Foundations of Reproducing Kernel Hilbert Spaces Advanced Topics in Machine Learning

D. Sejdinovic, A. Gretton

Gatsby Unit

March 12, 2013

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Foundations of RKHS

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Overview

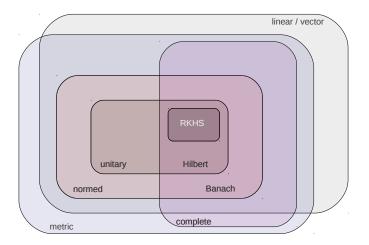
Elementary Hilbert space theory

- Norm. Inner product. Orthogonality
- Convergence. Complete spaces
- Linear operators. Riesz representation

What is an RKHS?

- Evaluation functionals view of RKHS
- Reproducing kernel
- Inner product between features
- Positive definite function
- Moore-Aronszajn Theorem

RKHS: a function space with a very special structure



Outline

Elementary Hilbert space theory

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- Convergence. Complete spaces
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Normed vector space

Definition (Norm)

Let \mathcal{F} be a vector space over the field \mathbb{R} of real numbers (or \mathbb{C}). A function $\|\cdot\|_{\mathcal{F}} : \mathcal{F} \to [0, \infty)$ is said to be *a norm* on \mathcal{F} if

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$$||f||_{\mathcal{F}} = 0$$
 if and only if $f = \mathbf{0}$ (norm separates points),

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In every normed vector space, one can define a metric induced by the norm:

$$d(f,g) = \|f-g\|_{\mathcal{F}}.$$

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• ($\mathbb{R}, |\cdot|$), ($\mathbb{C}, |\cdot|$)

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- ($\mathbb{R}, |\cdot|$), ($\mathbb{C}, |\cdot|$)
- $\mathcal{F} = \mathbb{R}^d$: $\|\mathbf{x}\|_p = \left(\sum_{i=1}^d |x_i|^p\right)^{1/p}, \ p \ge 1$ (only quasi-norm for 0)

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(only quasi-norm for $0)$

•
$$p \to \infty$$
: maximum norm, $\|\mathbf{x}\|_{\infty} = \max_i |x_i|$

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• $\mathcal{F} = \mathbb{R}^d$: $\|\mathbf{x}\|_p = \left(\sum_{i=1}^d |x_i|^p\right)^{1/p}, p \ge 1$
(only quasi-norm for $0)
• $p = 1$: Manhattan
• $p = 2$: Euclidean$

•
$$p \to \infty$$
: maximum norm, $\|\mathbf{x}\|_{\infty} = \max_i |x_i|$

•
$$\mathcal{F} = C[a,b]$$
: $||f||_p = \left(\int_a^b |f(x)|^p dx\right)^{1/p}, \ p \ge 1$

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Inner product

Definition (Inner product)

Let \mathcal{F} be a vector space over \mathbb{R} . A function $\langle \cdot, \cdot \rangle_{\mathcal{F}} : \mathcal{F} \times \mathcal{F} \to \mathbb{R}$ is said to be *an inner product* on \mathcal{F} if

$$(\alpha_1 f_1 + \alpha_2 f_2, \mathbf{g})_{\mathcal{F}} = \alpha_1 \langle f_1, \mathbf{g} \rangle_{\mathcal{F}} + \alpha_2 \langle f_2, \mathbf{g} \rangle_{\mathcal{F}}$$

$$(f,g)_{\mathcal{F}} = \langle g,f \rangle_{\mathcal{F}} \text{ (conjugate symmetry if over } \mathbb{C})$$

$$(f, f)_{\mathcal{F}} \geq 0 \text{ and } \langle f, f \rangle_{\mathcal{F}} = 0 \text{ if and only if } f = 0.$$

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In every inner product vector space, one can define *a norm* induced by the inner product:

$$\|f\|_{\mathcal{F}} = \langle f, f \rangle_{\mathcal{F}}^{1/2}$$
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Examples of inner product

•
$$\mathcal{F} = \mathbb{R}^d$$
: $\langle \mathbf{x}, \mathbf{y} \rangle = \sum_{i=1}^d x_i y_i$

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: $\langle \mathbf{x}, \mathbf{y} \rangle = \sum_{i=1}^d x_i y_i$
• $\mathcal{F} = C[\mathbf{a}, \mathbf{b}]$: $\langle f, g \rangle = \int_{\mathbf{a}}^b f(x)g(x)dx$

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• $\mathcal{F} = C[\mathbf{a}, \mathbf{b}]$: $\langle f, g \rangle = \int_a^b f(x)g(x)dx$
• $\mathcal{F} = \mathbb{R}^{d \times d}$: $\langle \mathbf{A}, \mathbf{B} \rangle = Tr(\mathbf{AB}^\top)$

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Angles. Orthogonality

Angle θ between $f, g \in \mathcal{F} \setminus \{0\}$ is given by:

$$\cos\theta = \frac{\langle f, g \rangle_{\mathcal{F}}}{\|f\|_{\mathcal{F}} \|g\|_{\mathcal{F}}}$$

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Definition

We say that f is orthogonal to g and write $f \perp g$, if $\langle f, g \rangle_{\mathcal{F}} = 0$. For $M \subset \mathcal{F}$, the orthogonal complement of M is:

$$M^{\perp}$$
 := { $g \in \mathcal{F}$: $f \perp g, \forall f \in M$ }.

