Foundations of Reproducing Kernel Hilbert Spaces II

Advanced Topics in Machine Learning

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Gatsby Unit

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Overview

1. What is an RKHS?
   - Reproducing kernel
   - 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

Outline

Will discuss three distinct concepts:

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

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

Outline

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

- $\forall x \in \mathcal{X}, \quad k_x = k(\cdot, x) \in \mathcal{H}$,
- $\forall x \in \mathcal{X}, \forall f \in \mathcal{H}, \quad \langle f, k(\cdot, x) \rangle_{\mathcal{H}} = f(x)$ (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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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 $k(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{F}}$.

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

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Corollary

*Every **reproducing kernel** is a **kernel**.*

Proof.

We can take (Aronszajn) feature map $\phi : x \mapsto k(\cdot, x)$. Then, $k(x, y) = \langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}}$, i.e., RKHS $\mathcal{H}$ is a feature space. □

Non-uniqueness of feature representation

Example

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

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k(x,y) &= x_1^2 y_1^2 + x_2^2 y_2^2 + 2 x_1 x_2 y_1 y_2 \\
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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* $\tilde{\phi}(x) = \begin{bmatrix} x_1^2 & x_2^2 & x_1 x_2 & x_1 x_2 \end{bmatrix}$, with feature spaces $\mathcal{H} = \mathbb{R}^3$ *or* $\tilde{\mathcal{H}} = \mathbb{R}^4$.

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Not RKHS!

Outline

Positive definite functions

Definition (Positive definite functions)

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

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

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.

Kernels are positive definite

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

Fact

Every kernel is a positive definite function.

So far

reproducing kernel $\implies$ kernel $\implies$ positive definite

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

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

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

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

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

Moore-Aronszajn Theorem

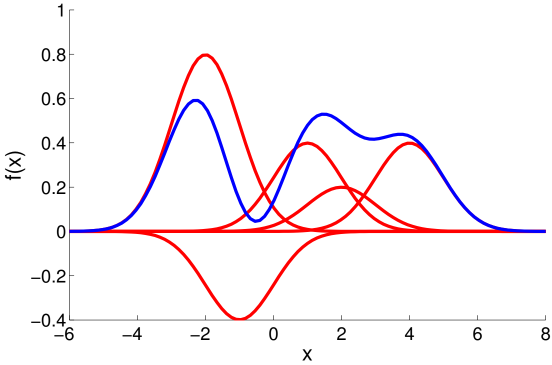
Starting with a positive def. k, construct a **pre-RKHS** (an inner product space of functions) $\mathcal{H}_0 \subset \mathbb{R}^{\mathcal{X}}$ with properties:

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

Moore-Aronszajn Theorem (2)

pre-RKHS $\mathcal{H}_0 = span\left\{k(\cdot, x) \,|\, x \in \mathcal{X}\right\}$ 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 a Cauchy sequence* $\{f_n\}$ *in* $\mathcal{H}_0$ *converging* ***pointwise*** *to* f*. Then,* $\mathcal{H}$ *is an RKHS.*

Moore-Aronszajn Theorem (4)

Theorem (Moore-Aronszajn - Step I)

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 Cauchy sequence f_n in $\mathcal{H}_0$ 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 a Cauchy sequence $\{f_n\} \in \mathcal{H}_0$ converging **pointwise** to f.

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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 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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4. Is $\mathcal{H}$ complete (i.e., is it a Hilbert space)?

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

Non-uniqueness of feature representation

Example

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so we can use the feature maps $\phi(x) = \begin{bmatrix} x_1^2 & x_2^2 & \sqrt{2} x_1 x_2 \end{bmatrix}$ *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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$\mathcal{H}$ and $\tilde{\mathcal{H}}$ are not RKHS - RKHS of k is unique

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!)

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

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

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

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

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

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- So far, no assumptions on:
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- Now, assume that:
  - $\mathcal{X}$ is a compact metric space (with metric $d_{\mathcal{X}}$)
    - such as $[a, b]$, continuity$\Rightarrow$uniform continuity
  - $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ 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

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

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.

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

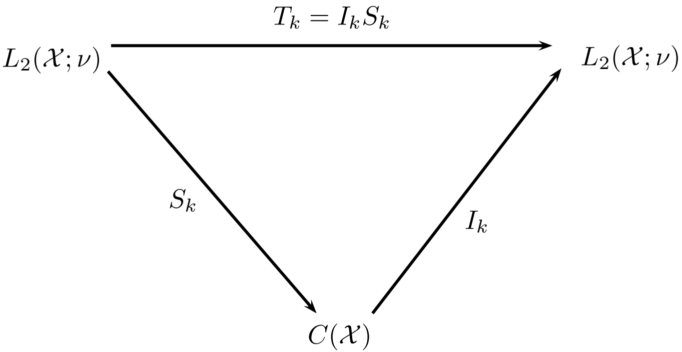
$$\begin{aligned} S_k : L_2(\mathcal{X};\nu) &\to \mathcal{C}(\mathcal{X}), \\ (S_k f)(x) &= \int k(x,y)f(y)d\nu(y), \;\; f \in L_2(\mathcal{X};\nu), \end{aligned}$$

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.

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

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

Integral operator of a kernel (2)



Properties of integral operator

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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 $\{e_j\}_{j \in J}$ of $\mathcal{F}$ and $\{\lambda_j\}_{j \in J}$ with $|\lambda_1| \geq |\lambda_2| \geq \cdots > 0$ converging to zero such that

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

Outline

Mercer's theorem

Let $\mathcal{X}$ be a compact metric space and $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ a continuous kernel. Fix a finite measure ν on $\mathcal{X}$ with $supp \nu = \mathcal{X}$. Integral operator T_k is then compact, positive and self-adjoint on $L_2(\mathcal{X}; \nu)$, so there exist ONS $\{\tilde{e}_j\}_{j \in J}$ and $\{\lambda_j\}_{j \in J}$ (strictly positive eigenvalues; J at most countable).

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Theorem (Mercer's theorem)

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

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- $\tilde{e}_j$ is an equivalence class in the ONS of $L_2(\mathcal{X}; \nu)$
- $e_j = \lambda_j^{-1} S_k \tilde{e}_j \in \mathcal{C}(\mathcal{X})$ is a continuous function in the class $\tilde{e}_j$: $I_k e_j = \lambda_j^{-1} T_k \tilde{e}_j = \lambda_j^{-1} \lambda_j \tilde{e}_j = \tilde{e}_j$.

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

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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:

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

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Does not depend on ν !

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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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$T_k^{1/2}$ 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 Aronszajn feature map.

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

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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:

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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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Summary

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

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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

Let $\phi : \mathbb{R}^d \to \mathbb{R}$, $\phi(x) = \exp(-\sigma \|x\|^2)$. Then, $\tilde{k}$ is representable as an inner product in $\mathbb{R}$:

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