Reproducing Kernel Hilbert Spaces

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9.520 Class 03

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About this class

Goal To introduce a particularly useful family of hypothesis spaces called Reproducing Kernel Hilbert Spaces (RKHS) We will discuss several perspectives on RKHS. In particular in this class we investigate the fundamental definition of RKHS as Hilbert spaces with bounded, continuous evaluation functionals and the intimate connection with symmetric positive definite kernels.

Plan

- Part I: RKHS are Hilbert spaces with bounded, continuous evaluation functionals.
- Part II: Reproducing Kernels
- Part III: Mercer Theorem
- Part IV: Feature Maps
- Part V: Representer Theorem

Regularization

The basic idea of regularization (originally introduced independently of the learning problem) is to restore well-posedness of ERM by constraining the hypothesis space $\mathcal{H}$.

Regularization

A possible way to do this is considering *regularized* empirical risk minimization, that is we look for solutions minimizing a two term functional

$$\underbrace{ERR(f)}_{\text{empirical error}} + \lambda \underbrace{R(f)}_{\text{regularizer}}$$

the regularization parameter λ trade-offs the two terms.

Tikhonov Regularization

Tikhonov regularization amounts to minimize

$$\frac{1}{n}\sum_{i=1}^{n} V(f(x_i), y_i) + \lambda \mathcal{R}(f) \qquad \lambda > 0 \tag{1}$$

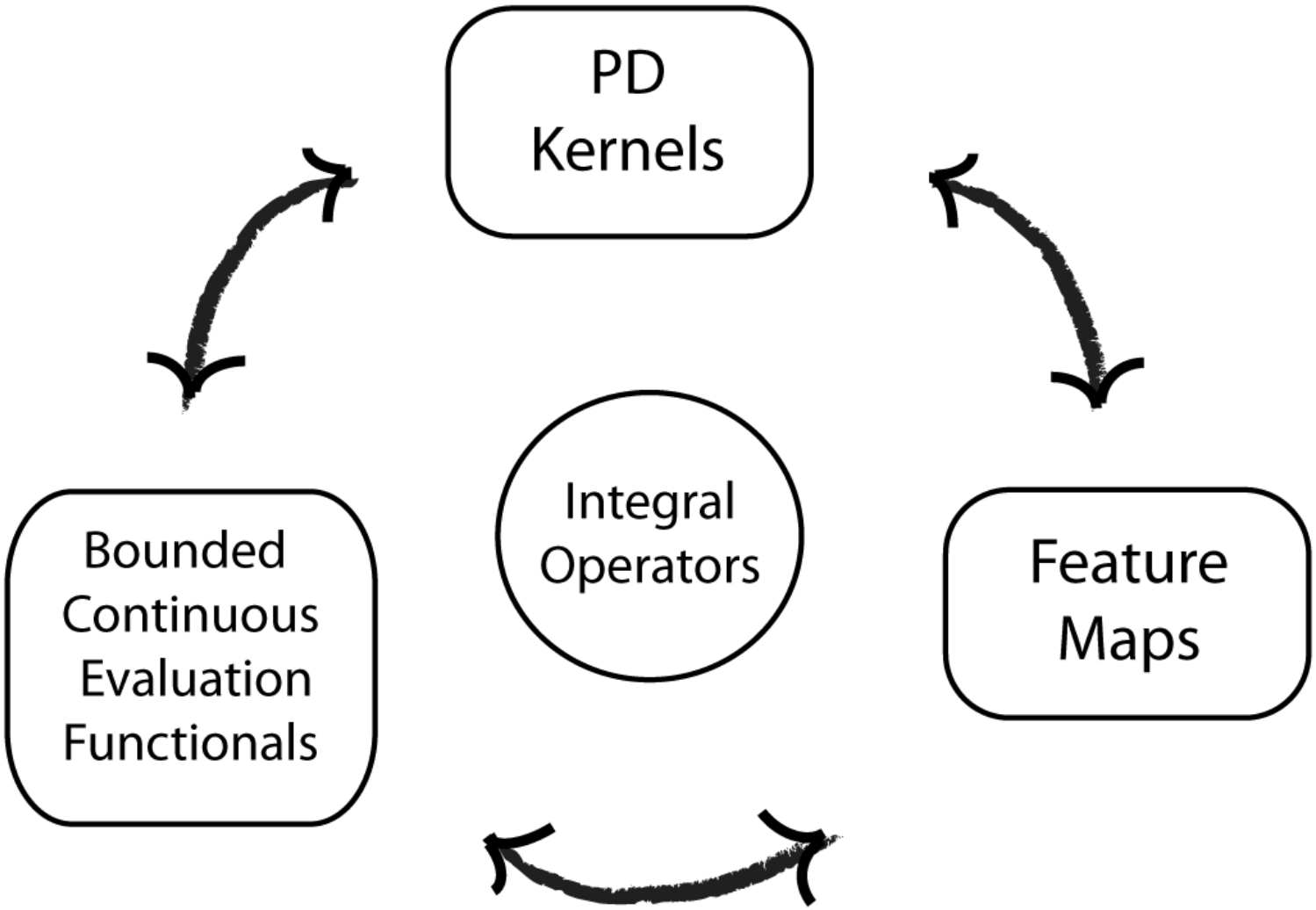
- $V(f(x), y)$ is the loss function, that is the price we pay when we predict $f(x)$ in place of y
- $\mathcal{R}(f)$ is a regularizer– often $\mathcal{R}(f) = \|\cdot\|_{\mathcal{H}}$, the norm in the *function space* $\mathcal{H}$