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• M^{\perp} is a linear subspace of \mathcal{F} ; $M \cap M^{\perp} = \{0\}$

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Key relations in inner product space

•
$$|\langle f,g \rangle| \le ||f|| \cdot ||g||$$
 (Cauchy-Schwarz inequality)
• $2 ||f||^2 + 2 ||g||^2 = ||f + g||^2 + ||f - g||^2$ (the parallelogram law)
• $4 \langle f,g \rangle = ||f + g||^2 - ||f - g||^2$ (the polarization identity)

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Key relations in inner product space

• $|\langle f,g \rangle| \le ||f|| \cdot ||g||$ (Cauchy-Schwarz inequality) • $2 ||f||^2 + 2 ||g||^2 = ||f + g||^2 + ||f - g||^2$ (the parallelogram law) • $4 \langle f,g \rangle = ||f + g||^2 - ||f - g||^2$ (the polarization identity) • $f \perp g \implies ||f||^2 + ||g||^2 = ||f + g||^2$ (Pythagorean theorem)

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Definition (Convergent sequence)

A sequence $\{f_n\}_{n=1}^{\infty}$ of elements of a normed vector space $(\mathcal{F}, \|\cdot\|_{\mathcal{F}})$ is said to *converge* to $f \in \mathcal{F}$ if for every $\epsilon > 0$, there exists $N = N(\varepsilon) \in \mathbb{N}$, such that for all $n \ge N$, $\|f_n - f\|_{\mathcal{F}} < \epsilon$.

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Definition (Cauchy sequence)

A sequence $\{f_n\}_{n=1}^{\infty}$ of elements of a normed vector space $(\mathcal{F}, \|\cdot\|_{\mathcal{F}})$ is said to be a Cauchy (fundamental) sequence if for every $\epsilon > 0$, there exists $N = N(\varepsilon) \in \mathbb{N}$, such that for all $n, m \ge N$, $\|f_n - f_m\|_{\mathcal{F}} < \epsilon$.

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Definition (Convergent sequence)

A sequence $\{f_n\}_{n=1}^{\infty}$ of elements of a normed vector space $(\mathcal{F}, \|\cdot\|_{\mathcal{F}})$ is said to converge to $f \in \mathcal{F}$ if for every $\epsilon > 0$, there exists $N = N(\varepsilon) \in \mathbb{N}$, such that for all $n \geq N$, $||f_n - f||_{\mathcal{F}} < \epsilon$.

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From
$$\|f_n - f_m\|_{\mathcal{F}} \le \|f_n - f\|_{\mathcal{F}} + \|f - f_m\|_{\mathcal{F}}$$
, convergent \Rightarrow Cauchy.

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Cauchy⇒convergent

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Foundations of RKHS

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Examples

Example

1, 1.4, 1.41, 1.414, 1.4142, ... is a Cauchy sequence in $\mathbb Q$ which does not converge - because $\sqrt{2}\notin\mathbb Q.$

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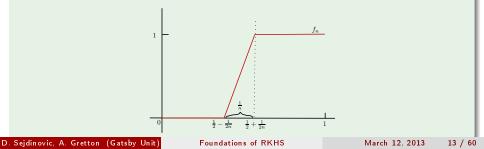
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Example

C[0,1] with the norm $||f||_2 = \left(\int_0^1 |f(x)|^2 dx\right)^{1/2}$, a sequence $\{f_n\}$ does not have a continuous limit!



Complete space

Definition (Complete space)

A metric space \mathcal{F} is said to be *complete* if every Cauchy sequence $\{f_n\}_{n=1}^{\infty}$ in \mathcal{F} converges: it has a limit, and this limit is in \mathcal{F} .

• i.e., one can find
$$f \in \mathcal{F}$$
, s.t. $\lim_{n \to \infty} \|f_n - f\|_{\mathcal{F}} = 0$.

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- Complete + norm = Banach
- Complete + inner product = Hilbert

Closed vs. Complete

- Closed: M ⊆ F is closed (in F) if it contains limits of all sequences in M that converge in F
- **Complete**: *M* is complete (with no reference to a larger space) if all Cauchy sequences in *M* converge in *M*

Closed vs. Complete

- Closed: M ⊆ F is closed (in F) if it contains limits of all sequences in M that converge in F
- **Complete**: *M* is complete (with no reference to a larger space) if all Cauchy sequences in *M* converge in *M*
- If M is a **closed subspace** of a Hilbert space \mathcal{F} , then:

$$M + M^{\perp} = \left\{ m + m^{\perp} : m \in M, m^{\perp} \in M^{\perp} \right\} = \mathcal{F}.$$

• In particular, for closed subspace $M \underset{\neq}{\subseteq} \mathcal{F}, \ M^{\perp} \neq \{0\}.$

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Examples of Hilbert spaces

Example

For an index set A, the space $\ell^2(A)$ of sequences $\{x_\alpha\}_{\alpha \in A}$ of real numbers, satisfying $\sum_{\alpha \in A} |x_\alpha|^2 < \infty$, endowed with the inner product

$$\langle \{x_{\alpha}\}, \{y_{\alpha}\} \rangle_{\ell^{2}(\mathcal{A})} = \sum_{\alpha \in \mathcal{A}} x_{\alpha} y_{\alpha}$$

is a Hilbert space.

