

Foundations of Reproducing Kernel Hilbert Spaces II

Advanced Topics in Machine Learning

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Gatsby Unit

slides and notes are available at www.gatsby.ucl.ac.uk/~dino/teaching

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The story so far

- Hilbert space:

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 - define $k(\cdot, x)$ as that representer of evaluation: **reproducing kernel**
- **kernel** as an inner product between features: $k(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{H}}$

Overview

- 1 What is an RKHS?
 - Reproducing kernel
 - Inner product between features
 - Positive definite function
- 2 Moore-Aronszajn Theorem
- 3 Mercer representation of RKHS
 - Integral operator
 - Mercer's theorem
 - Relation between \mathcal{H}_k and $L_2(\mathcal{X}; \nu)$
- 4 Operations with kernels
 - Sum and product
 - Constructing new kernels

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RKHS

Definition (Reproducing kernel Hilbert space)

Let \mathcal{X} be a non-empty set. A Hilbert space \mathcal{H} of functions $f : \mathcal{X} \rightarrow \mathbb{R}$ is said to be a Reproducing Kernel Hilbert Space (RKHS) if evaluation functionals $\delta_x : f \mapsto f(x)$ are continuous $\forall x \in \mathcal{X}$.

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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
- positive definite function

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

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Reproducing kernel

Definition (Reproducing kernel)

Let \mathcal{H} be a Hilbert space of functions $f : \mathcal{X} \rightarrow \mathbb{R}$ defined on a non-empty set \mathcal{X} . A function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ 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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In particular, for any $x, y \in \mathcal{X}$,

$$k(x, y) = \langle k(\cdot, y), k(\cdot, x) \rangle_{\mathcal{H}} = \langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}}.$$

Reproducing kernel of an RKHS

Theorem

If it exists, reproducing kernel is unique.

Theorem

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

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Feature space inner product

Definition (Kernel)

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

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- \mathcal{F} is called a **feature space**.

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- \mathcal{F} is called a **feature space**.

Fact

Every reproducing kernel is a kernel (every RKHS is a valid feature space).

Non-uniqueness of feature representation

Example

Consider $\mathcal{X} = \mathbb{R}^2$, and $k(x, y) = \langle x, y \rangle^2$

$$\begin{aligned}
 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_1 x_2 \end{bmatrix} \begin{bmatrix} y_1^2 \\ y_2^2 \\ \sqrt{2}y_1 y_2 \end{bmatrix} \\
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so we can use the feature maps $\phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1 x_2)$ or

$\tilde{\phi}(x) = [x_1^2 \quad x_2^2 \quad x_1 x_2 \quad x_1 x_2]$, with feature spaces $\mathcal{H} = \mathbb{R}^3$ or $\tilde{\mathcal{H}} = \mathbb{R}^4$.

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Not RKHS!

Evaluation is not defined on \mathbb{R}^3 or \mathbb{R}^4 .

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Positive definite functions

Definition (Positive definite functions)

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

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

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h is *strictly* positive definite if for mutually distinct x_i , the equality holds only when all the a_i are zero.

Kernels are positive definite

Fact

Every kernel is a positive definite function.

Kernels are positive definite

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$$\begin{aligned}
 \sum_{i=1}^n \sum_{j=1}^n a_i a_j k(x_i, x_j) &= \sum_{i=1}^n \sum_{j=1}^n a_i a_j \langle \phi(x_i), \phi(x_j) \rangle_{\mathcal{F}} \\
 &= \left\langle \sum_{i=1}^n a_i \phi(x_i), \sum_{j=1}^n a_j \phi(x_j) \right\rangle_{\mathcal{F}} \\
 &= \left\| \sum_{i=1}^n a_i \phi(x_i) \right\|_{\mathcal{F}}^2 \geq 0.
 \end{aligned}$$

So far

reproducing kernel \implies kernel \implies positive definite

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

So far

reproducing kernel \iff kernel \iff positive definite

Yes (Moore-Aronszajn)!