The regularizer should encode some notion of smoothness of f.

The "Ingredients" of Tikhonov Regularization

- The scheme we just described is very general and by choosing different loss functions $V(f(x), y)$ we can recover different algorithms
- The main point we want to discuss is how to choose a norm encoding some notion of smoothness/complexity of the solution
- Reproducing Kernel Hilbert Spaces allow us to do this in a very powerful way

Different Views on RKHS



Part I: Evaluation Functionals

Some Functional Analysis

A **function space** $\mathcal{F}$ is a space whose elements are functions f, for example $f : \mathbb{R}^d \to \mathbb{R}$.

A **norm** is a nonnegative function $\|\cdot\|$ such that $\forall f, g \in \mathcal{F}$ and $\alpha \in \mathbb{R}$

1. $\|f\| \geq 0$ and $\|f\| = 0$ *iff* $f = 0$;
2. $\|f + g\| \leq \|f\| + \|g\|$;
3. $\|\alpha f\| = |\alpha| \, \|f\|$.

A norm can be defined via a **inner product** $\|f\| = \sqrt{\langle f, f \rangle}$.

A **Hilbert space** is a complete inner product space.

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Examples

- Continuous functions $C[a, b]$:
  a norm can be established by defining

$$\|f\| = \max_{a \leq x \leq b} |f(x)|$$

  (not a Hilbert space!)

- Square integrable functions $L_2[a, b]$:
  it is a Hilbert space where the norm is induced by the dot product

$$\langle f, g \rangle = \int_a^b f(x)g(x)dx$$

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Hypothesis Space: Desiderata

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An evaluation functional over the *Hilbert space of functions* $\mathcal{H}$ is a linear functional $\mathcal{F}_t : \mathcal{H} \rightarrow \mathbb{R}$ that *evaluates* each function in the space at the point t, or

$$\mathcal{F}_t[f] = f(t).$$

Definition

A Hilbert space $\mathcal{H}$ is a reproducing kernel Hilbert space (RKHS) if the evaluation functionals are bounded and continuous, i.e. if there exists a M s.t.

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Evaluation functionals

Evaluation functionals are not always bounded.
Consider $L_2[a, b]$:

- Each element of the space is an equivalence class of functions with the same integral $\int |f(x)|^2 dx$.
- An integral remains the same if we change the function in a countable set of points.