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Examples of Hilbert spaces (2)

Example

If ν is a positive measure on $\mathcal{X} \subset \mathbb{R}^d$, then the space

$$L_2(\mathcal{X};\nu) := \left\{ f: \mathcal{X} \to \mathbb{R} \mid \left\| f \right\|_2 = \left(\int_{\mathcal{X}} |f(x)|^2 d\nu(x) \right)^{1/2} < \infty \right\}$$

is a Hilbert space with inner product

$$\langle f,g\rangle_2 = \int_{\mathcal{X}} f(x)g(x)d\nu(x).$$

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is a Hilbert space with inner product

$$\langle f,g\rangle_2 = \int_{\mathcal{X}} f(x)g(x)d\nu(x).$$

• Strictly speaking, $L_2(\mathcal{X}; \nu)$ is the space of equivalence classes of functions that differ by at most a set of ν -measure zero.

Outline



Elementary Hilbert space theory

- Norm. Inner product. Orthogonality
- Convergence. Complete spaces
- Linear operators. Riesz representation

What is an RKHS?

- Evaluation functionals view of RKHS
- Reproducing kernel
- Inner product between features
- Positive definite function
- Moore-Aronszajn Theorem

Linear operators

Definition (Linear operator)

Consider a function $A : \mathcal{F} \to \mathcal{G}$, where \mathcal{F} and \mathcal{G} are both vector spaces over \mathbb{R} . A is said to be a **linear operator** if

 $A(\alpha_1 f_1 + \alpha_2 f_2) = \alpha_1 (Af_1) + \alpha_2 (Af_2) \quad \forall \alpha_1, \alpha_2 \in \mathbb{R}, f_1, f_2 \in \mathcal{F}.$

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Operators with $\mathcal{G} = \mathbb{R}$ are called **functionals**.

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Operators with $\mathcal{G} = \mathbb{R}$ are called **functionals**.

Example

For $g \in \mathcal{F}$, $A_g : \mathcal{F} \to \mathbb{R}$, defined with $A_g f = \langle f, g \rangle_{\mathcal{F}}$ is a linear functional.

$$\begin{aligned} A_{g}(\alpha_{1}f_{1} + \alpha_{2}f_{2}) &= \langle \alpha_{1}f_{1} + \alpha_{2}f_{2}, g \rangle_{\mathcal{F}} \\ &= \alpha_{1} \langle f_{1}, g \rangle_{\mathcal{F}} + \alpha_{2} \langle f_{2}, g \rangle_{\mathcal{F}} \\ &= \alpha_{1}A_{g}f_{1} + \alpha_{2}A_{g}f_{2}. \end{aligned}$$

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Boundedness

Definition (Operator norm)

The operator norm of a linear operator $A\,:\,\mathcal{F}
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$$\|A\| = \sup_{f \in \mathcal{F}} \frac{\|Af\|_{\mathcal{G}}}{\|f\|_{\mathcal{F}}}$$

If $||A|| < \infty$, A is called a **bounded linear operator**.

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bounded operator \neq bounded function

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Foundations of RKHS

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Continuity

Definition (Continuity)

Consider a function $A : \mathcal{F} \to \mathcal{G}$, where \mathcal{F} and \mathcal{G} are both normed vector spaces over \mathbb{R} . A is said to be **continuous** at $f_0 \in \mathcal{F}$, if for every $\epsilon > 0$, there exists a $\delta = \delta(\epsilon, f_0) > 0$, s.t.

$$\|f - f_0\|_{\mathcal{F}} < \delta \qquad \Longrightarrow \qquad \|Af - Af_0\|_{\mathcal{G}} < \epsilon$$

A is said to be **continuous** on \mathcal{F} , if it is continuous at every point of \mathcal{F} .

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Example

For $g \in \mathcal{F}$, $A_g : \mathcal{F} \to \mathbb{R}$, defined with $A_g(f) := \langle f, g \rangle_{\mathcal{F}}$ is continuous on \mathcal{F} : $|A_g f_1 - A_g f_2| = |\langle f_1 - f_2, g \rangle_{\mathcal{F}}| \le ||g||_{\mathcal{F}} ||f_1 - f_2||_{\mathcal{F}}$, so can take $\delta = \varepsilon / ||g||_{\mathcal{F}}$ (also Lipschitz!).

- ullet Linear operator $A\,:\,\mathcal{F} o\mathcal{G}$ maps linear subspaces to linear subspaces
 - $Null(A) = A^{-1}(\{0\})$ is a linear subspace of $\mathcal F$
 - $Im(A) = A(\mathcal{F})$ is a linear subspace of \mathcal{G} .

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- Continuous function A : F → G maps to open (closed) sets from open (closed) sets
 - If A is also linear, Null(A) = A⁻¹({0}) is a closed linear subspace of *F*.