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Moore-Aronszajn Theorem

Theorem (Moore-Aronszajn)

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

Moore-Aronszajn Theorem: pre-RKHS

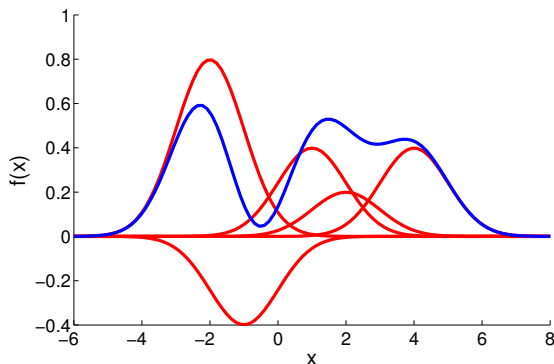
Starting with a positive def. k , construct a **pre-RKHS** (an inner product space) $\mathcal{H}_0 \subset \mathbb{R}^{\mathcal{X}}$ with properties:

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

Moore-Aronszajn Theorem: pre-RKHS

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

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



Moore-Aronszajn Theorem: Steps

Theorem (Moore-Aronszajn - Step A)

Space $\mathcal{H}_0 = \text{span} \{k(\cdot, x) \mid x \in \mathcal{X}\}$, 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 $g = \sum_{j=1}^m \beta_j k(\cdot, y_j)$, is a valid pre-RKHS.

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Theorem (Moore-Aronszajn - Step B)

Let \mathcal{H}_0 be a pre-RKHS space. Define \mathcal{H} to be the set of functions $f \in \mathbb{R}^{\mathcal{X}}$ for which there exists an \mathcal{H}_0 -Cauchy sequence $\{f_n\}$ converging **pointwise** to f . Then, \mathcal{H} is an RKHS.

Moore-Aronszajn Theorem - Step A

- Is $\langle f, g \rangle_{\mathcal{H}_0}$ a valid inner product?
- Are evaluation functionals δ_x continuous on \mathcal{H}_0 ?
- Does every \mathcal{H}_0 -Cauchy sequence f_n which converges pointwise to 0 also converge in \mathcal{H}_0 -norm to 0?

Moore-Aronszajn Theorem- Step B

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

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- 1 We define the inner product between $f, g \in \mathcal{H}$ as the limit of an inner product of the \mathcal{H}_0 -Cauchy sequences $\{f_n\}, \{g_n\}$ converging to f and g respectively. Is this inner product well defined, i.e., independent of the sequences used?

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 - ② 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?
 - ③ Are the evaluation functionals still continuous on \mathcal{H} ?
 - ④ Is \mathcal{H} complete (i.e., does every \mathcal{H} -Cauchy sequence converge)?
- (1)+(2)+(3)+(4) $\implies \mathcal{H}$ is RKHS!

Summary

reproducing kernel \iff kernel \iff positive definite

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set of all pd functions: $\mathbb{R}_+^{\mathcal{X} \times \mathcal{X}}$

$\xleftrightarrow{1-1}$

set of all RKHSs: $\text{Hilb}(\mathbb{R}^{\mathcal{X}})$

Non-uniqueness of feature representation

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

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

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

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- Different feature maps give *coefficients* of canonical feature map $k(\cdot, x)$ in terms of (different) simpler functions.
- RKHS of k remains **unique**, regardless of the representation.

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Assumptions

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 - nor on k (apart from it being a positive definite function)
- Now, assume that:

Assumptions

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 - \mathcal{X} (apart from it being a non-empty set)
 - nor on k (apart from it being a positive definite function)
- Now, assume that:
 - \mathcal{X} is a compact metric space
 - such as $[a, b]^d$, **key**: every continuous function on \mathcal{X} is bounded and uniformly continuous

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 - $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a continuous positive definite function

Integral operator of a kernel

Definition (Integral operator)

Let ν be a finite Borel measure on \mathcal{X} . For the linear map

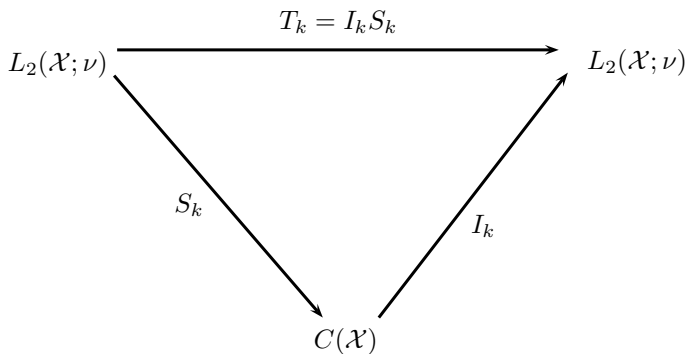
$$S_k : L_2(\mathcal{X}; \nu) \rightarrow \mathcal{C}(\mathcal{X}),$$
$$(S_k \tilde{f})(x) = \int k(x, y) f(y) d\nu(y), \quad f \in \tilde{f} \in L_2(\mathcal{X}; \nu),$$

