the evaluation functional on H. Indeed, for f and f_n as in Lemma1.10, we have

$$T_x(f) = \lim_{n \to \infty} \operatorname{ev}_x(f_n) = \lim_{n \to \infty} f_n(x) = f(x).$$

Lemma 1.12. H is a RKHS.

Proof. In light of Theorem1.2 and Lemma1.11, it suffices to show that H is complete. Let $\{f_n\}$ be a Cauchy sequence in H. Let $x \in E$. $\{f_n(x)\}$ is also a Cauchy in \mathbb{F} , and hence converges to some f(x). By Lemma1.10, for every $n \in \mathbb{N}$, there is $g_n \in H_0$ such that $||f_n - g_n||_H < n^{-1}$. In view of the inequality

$$||f - f_n||_H \le ||f - g_n||_H + ||g_n - f_n||_H$$

it suffices to prove that $||f - g_n||_H \to 0$. To this end, we show that $\{g_n\}$ is a Cauchy sequence converging pointwise to f (and then apply Lemma1.10).

For fixed $x \in E$, we have

$$|g_n(x) - f(x)| \le |g_n(x) - f_n(x)| + |f_n(x) - f(x)|$$

= $|\operatorname{ev}_x(g_n - f_n)| + |f_n(x) - f(x)| \to 0$

as $n \to \infty$, since ev_x is continuous and $f_n(x) \to f(x)$ pointwise. Moreover,

$$||g_n - g_m||_{H_0} = ||g_n - g_m||_H$$

$$\leq ||g_n - f_n|| + ||f_n - f_m|| + ||g_m - f_m||$$

$$= n^{-1} + ||f_n - f_m|| + n^{-1} \to 0$$

when $n \to \infty$, as required.

2 Reconstruction of RKHS

References

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