Norms in RKHS and Smoothness

Choosing different kernels one can show that the norm in the corresponding RKHS encodes different notions of smoothness.

- Band limited functions. Consider the set of functions

$$\mathcal{H} := \{f \in L^2(\mathbb{R}) \mid F(\omega) \in [-a, a], a < \infty\}$$

with the usual L^2 inner product. the function at every point is given by the convolution with a sinc function $sin(ax)/ax$. The norm

$$\|f\|_{\mathcal{H}}^2 = \int f(x)^2 dx = \int_a^a |F(\omega)|^2 d\omega$$

Where $F(\omega) = \mathcal{F}\{f\}(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t}\, dt$ is the Fourier tranform of f.

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Norms in RKHS and Smoothness

- Sobolev Space: consider $f : [0, 1] \rightarrow \mathbb{R}$ with $f(0) = f(1) = 0$. The norm

$$\|f\|_{\mathcal{H}}^2 = \int (f'(x))^2 dx = \int \omega^2 |F(\omega)|^2 d\omega$$

- Gaussian Space: the norm can be written as

$$\|f\|_{\mathcal{H}}^2 = \frac{1}{2\pi^d} \int |F(\omega)|^2 exp^{\frac{\sigma^2\omega^2}{2}} d\omega$$

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Linear RKHS

Our function space is 1-dimensional lines

$$f(x) = w\,x$$

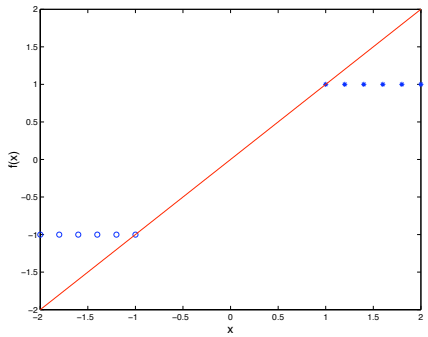
where the RKHS norm is simply

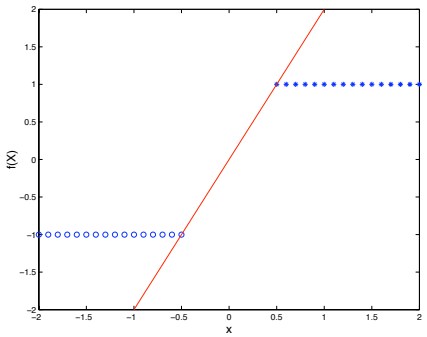
$$\|f\|_{\mathcal{H}}^2 = \langle f, f \rangle_{\mathcal{H}} = w^2$$

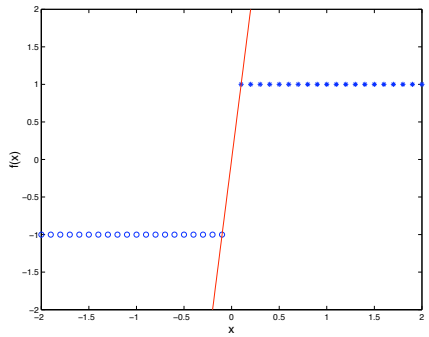
so that our measure of complexity is the slope of the line.
We want to separate two classes using lines and see how the magnitude of the slope corresponds to a measure of complexity.
We will look at three examples and see that each example requires more "complicated functions, functions with greater slopes, to separate the positive examples from negative examples.

Linear case (cont.)

here are three datasets: a linear function should be used to separate the classes. Notice that as the class distinction becomes finer, a larger slope is required to separate the classes.