its composition $T_k = I_k \circ S_k$ with the inclusion $I_k : \mathcal{C}(\mathcal{X}) \hookrightarrow L_2(\mathcal{X}; \nu)$ is said to be the *integral operator* of k .

Proof that $S_k \tilde{f}$ is continuous

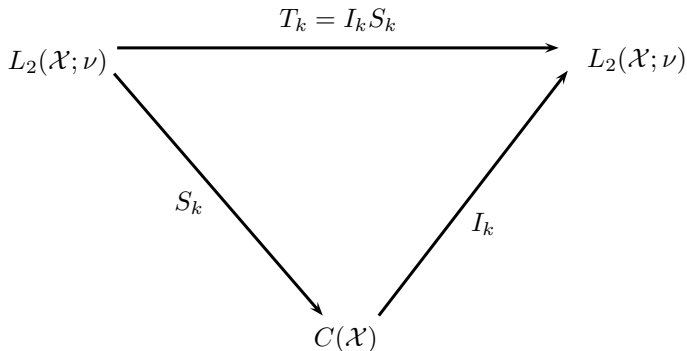
$$\begin{aligned}
 |(S_k \tilde{f})(x) - (S_k \tilde{f})(x')| &= \left| \int (k(x, y) - k(x', y)) f(y) d\nu(y) \right| \\
 &= \left| \langle I_k(k_x - k_{x'}), \tilde{f} \rangle_{L^2} \right| \\
 &\leq \|I_k(k_x - k_{x'})\|_{L^2} \|\tilde{f}\|_{L^2} \\
 &= \|\tilde{f}\|_{L^2} \sqrt{\int (k(x, y) - k(x', y))^2 d\nu(y)} \\
 &\leq \nu(\mathcal{X}) \|\tilde{f}\|_{L^2} \max_y |k(x, y) - k(x', y)|
 \end{aligned}$$

Integral operator of a kernel (2)



$$T_k : L_2(\mathcal{X}; \nu) \rightarrow L_2(\mathcal{X}; \nu)$$

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$T_k \neq S_k$: $(S_k \tilde{f})(x)$ is defined, while $(T_k \tilde{f})(x)$ is **not**!

Properties of integral operators

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Theorem (Spectral theorem)

Let \mathcal{F} be a Hilbert space, and $T : \mathcal{F} \rightarrow \mathcal{F}$ a compact, self-adjoint operator. There is an **at most countable** ONS $\{u_j\}_{j \in J}$ of \mathcal{F} and $\{\lambda_j\}_{j \in J}$ with $|\lambda_1| \geq |\lambda_2| \geq \dots > 0$ converging to zero such that

$$Tf = \sum_{j \in J} \lambda_j \langle f, u_j \rangle_{\mathcal{F}} u_j, \quad f \in \mathcal{F}.$$

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- $e_j = \lambda_j^{-1} S_k \tilde{e}_j \in \mathcal{C}(\mathcal{X})$ is a continuous function in the class \tilde{e}_j :

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 $I_k e_j = \tilde{e}_j$.

Theorem (Mercer's theorem)

$\forall x, y \in \mathcal{X}$ with convergence uniform on $\mathcal{X} \times \mathcal{X}$:

$$k(x, y) = \sum_{j \in J} \lambda_j e_j(x) e_j(y).$$

Mercer's theorem (2)

$$\begin{aligned}k(x, y) &= \sum_{j \in J} \lambda_j e_j(x) e_j(y) \\ &= \left\langle \left\{ \sqrt{\lambda_j} e_j(x) \right\}, \left\{ \sqrt{\lambda_j} e_j(y) \right\} \right\rangle_{\ell^2(J)}\end{aligned}$$

