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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Non-closed subspaces

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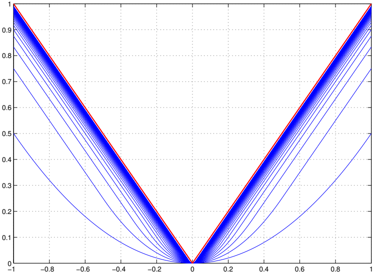
Example

Let $\mathcal{F} = \{f : [-1,1] \to \mathbb{R}, f \text{ continuous}\}$, with $\|f\|_\infty = \sup |f(x)|$, and $\mathcal{F}^1$ its subspace of **differentiable functions**. *Then $\mathcal{F}^1$ is not closed.*

- Idea: construct a sequence of differentiable functions converging in $\|\cdot\|_\infty$ to $f(x) = |x|$:

$$f_n(x) = \begin{cases} -x - \frac{1}{2n}, & x \leq -1/n, \\ \frac{n}{2}x^2, & |x| < 1/n, \\ x - \frac{1}{2n}, & x \geq 1/n. \end{cases}$$



Non-closed subspaces

Example

Let $\mathcal{H}$ be an infinite-dimensional Hilbert space with orthonormal basis $\mathcal{U} = \{u_j\}_{j=1}^{\infty}$. Then span$[\mathcal{U}]$ (finite linear combinations of elements of $\mathcal{U}$) is not closed.

- Take $h = \sum_{j=1}^{\infty} a_j u_j$ with $a_j > 0$ and $\sum_{j=1}^{\infty} a_j^2 < \infty$. Then $h_n = \sum_{j=1}^{n} a_j u_j$ converges to $h \notin span[\mathcal{U}]$.

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Recall:

- In the proof of *Riesz Theorem*, we used: M closed subspace $\implies M^{\perp}$contains a non-zero element.
- Here: $span[\mathcal{U}]^{\perp} = \{0\}$ (i.e., $span[\mathcal{U}]$ is dense in $\mathcal{H}$).

The story so far

- **Hilbert space:**

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  - reproducing kernel $\Longrightarrow$ kernel
  - canonical feature $\phi : x \mapsto k(\cdot, x)$

Overview

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

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(Just) Kernel

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 $k(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{F}}$.

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

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Corollary

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 $k(x,y) = \langle x, y \rangle^2$

$$\begin{aligned} k(x,y) &= x_1^2 y_1^2 + x_2^2 y_2^2 + 2 x_1 x_2 y_1 y_2 \\ &= \begin{bmatrix} x_1^2 & x_2^2 & \sqrt{2} x_1 x_2 \end{bmatrix} \begin{bmatrix} y_1^2 \\ y_2^2 \\ \sqrt{2} y_1 y_2 \end{bmatrix} \\ &= \begin{bmatrix} x_1^2 & x_2^2 & x_1 x_2 & x_1 x_2 \end{bmatrix} \begin{bmatrix} y_1^2 \\ y_2^2 \\ y_1 y_2 \\ y_1 y_2 \end{bmatrix}. \end{aligned}$$

so we can use the feature maps $\phi(x) = (x_1^2, x_2^2, \sqrt{2} x_1 x_2)$ *or* $\tilde{\phi}(x) = \begin{bmatrix} x_1^2 & x_2^2 & x_1 x_2 & x_1 x_2 \end{bmatrix}$, with feature spaces $\mathcal{H} = \mathbb{R}^3$ *or* $\tilde{\mathcal{H}} = \mathbb{R}^4$.

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&= \left[\begin{array}{cccc} x_1^2 & x_2^2 & x_1x_2 & x_1x_2 \end{array}\right] \left[\begin{array}{c} y_1^2 \\ y_2^2 \\ y_1y_2 \\ y_1y_2 \end{array}\right].
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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 $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is *positive definite* if $\forall n \geq 1$, $\forall (a_1, \ldots a_n) \in \mathbb{R}^n$, $\forall (x_1, \ldots, x_n) \in \mathcal{X}^n$,

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

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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

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

Fact

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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 \left\langle \phi(x_i), \phi(x_j) \right\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

$$\text{reproducing kernel} \implies \text{kernel} \implies \text{positive definite}$$

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

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Moore-Aronszajn Theorem

Theorem (Moore-Aronszajn)

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.*

Summary

reproducing kernel $\iff$ kernel $\iff$ positive definite

Summary

reproducing kernel $\Longleftrightarrow$ kernel $\Longleftrightarrow$ positive definite

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

$$\overset{1-1}{\longleftrightarrow}$$

set of all subspaces of $\mathbb{R}^{\mathcal{X}}$ with continuous evaluation: $Hilb(\mathbb{R}^{\mathcal{X}})$

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!)

$$\langle \phi(x), \phi(y) \rangle_{\mathbb{R}^3} = a y_1^2 + b y_2^2 + c\sqrt{2} y_1 y_2 \quad = \quad k_x(y) = \langle k_x, k_y \rangle_{\mathcal{H}_k}$$