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- Continuous function A : F → G maps to open (closed) sets from open (closed) sets
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- \bullet Bounded linear operator $A\,:\,\mathcal{F}\to\mathcal{G}$ maps bounded sets to bounded sets

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Continuous operator \equiv Bounded operator

Theorem

Let $(\mathcal{F}, \|\cdot\|_{\mathcal{F}})$ and $(\mathcal{G}, \|\cdot\|_{\mathcal{G}})$ be normed linear spaces. If L is a linear operator, then the following three conditions are equivalent:

- L is a bounded operator.
- 2 L is continuous on \mathcal{F} .
- **()** L is continuous at one point of \mathcal{F} .

Proof

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Dual space

Definition (Topological dual)

If \mathcal{F} is a normed space, then the space \mathcal{F}' of *continuous linear* functionals $A : \mathcal{F} \to \mathbb{R}$ is called the topological dual space of \mathcal{F} .

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We have seen that $A_g:=\langle\cdot,g
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angle_{\mathcal{F}}$ are continuous linear functionals.

Theorem (Riesz representation)

In a Hilbert space \mathcal{F} , for every continous linear functional $L \in \mathcal{F}'$, there exists a unique $g \in \mathcal{F}$, such that

$$Lf \equiv \langle f, g \rangle_{\mathcal{F}}$$
.

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Proof of Riesz representation

Proof.

Let $L \in \mathcal{F}'$. If $Lf \equiv 0$, then $Lf = \langle f, 0 \rangle_{\mathcal{F}}$, so g = 0. Otherwise, $M = Null(L) \subsetneq \mathcal{F}$ is a closed linear linear subspace of \mathcal{F} , so there must exist $h \in M^{\perp}$, with $||h||_{\mathcal{F}} = 1$. We claim that we can take g = (Lh)h. Indeed, for $f \in \mathcal{F}$, take $u_f = (Lf)h - (Lh)f$. Clearly $u_f \in M$. Thus,

$$0 = \langle u_f, h \rangle_{\mathcal{F}} = \langle (Lf)h - (Lh)f, h \rangle_{\mathcal{F}} = (Lf) ||h||_{\mathcal{F}}^2 - (Lh) \langle f, h \rangle_{\mathcal{F}} = Lf - \langle f, (Lh)h \rangle_{\mathcal{F}}.$$

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Orthonormal basis

• orthonormal set $\{u_{\alpha}\}_{\alpha\in \mathcal{A}}$, s.t.

$$\langle u_{\alpha}, u_{\beta} \rangle_{\mathcal{F}} = \begin{cases} 1, & \alpha = \beta \\ 0, & \alpha \neq \beta \end{cases}$$

• if also basis, define $\widehat{f}(lpha) = \langle f, u_lpha
angle_{\mathcal{F}}$

$$f = \sum_{\alpha \in A} \hat{f}(\alpha) u_{\alpha}$$

$$\langle f, g \rangle_{\mathcal{F}} = \sum_{\alpha \in A} \hat{f}(\alpha) \hat{g}(\alpha)$$

$$= \left\langle \left\{ \hat{f}(\alpha) \right\}, \left\{ \hat{g}(\alpha) \right\} \right\rangle_{\ell^{2}(A)}$$

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Isometric isomorphism

Definition (Hilbert space isomorphism)

Two Hilbert spaces \mathcal{H} and \mathcal{F} are said to be *isometrically isomorphic* if there is a **linear bijective map** $U : \mathcal{H} \to \mathcal{F}$, which **preserves the inner product**, i.e., $\langle h_1, h_2 \rangle_{\mathcal{H}} = \langle Uh_1, Uh_2 \rangle_{\mathcal{F}}$.

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Riesz representation gives an isomorphism $g \mapsto \langle \cdot, g \rangle_{\mathcal{F}}$ between \mathcal{F} and \mathcal{F}' : dual space of a Hilbert space is also a Hilbert space.

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Riesz representation gives an isomorphism $g \mapsto \langle \cdot, g \rangle_{\mathcal{F}}$ between \mathcal{F} and \mathcal{F}' : dual space of a Hilbert space is also a Hilbert space.

Theorem

Every Hilbert space has an orthonormal basis. Thus, all Hilbert spaces are isometrically isomorphic to $\ell^2(A)$, for some set A. We can take $A = \mathbb{N}$ iff Hilbert space is separable.

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Hilbert space:

• is a vector space over \mathbb{R} (or \mathbb{C})

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Hilbert space:

- is a vector space over \mathbb{R} (or \mathbb{C})
- comes equipped with an inner product, a norm and a metric

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Hilbert space:

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- comes equipped with an inner product, a norm and a metric
- is complete with respect to its metric

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- comes equipped with an inner product, a norm and a metric
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- continuity and boundedness of linear operators are equivalent
- all continuous linear functionals arise from the inner product

Outline

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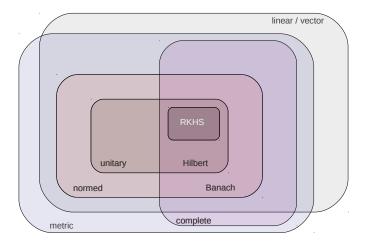
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RKHS: a function space with a very special structure



Evaluation functional

Definition (Evaluation functional)

Let \mathcal{H} be a Hilbert space of functions $f : \mathcal{X} \to \mathbb{R}$, defined on a non-empty set \mathcal{X} . For a fixed $x \in \mathcal{X}$, map $\delta_x : \mathcal{H} \to \mathbb{R}$, $\delta_x : f \mapsto f(x)$ is called the (Dirac) evaluation functional at x.