Part II: Kernels

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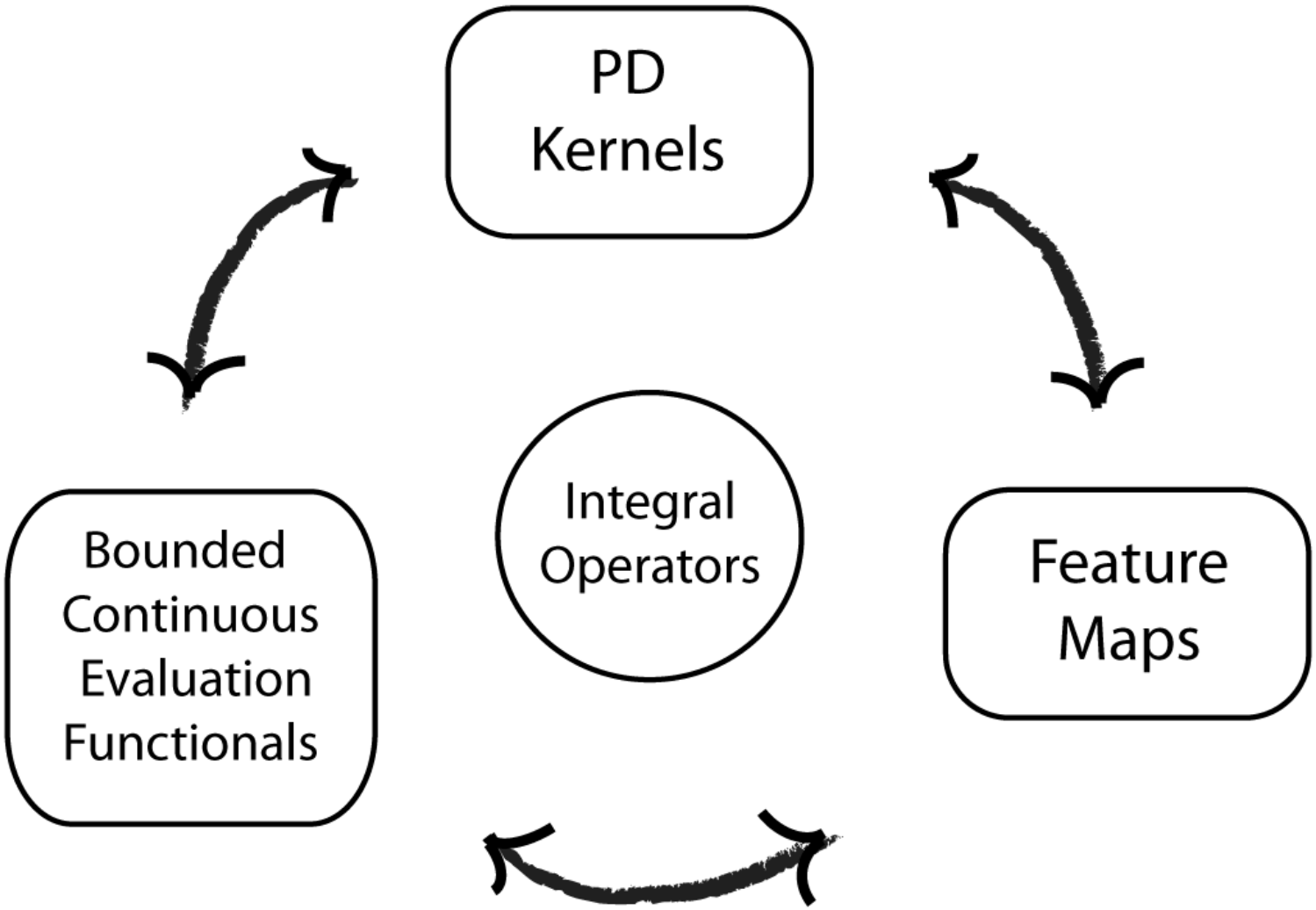

Representation of Continuous Functionals

Let $\mathcal{H}$ be a Hilbert space and $g \in \mathcal{H}$, then

$$\Phi_g(f) = \langle f, g \rangle, \qquad f \in \mathcal{H}$$

is a continuous linear functional.