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Another (Mercer) feature map:

$$\begin{aligned}\phi : \mathcal{X} &\rightarrow \ell^2(J) \\ \phi : x &\mapsto \left\{ \sqrt{\lambda_j} e_j(x) \right\}_{j \in J}\end{aligned}$$

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$$\sum_{j \in J} \left(\sqrt{\lambda_j} e_j(x) \right)^2 = k(x, x) < \infty$$

Mercer's theorem (3)

- Sum $\sum_{j \in J} a_j e_j(x)$ converges absolutely $\forall x \in \mathcal{X}$ whenever sequence $\{a_j / \sqrt{\lambda_j}\} \in \ell^2(J)$:

$$\begin{aligned} \sum_{j \in J} |a_j e_j(x)| &\leq \left[\sum_{j \in J} |a_j / \sqrt{\lambda_j}|^2 \right]^{1/2} \cdot \left[\sum_{j \in J} |\sqrt{\lambda_j} e_j(x)|^2 \right]^{1/2} \\ &= \left\| \{a_j / \sqrt{\lambda_j}\} \right\|_{\ell^2(J)} \sqrt{k(x, x)}. \end{aligned}$$

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$\sum_{j \in J} a_j e_j$ is a well defined function on \mathcal{X}

Mercer representation of RKHS

Theorem

Let \mathcal{X} be a compact metric space and $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ a continuous kernel. Define:

$$\mathcal{H} = \left\{ f = \sum_{j \in J} a_j e_j : \{a_j / \sqrt{\lambda_j}\} \in \ell^2(J) \right\},$$

with inner product:

$$\left\langle \sum_{j \in J} a_j e_j, \sum_{j \in J} b_j e_j \right\rangle_{\mathcal{H}} = \sum_{j \in J} \frac{a_j b_j}{\lambda_j}.$$

Then \mathcal{H} is the RKHS of k .

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RKHS is unique, so does not depend on ν !

Proof

- 1 $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ is an inner product: if $f = \sum_{j \in J} a_j e_j$
then $\langle f, f \rangle_{\mathcal{H}} = \sum_{j \in J} \frac{a_j^2}{\lambda_j} > 0$ if some $a_j > 0$
- 2 Let $\{f_n\}$ be Cauchy, $f_n = \sum_{j \in J} a_j^{(n)} e_j$. Then $\|f_n - f_m\|_{\mathcal{H}}^2 =$
 $\sum_{j \in J} \frac{(a_j^{(n)} - a_j^{(m)})^2}{\lambda_j} = \left\| \left\{ a_j^{(n)} / \sqrt{\lambda_j} \right\} - \left\{ a_j^{(m)} / \sqrt{\lambda_j} \right\} \right\|_{\ell^2}^2 < \epsilon$, so must
have a limit because ℓ^2 is a Hilbert space.
- 3 $k(\cdot, x) = \sum_{j \in J} [\lambda_j e_j(x)] e_j \in \mathcal{H}$ since $\sum_{j \in J} \left(\frac{\lambda_j e_j(x)}{\sqrt{\lambda_j}} \right)^2 = k(x, x) < \infty$
- 4 $\langle f, k(\cdot, x) \rangle_{\mathcal{H}} = \left\langle \sum_{j \in J} a_j e_j, \sum_{j \in J} [\lambda_j e_j(x)] e_j \right\rangle_{\mathcal{H}} = \sum_{j \in J} \frac{a_j \lambda_j e_j(x)}{\lambda_j} =$
 $\sum_{j \in J} a_j e_j(x) = f(x)$.

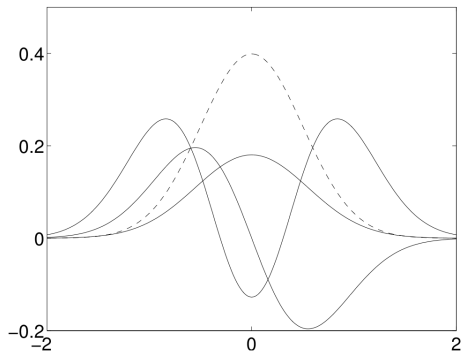
Smoothness interpretation

Gaussian kernel, $k(x, y) = \exp(-\sigma \|x - y\|^2)$,

$$\lambda_j \propto b^j \quad b < 1$$

$$e_j(x) \propto \exp(-(c - a)x^2) H_j(x\sqrt{2c}),$$

a, b, c are functions of σ , and H_j is j th order Hermite polynomial.