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• Evaluation functional is always linear: For $f, g \in \mathcal{H}$ and $\alpha, \beta \in \mathbb{R}$, $\delta_x(\alpha f + \beta g) = (\alpha f + \beta g)(x) = \alpha f(x) + \beta g(x) = \alpha \delta_x(f) + \beta \delta_x(g).$

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Evaluation functional

Definition (Evaluation functional)

Let \mathcal{H} be a Hilbert space of functions $f : \mathcal{X} \to \mathbb{R}$, defined on a non-empty set \mathcal{X} . For a fixed $x \in \mathcal{X}$, map $\delta_x : \mathcal{H} \to \mathbb{R}$, $\delta_x : f \mapsto f(x)$ is called the (Dirac) evaluation functional at x.

- Evaluation functional is always linear: For $f, g \in \mathcal{H}$ and $\alpha, \beta \in \mathbb{R}$, $\delta_x(\alpha f + \beta g) = (\alpha f + \beta g)(x) = \alpha f(x) + \beta g(x) = \alpha \delta_x(f) + \beta \delta_x(g).$
- But is it continuous?

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Discontinuous evaluation

Example

 \mathcal{F} : the space of polynomials over [0, 1], endowed with the L_p norm, i.e.,

$$||f_1 - f_2||_p = \left(\int_0^1 |f_1(x) - f_2(x)|^p dx\right)^{1/p}$$

Consider the sequence of functions $\{q_n\}_{n=1}^{\infty}$, where $q_n = x^n$. Then: $\lim_{n\to\infty} ||q_n - 0||_p = 0$, i.e., $\{q_n\}$ converges to "zero function" in L_p norm, but does not get close to zero function everywhere:

$$1 = \lim_{n \to \infty} \delta_1(q_n) \neq \delta_1(\lim_{n \to \infty} q_n) = 0.$$

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Discontinuous evaluation

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$$1 = \lim_{n \to \infty} \delta_1(q_n) \neq \delta_1(\lim_{n \to \infty} q_n) = 0.$$

 $\delta_1: f \mapsto f(1)$ is not continuous!

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Foundations of RKHS

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RKHS

Definition (Reproducing kernel Hilbert space)

A Hilbert space \mathcal{H} of functions $f : \mathcal{X} \to \mathbb{R}$, defined on a non-empty set \mathcal{X} is said to be a Reproducing Kernel Hilbert Space (RKHS) if $\delta_x \in \mathcal{H}'$, $\forall x \in \mathcal{X}$.

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Theorem (Norm convergence implies pointwise convergence) If $\lim_{n\to\infty} \|f_n - f\|_{\mathcal{H}} = 0$, then $\lim_{n\to\infty} f_n(x) = f(x), \forall x \in \mathcal{X}$.

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RKHS

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Theorem (Norm convergence implies pointwise convergence) If $\lim_{n\to\infty} \|f_n - f\|_{\mathcal{H}} = 0$, then $\lim_{n\to\infty} f_n(x) = f(x), \forall x \in \mathcal{X}$.

If two functions $f, g \in \mathcal{H}$ are close in the norm of \mathcal{H} , then f(x) and g(x)are close for all $x \in \mathcal{X}$

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Will discuss three distinct concepts:

- reproducing kernel
- inner product between features (kernel)
- positive definite function

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Will discuss three distinct concepts:

- reproducing kernel
- inner product between features (kernel)
- positive definite function

...and then show that they are all equivalent.

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Elementary Hilbert space theory

- Norm. Inner product. Orthogonality
- Convergence. Complete spaces
- Linear operators. Riesz representation

What is an RKHS?

• Evaluation functionals view of RKHS

Reproducing kernel

- Inner product between features
- Positive definite function
- Moore-Aronszajn Theorem

Reproducing kernel

Definition (Reproducing kernel)

Let \mathcal{H} be a Hilbert space of functions $f : \mathcal{X} \to \mathbb{R}$ defined on a non-empty set \mathcal{X} . A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called *a reproducing kernel* of \mathcal{H} if it satisfies

- $\forall x \in \mathcal{X}, k_x = k(\cdot, x) \in \mathcal{H},$
- $\forall x \in \mathcal{X}, \forall f \in \mathcal{H}, \langle f, k(\cdot, x) \rangle_{\mathcal{H}} = f(x)$ (the reproducing property).

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• $\forall x \in \mathcal{X}, \forall f \in \mathcal{H}, \langle f, k(\cdot, x) \rangle_{\mathcal{H}} = f(x)$ (the reproducing property).

In particular, for any
$$x, y \in \mathcal{X}$$
,
 $k(x, y) = \langle k(\cdot, y), k(\cdot, x) \rangle_{\mathcal{H}} = \langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}}.$

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Reproducing kernel

Reproducing kernel of an RKHS

Theorem

If it exists, reproducing kernel is unique.

Theorem

 ${\cal H}$ is a reproducing kernel Hilbert space if and only if it has a reproducing kernel.

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Elementary Hilbert space theory

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Functions representable as inner products

Definition (Kernel)

A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called *a kernel* on \mathcal{X} if there exists a Hilbert space (not necessarilly an RKHS) \mathcal{F} and a map $\phi : \mathcal{X} \to \mathcal{F}$, such that $k(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{F}}$.