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

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    - such as $[a, b]$, every continuous function on $\mathcal{X}$ is bounded and uniformly continuous
  - $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ 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

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

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

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

Integral operator of a kernel (2)

$$
\begin{tikzcd}
L_2(\mathcal{X};\nu) \arrow[rr, "T_k = I_k S_k"] \arrow[dr, "S_k"'] & & L_2(\mathcal{X};\nu) \\
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$$T_k \ : \ L_2(\mathcal{X};\nu) \ \to \ L_2(\mathcal{X};\nu)$$

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

Properties of integral operators

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- k continuous $\implies$ T_k **compact**: if $\{f_n\}$ is bounded, then $\{T_k f_n\}$ has a convergent subsequence

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Theorem (Spectral theorem)

Let $\mathcal{F}$ be a Hilbert space,and $T : \mathcal{F} \to \mathcal{F}$ 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 $|\lambda_1| \geq |\lambda_2| \geq \cdots > 0$ converging to zero such that

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

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Mercer's theorem

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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)

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\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)}
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Another (Mercer) feature map:

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\phi : \mathcal{X} &\to \ell^2(J) \\
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\sum_{j\in J} \left(\sqrt{\lambda_j} e_j(x)\right)^2 = k(x,x) < \infty
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Mercer's theorem (3)

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

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

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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 $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ a continuous kernel. Define:

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

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

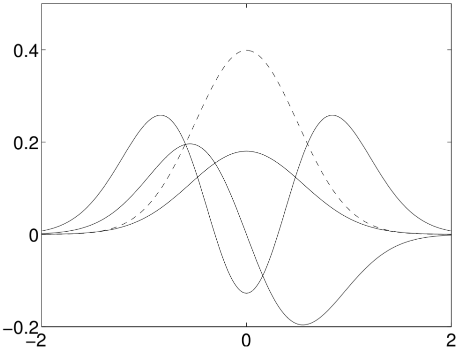
1. $\langle\cdot,\cdot\rangle_{\mathcal{H}}$ is an inner product: if $f = \sum_{j\in J} a_j e_j$ then $\langle f, f\rangle_{\mathcal{H}} = \sum_{j\in J} \frac{a_j^2}{\lambda_j} > 0$ if some $a_j > 0$
2. Let $\{f_n\}$ be Cauchy, $f_n = \sum_{j\in J} a_j^{(n)} e_j$. Then $\|f_n - f_m\|_{\mathcal{H}}^2 = \sum_{j\in J} \frac{\left(a_j^{(n)} - a_j^{(m)}\right)^2}{\lambda_j} = \left\| \left\{ a_j^{(n)}/\sqrt{\lambda_j} \right\} - \left\{ a_j^{(m)}/\sqrt{\lambda_j} \right\} \right\|_{\ell^2}^2 < \epsilon$, 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, $k(x,y) = \exp\left(-\sigma \|x-y\|^2\right)$,

$$\begin{aligned} \lambda_j &\propto b^j \qquad b < 1 \\ e_j(x) &\propto \exp(-(c-a)x^2)H_j(x\sqrt{2c}), \end{aligned}$$

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



NOTE that $\|f\|_{\mathcal{H}_k} < \infty$ is a "smoothness" constraint: λ_j decay as e_j become "rougher" and

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

(Figure from Rasmussen and Williams)

Outline

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

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

$$T_k f = \sum_{j\in J} \lambda_j \hat{f}(j)\tilde{e}_j, \qquad f \in L_2(\mathcal{X};\nu)$$

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

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$T_k^{1/2}$ induces an isometric isomorphism between *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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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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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:

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

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Gaussian kernel

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

Outline

Moore-Aronszajn Theorem

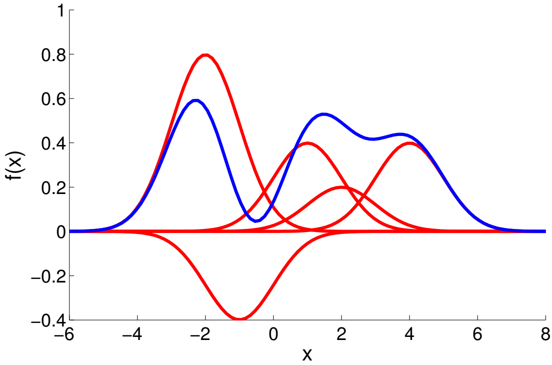
Starting with a positive def. k, construct a **pre-RKHS** (an inner product space of functions) $\mathcal{H}_0 \subset \mathbb{R}^{\mathcal{X}}$ with properties:

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

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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 (5)

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

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$$\text{all pd functions } \mathbb{R}_+^{\mathcal{X}\times\mathcal{X}}$$

$$\overset{1-1}{\longleftrightarrow}$$

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