NOTE that $\|f\|_{\mathcal{H}_k} < \infty$ is a “smoothness” constraint:

λ_j decay as e_j become “rougher” and

$$\|f\|_{\mathcal{H}_k}^2 = \sum_{j \in J} \frac{a_j^2}{\lambda_j}$$

(Figure from Rasmussen and Williams)

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\mathcal{H}_k and $L_2(\mathcal{X}; \nu)$

Assume $\{\tilde{e}_j\}_{j \in J}$ is ONB of $L_2(\mathcal{X}; \nu)$, and write $\hat{f}(j) = \langle f, \tilde{e}_j \rangle_{L_2}$

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$$\sum_{j \in J} |\hat{f}(j)|^2 = \|f\|_2^2 < \infty \Rightarrow \{\hat{f}(j)\} \in \ell^2(J) \Rightarrow \sum_{j \in J} \sqrt{\lambda_j} \hat{f}(j) e_j \in \mathcal{H}_k$$

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$T_k^{1/2}$ induces an isometric isomorphism between $\text{span}\{\tilde{e}_j : j \in J\} \subseteq L_2(\mathcal{X}; \nu)$ and \mathcal{H}_k (and both are isometrically isomorphic to $\ell^2(J)$).

Canonical feature map

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Mercer feature map gives Fourier coefficients of the **canonical feature map**.

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Operations with kernels

Fact (Sum and scaling of kernels)

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

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

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

Operations with kernels (2)

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

Summary

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\longleftrightarrow

all function spaces with continuous evaluation $Hilb(\mathbb{R}^{\mathcal{X}})$

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bijection between $\mathbb{R}_+^{\mathcal{X} \times \mathcal{X}}$ and $Hilb(\mathbb{R}^{\mathcal{X}})$ preserves geometric structure

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Kernels on \mathbb{R}^d

New kernels from old:

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$$\begin{aligned} k_{\text{gauss}}(x, x') &= \tilde{k}(x, x')k_{\text{exp}}(x, x') \\ &= \exp\left(-\sigma \left[\|x\|^2 + \|x'\|^2 - 2\langle x, x' \rangle\right]\right) \\ &= \exp\left(-\sigma \|x - x'\|^2\right) \quad \text{kernel!} \end{aligned}$$

Moore-Aronszajn Theorem

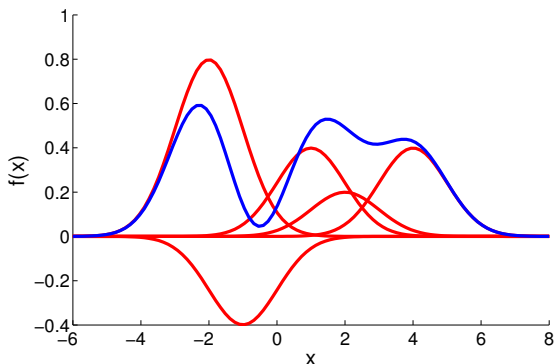
Starting with a positive def. k , construct a **pre-RKHS** (an inner product space of functions) $\mathcal{H}_0 \subset \mathbb{R}^{\mathcal{X}}$ with properties:

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

Moore-Aronszajn Theorem (2)

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

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



Moore-Aronszajn Theorem (3)

Theorem (Moore-Aronszajn - Step I)

Space $\mathcal{H}_0 = \text{span} \{k(\cdot, x) \mid x \in \mathcal{X}\}$, 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 $g = \sum_{j=1}^m \beta_j k(\cdot, y_j)$, is a valid pre-RKHS.

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Theorem (Moore-Aronszajn - Step II)

Let \mathcal{H}_0 be a pre-RKHS space. Define \mathcal{H} to be the set of functions $f \in \mathbb{R}^{\mathcal{X}}$ for which there exists an \mathcal{H}_0 -Cauchy sequence $\{f_n\}$ converging **pointwise** to f . Then, \mathcal{H} is an RKHS.

Moore-Aronszajn Theorem (4)

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- (1)+(2)+(3)+(4) $\implies \mathcal{H}$ is RKHS!

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$\xleftrightarrow{1-1}$

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