Functions representable as inner products

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- ullet note that we dropped 'reproducing', as ${\mathcal F}$ may not be an RKHS.
- ϕ : $\mathcal{X} \to \mathcal{F}$ is called a **feature map**,
- \mathcal{F} is called a **feature space**.

Functions representable as inner products

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- ϕ : $\mathcal{X} \to \mathcal{F}$ is called a **feature map**,
- \mathcal{F} is called a **feature space**.

Corollary

Every **reproducing kernel** is a **kernel** (can take $\phi : x \mapsto k(\cdot, x)$, $k(x, y) = \langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}}$, i.e., RKHS \mathcal{H} is a feature space).

Example Consider $\mathcal{X} = \mathbb{R}^2$, and $k(x, y) = \langle x, y \rangle^2$ $k(x, y) = x_1^2 y_1^2 + x_2^2 y_2^2 + 2x_1 x_2 y_1 y_2$ $= \begin{bmatrix} x_1^2 & x_2^2 & \sqrt{2}x_1x_2 \end{bmatrix} \begin{bmatrix} y_1^2 \\ y_2^2 \\ \sqrt{2}y_1y_2 \end{bmatrix}$ $= \begin{bmatrix} x_1^2 & x_2^2 & x_1x_2 & x_1x_2 \end{bmatrix} \begin{bmatrix} y_1^2 \\ y_2^2 \\ y_1y_2 \\ y_1y_2 \\ y_1y_2 \end{bmatrix}.$ so we can use the feature maps $\phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$ or $ilde{\phi}(x) = \begin{bmatrix} x_1^2 & x_2^2 & x_1x_2 & x_1x_2 \end{bmatrix}$, with feature spaces $\mathcal{H} = \mathbb{R}^3$ or $ilde{\mathcal{H}} = \mathbb{R}^4$.

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Example Consider $\mathcal{X} = \mathbb{R}^2$, and $k(x, y) = \langle x, y \rangle^2$ $k(x, y) = x_1^2 y_1^2 + x_2^2 y_2^2 + 2x_1 x_2 y_1 y_2$ $= \begin{bmatrix} x_1^2 & x_2^2 & \sqrt{2}x_1x_2 \end{bmatrix} \begin{bmatrix} y_1^2 \\ y_2^2 \\ \sqrt{2}y_1y_2 \end{bmatrix}$ $= \begin{bmatrix} x_1^2 & x_2^2 & x_1x_2 & x_1x_2 \end{bmatrix} \begin{bmatrix} y_1^2 \\ y_2^2 \\ y_1y_2 \\ y_1y_2 \\ y_1y_2 \end{bmatrix}.$ so we can use the feature maps $\phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$ or $ilde{\phi}(x) = \begin{bmatrix} x_1^2 & x_2^2 & x_1x_2 & x_1x_2 \end{bmatrix}$, with feature spaces $\mathcal{H} = \mathbb{R}^3$ or $ilde{\mathcal{H}} = \mathbb{R}^4$.

Not RKHS!

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Foundations of RKHS

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Elementary Hilbert space theory

- Norm. Inner product. Orthogonality
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- Linear operators. Riesz representation

What is an RKHS?

- Evaluation functionals view of RKHS
- Reproducing kernel
- Inner product between features
- Positive definite function
- Moore-Aronszajn Theorem

Positive definite functions

Definition (Positive definite functions)

A symmetric function $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is positive definite if $\forall n \geq 1, \ \forall (a_1, \dots a_n) \in \mathbb{R}^n, \ \forall (x_1, \dots, x_n) \in \mathcal{X}^n$,

$$\sum_{i=1}^n \sum_{j=1}^n a_i a_j h(x_i, x_j) = \mathbf{a}^\top \mathbf{H} \mathbf{a} \ge 0.$$

The function $h(\cdot, \cdot)$ is *strictly* positive definite if for mutually distinct x_i , the equality holds only when all the a_i are zero.

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Kernels are positive definite

Every inner product is a positive definite function, and more generally:

Fact

Every kernel is a positive definite function.

reproducing kernel \implies kernel \implies positive definite

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Foundations of RKHS

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reproducing kernel \implies kernel \implies positive definite

Is every positive definite function a reproducing kernel for some RKHS?

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Theorem (Moore-Aronszajn - Part I)

Let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be positive definite. There is a **unique RKHS** $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ with reproducing kernel k.

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Example Consider $\mathcal{X} = \mathbb{R}^2$, and $k(x, y) = \langle x, y \rangle^2$ $k(x, y) = x_1^2 y_1^2 + x_2^2 y_2^2 + 2x_1 x_2 y_1 y_2$ $= \begin{bmatrix} x_1^2 & x_2^2 & \sqrt{2}x_1x_2 \end{bmatrix} \begin{vmatrix} y_1^2 \\ y_2^2 \\ \sqrt{2}y_1y_2 \end{vmatrix}$ $= \begin{bmatrix} x_1^2 & x_2^2 & x_1x_2 & x_1x_2 \end{bmatrix} \begin{bmatrix} y_1^2 \\ y_2^2 \\ y_1y_2 \\ y_1y_2 \\ y_1y_2 \end{bmatrix}.$ so we can use the feature maps $\phi(x) = \begin{bmatrix} x_1^2 & x_2^2 & \sqrt{2}x_1x_2 \end{bmatrix}$ or $ilde{\phi}(x) = \begin{bmatrix} x_1^2 & x_2^2 & x_1x_2 & x_1x_2 \end{bmatrix}$, with feature spaces $\mathcal{H} = \mathbb{R}^3$ or $ilde{\mathcal{H}} = \mathbb{R}^4$.