Riesz representation theorem

The theorem states that every continuous linear functional Φ can be written uniquely in the form,

$$\Phi(f) = \langle f, g \rangle$$

for some appropriate element $g \in \mathcal{H}$.

Reproducing kernel (rk)

- If $\mathcal{H}$ is a RKHS, then for each $t \in X$ there exists, by the *Riesz representation theorem* a function K_t in $\mathcal{H}$ (called *representer*) with the **reproducing** property

$$\mathcal{F}_t[f] = \langle K_t, f \rangle_{\mathcal{H}} = f(t).$$

- Since K_t is a function in $\mathcal{H}$, by the reproducing property, for each $x \in X$

$$K_t(x) = \langle K_t, K_x \rangle_{\mathcal{H}}$$

The *reproducing kernel* (rk) of $\mathcal{H}$ is

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Positive definite kernels

Let X be some set, for example a subset of $\mathbb{R}^d$ or $\mathbb{R}^d$ itself. A *kernel* is a symmetric function $K : X \times X \to \mathbb{R}$.

Definition

A kernel $K(t, s)$ is *positive definite (pd)* if

$$\sum_{i,j=1}^{n} c_i c_j K(t_i, t_j) \geq 0$$

for any $n \in \mathbb{N}$ and choice of $t_1, ..., t_n \in X$ and $c_1, ..., c_n \in \mathbb{R}$.

RKHS and kernels

The following theorem relates pd kernels and RKHS

Theorem

a) For every RKHS there exist an associated reproducing kernel which is symmetric and positive definite

b) Conversely every symmetric, positive definite kernel K on $X \times X$ defines a unique RKHS on X with K as its reproducing kernel

Sketch of proof

a) We must prove that the rk $K(t,x) = \langle K_t, K_x \rangle_{\mathcal{H}}$ is *symmetric* and *pd*.

- Symmetry follows from the symmetry property of dot products

$$\langle K_t, K_x \rangle_{\mathcal{H}} = \langle K_x, K_t \rangle_{\mathcal{H}}$$

- K is pd because

$$\sum_{i,j=1}^{n} c_i c_j K(t_i, t_j) = \sum_{i,j=1}^{n} c_i c_j \langle K_{t_i}, K_{t_j} \rangle_{\mathcal{H}} = || \sum c_j K_{t_j} ||^2_{\mathcal{H}} \geq 0.$$

Sketch of proof (cont.)

b) Conversely, given K one can construct the RKHS $\mathcal{H}$ as the *completion* of the space of functions spanned by the set $\{K_x | x \in X\}$ with a inner product defined as follows.
The dot product of two functions f and g in $\text{span}\{K_x | x \in X\}$

$$f(x) = \sum_{i=1}^{s} \alpha_i K_{x_i}(x)$$

$$g(x) = \sum_{i=1}^{s'} \beta_i K_{x'_i}(x)$$

is *by definition*

$$\langle f, g \rangle_{\mathcal{H}} = \sum_{i=1}^{s} \sum_{j=1}^{s'} \alpha_i \beta_j K(x_i, x'_j).$$

Examples of pd kernels

Very common examples of symmetric pd kernels are

- **Linear kernel**

$$K(x, x') = x \cdot x'$$

- **Gaussian kernel**

$$K(x, x') = \mathrm{e}^{-\frac{\|x-x'\|^2}{\sigma^2}}, \qquad \sigma > 0$$

- **Polynomial kernel**

$$K(x, x') = (x \cdot x' + 1)^d, \qquad d \in \mathbb{N}$$

For specific applications, designing an effective kernel is a challenging problem.

Examples of pd kernels

- Kernel are a very general concept. We can have kernel on vectors, string, matrices, graphs, probabilities...
- Combinations of Kernels allow to do integrate different kinds of data.
- Often times Kernel are views and designed to be similarity measure (in this case it make sense to have normalized kernels)

$$d(x, x')^2 = \left\| K_x - K'_x \right\|^2 = 2(1 - K(x, x')).$$