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Example Consider $\mathcal{X} = \mathbb{R}^2$, and $k(x, y) = \langle x, y \rangle^2$ $k(x, y) = x_1^2 y_1^2 + x_2^2 y_2^2 + 2x_1 x_2 y_1 y_2$ $= \begin{bmatrix} x_1^2 & x_2^2 & \sqrt{2}x_1x_2 \end{bmatrix} \begin{vmatrix} y_1^2 \\ y_2^2 \\ \sqrt{2}y_1y_2 \end{vmatrix}$ $= \begin{bmatrix} x_1^2 & x_2^2 & x_1x_2 & x_1x_2 \end{bmatrix} \begin{bmatrix} y_1^2 \\ y_2^2 \\ y_1y_2 \\ y_1y_2 \\ y_1y_2 \end{bmatrix}.$ so we can use the feature maps $\phi(x) = \begin{bmatrix} x_1^2 & x_2^2 & \sqrt{2}x_1x_2 \end{bmatrix}$ or $ilde{\phi}(x) = \begin{bmatrix} x_1^2 & x_2^2 & x_1x_2 & x_1x_2 \end{bmatrix}$, with feature spaces $\mathcal{H} = \mathbb{R}^3$ or $ilde{\mathcal{H}} = \mathbb{R}^4$.

 ${\mathcal H}$ and ${ ilde{{\mathcal H}}}$ are not RKHS - RKHS of k is unique

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Foundations of RKHS

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• There are (infinitely) many feature space representations (and we can even work in one or more of them, if it's convenient!)

$$\langle \phi(x), \phi(y) \rangle_{\mathbb{R}^3} = ay_1^2 + by_2^2 + c\sqrt{2}y_1y_2 = k_x(y) = \langle k_x, k_y \rangle_{\mathcal{H}_k}$$

 $\phi(x) = [a = x_1^2 \quad b = x_2^2 \quad c = \sqrt{2}x_1x_2]$

• There are (infinitely) many feature space representations (and we can even work in one or more of them, if it's convenient!)

$$\left\langle \tilde{\phi}(x), \tilde{\phi}(y) \right\rangle_{\mathbb{R}^4} = \tilde{a}y_1^2 + \tilde{b}y_2^2 + \tilde{c}y_1y_2 + \tilde{d}y_1y_2 = k_x(y) = \langle k_x, k_y \rangle_{\mathcal{H}_k}$$
$$\tilde{\phi}(x) =$$
$$\begin{bmatrix} \tilde{a} = x_1^2 & \tilde{b} = x_2^2 & \tilde{c} = x_1x_2 & \tilde{d} = x_1x_2 \end{bmatrix}$$

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• There are (infinitely) many feature space representations (and we can even work in one or more of them, if it's convenient!)

$$\begin{aligned} \langle \phi(x), \phi(y) \rangle_{\mathbb{R}^3} &= a y_1^2 + b y_2^2 + c \sqrt{2} y_1 y_2 &= k_x(y) = \langle k_x, k_y \rangle_{\mathcal{H}_k} \\ \phi(x) &= \\ \begin{bmatrix} a = x_1^2 & b = x_2^2 & c = \sqrt{2} x_1 x_2 \end{bmatrix} \end{aligned}$$

$$\left\langle \tilde{\phi}(x), \tilde{\phi}(y) \right\rangle_{\mathbb{R}^4} = \tilde{a}y_1^2 + \tilde{b}y_2^2 + \tilde{c}y_1y_2 + \tilde{d}y_1y_2 = k_x(y) = \left\langle k_x, k_y \right\rangle_{\mathcal{H}_k}$$
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• But what remains unique?

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- But what remains unique?
- Kernel and its RKHS!

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Foundations of RKHS

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Summary

reproducing kernel \iff kernel \iff positive definite

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Foundations of RKHS

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reproducing kernel \iff kernel \iff positive definite set of all kernels: $\mathbb{R}^{\mathcal{X} \times \mathcal{X}}_+$ set of all subspaces of $\mathbb{R}^{\mathcal{X}}$ with continuous evaluation: $Hilb(\mathbb{R}^{\mathcal{X}})$

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Foundations of RKHS

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Elementary Hilbert space theory

- Norm. Inner product. Orthogonality
- Convergence. Complete spaces
- Linear operators. Riesz representation

What is an RKHS?

- Evaluation functionals view of RKHS
- Reproducing kernel
- Inner product between features
- Positive definite function
- Moore-Aronszajn Theorem

Theorem (Moore-Aronszajn - Part I)

Let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be positive definite. There is a **unique RKHS** $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ with reproducing kernel k.

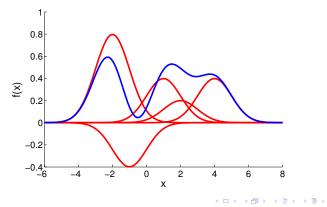
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Starting with a positive def. k, construct a **pre-RKHS** \mathcal{H}_0 with properties:

- **①** The evaluation functionals δ_x are continuous on \mathcal{H}_0 ,
- 2 Any Cauchy sequence f_n in \mathcal{H}_0 which converges pointwise to 0 also converges in \mathcal{H}_0 -norm to 0.

pre-RKHS $\mathcal{H}_0 = span \{k(\cdot, x) | x \in \mathcal{X}\}$ will be taken to be the set of functions:

$$f(x) = \sum_{i=1}^{n} \alpha_i k(x_i, x)$$



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Theorem (Moore-Aronszajn - Part II)

Space $\mathcal{H}_0 = \text{span}\left\{k(\cdot,x) \,|\, x \in \mathcal{X}
ight\}$ is endowed with the inner product

$$\langle f, g \rangle_{\mathcal{H}_0} = \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j k(x_i, y_j),$$

where $f = \sum_{i=1}^{n} \alpha_i k(\cdot, x_i)$ and $g = \sum_{j=1}^{m} \beta_j k(\cdot, y_j)$, then \mathcal{H}_0 is dense in RKHS \mathcal{H} of k.

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Define \mathcal{H} to be the set of functions $f \in \mathbb{R}^{\mathcal{X}}$ for which there exists a Cauchy sequence $\{f_n\} \in \mathcal{H}_0$ converging **pointwise** to f.

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We define the inner product between f, g ∈ H as the limit of an inner product of the Cauchy sequences {f_n}, {g_n} converging to f and g respectively. Is the inner product well defined, and independent of the sequences used?

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- 3 An inner product space must satisfy $\langle f, f \rangle_{\mathcal{H}} = 0$ iff f = 0. Is this true when we define the inner product on \mathcal{H} as above?

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- An inner product space must satisfy \$\langle f, f \rangle_{\mathcal{H}} = 0\$ iff \$f = 0\$. Is this true when we define the inner product on \$\mathcal{H}\$ as above?
- ${f 0}$ Are the evaluation functionals still continuous on ${\cal H}?$
- Is H complete (a Hilbert space)?

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reproducing kernel \iff kernel \iff positive definite

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Foundations of RKHS

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Summary

reproducing kernel \iff kernel \iff positive definite all kernels $\mathbb{R}^{\mathcal{X} \times \mathcal{X}}_+$ $\stackrel{1-1}{\longleftrightarrow}$ all function spaces with continuous evaluation $Hilb(\mathbb{R}^{\mathcal{X}})$

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Fact (Sum and scaling of kernels)

If k, k_1 , and k_2 are kernels on \mathcal{X} , and $\alpha \ge 0$ is a scalar, then αk , $k_1 + k_2$ are kernels.

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- A difference of kernels is not necessarily a kernel! This is because we cannot have $k_1(x,x) k_2(x,x) = \langle \phi(x), \phi(x) \rangle_{\mathcal{H}} < 0$.
- This gives the set of all kernels the geometry of a *closed convex cone*.

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- This gives the set of all kernels the geometry of a *closed convex cone*.

$$\mathcal{H}_{k_1+k_2} = \mathcal{H}_{k_1} + \mathcal{H}_{k_2} = \{f_1 + f_2 : f_1 \in \mathcal{H}_{k_1}, f_2 \in \mathcal{H}_{k_2}\}$$

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Fact (Product of kernels)

If k_1 and k_2 are kernels on \mathcal{X} and \mathcal{Y} , then $k = k_1 \otimes k_2$, given by:

$$k((x,y),(x',y')) := k_1(x,x')k_2(y,y')$$

is a kernel on $\mathcal{X} \times \mathcal{Y}$. If $\mathcal{X} = \mathcal{Y}$, then $k = k_1 \cdot k_2$, given by:

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$$\mathcal{H}_{k_1\otimes k_2}\cong \mathcal{H}_{k_1}\otimes \mathcal{H}_{k_2}$$

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Summary

all kernels $\mathbb{R}^{\mathcal{X}\times\mathcal{X}}_+$ $\stackrel{1-1}{\longleftrightarrow}$ all function spaces with continuous evaluation $Hilb(\mathbb{R}^{\mathcal{X}})$

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Foundations of RKHS

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Summary

all kernels $\mathbb{R}^{\mathcal{X} \times \mathcal{X}}_+$ $\stackrel{1-1}{\longleftrightarrow}$ all function spaces with continuous evaluation $Hilb(\mathbb{R}^{\mathcal{X}})$ bijection between $\mathbb{R}^{\mathcal{X} \times \mathcal{X}}_+$ and $Hilb(\mathbb{R}^{\mathcal{X}})$ preserves geometric structure

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Foundations of RKHS

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New kernels from old:

• trivial (linear) kernel on \mathbb{R}^d is $k(x,x')=\langle x,x'
angle$

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New kernels from old:

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• for any
$$p(t) = a_m t^m + \dots + a_1 t + a_0$$
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- polynomial kernel: $k(x,x') = (\langle x,x' \rangle + c)^m$, for $c \ge 0$

Image: A matrix and a matrix

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