Reproducing Kernel Hilbert Spaces

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9.520 Class 03

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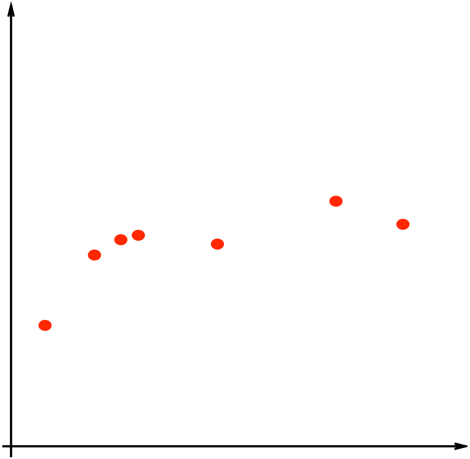
About this class

Goal To introduce a particularly useful family of hypothesis spaces called Reproducing Kernel Hilbert Spaces (RKHS) and to derive the general solution of Tikhonov regularization in RKHS.

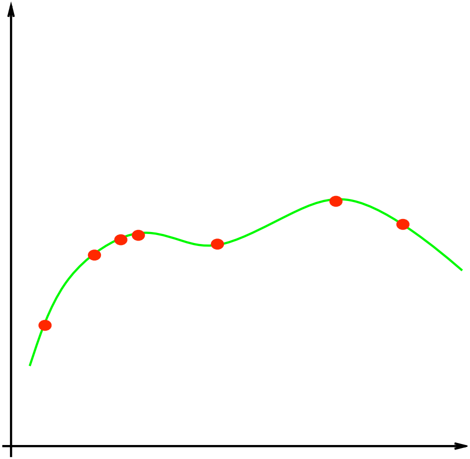
Function Approximation from Samples

Here is a graphical example for generalization: given a certain number of samples...



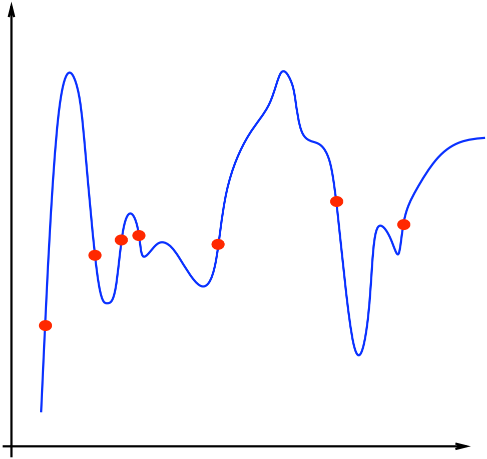
Function Approximation from Samples (cont.)

Suppose this is the “true” solution...



The Problem is Ill-Posed

... but suppose ERM gives this solution!



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 $\mathcal{H}$.

Penalized Minimization

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

$$\underbrace{ERR(f)}_{empirical\ error} + \lambda \underbrace{pen(f)}_{penalization\ term}$$

the regularization parameter λ trade-offs the two terms.

Tikhonov Regularization

Tikhonov regularization amounts to minimize

$$\frac{1}{n}\sum_{i=1}^{n} V(f(x_i), y_i) + \lambda\|f\|_{\mathcal{H}}^2, \qquad \lambda > 0 \tag{1}$$

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

Such a penalization term 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

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 **dot product** $\|f\| = \sqrt{\langle f, f \rangle}$.

A **Hilbert space** (besides other technical conditions) is a (possibly) infinite dimensional linear space endowed with a dot product.

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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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RKHS

A linear evaluation functional over the *Hilbert space of functions* $\mathcal{H}$ is a linear functional $\mathcal{F}_t : \mathcal{H} \to \mathbb{R}$ 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, i.e. if there exists a M s.t.

$$|\mathcal{F}_t[f]| = |f(t)| \leq M\|f\|_{\mathcal{H}} \ \ \forall f \in \mathcal{H}$$

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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.

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 of $\mathcal{H}$ (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 $x \in X$

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

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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 the reproducing kernel is a positive definite kernel

b) Conversely for every positive definite kernel K on $X \times X$ there is 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 $\mathrm{span}\{K_x | x \in X\}$

$$
\begin{aligned}
f(x) &= \sum_{i=1}^{s} \alpha_i K_{x_i}(x) \\
g(x) &= \sum_{i=1}^{s'} \beta_i K_{x'_i}(x)
\end{aligned}
$$

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.

Historical Remarks

RKHS were explicitly introduced in learning theory by Girosi (1997). Poggio and Girosi (1989) introduced Tikhonov regularization in learning theory and worked with RKHS only implicitly, because they dealt mainly with hypothesis spaces on unbounded domains, which we will not discuss here. Of course, RKHS were used much earlier in approximation theory (eg Wahba, 1990...) and computer vision (eg Bertero, Torre, Poggio, 1988...).

Norms in RKHS and Smoothness

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

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

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

  is induced by the kernel $K(x,y) = \Theta(y-x)(1-y)x + \Theta(x-y)(1-x)y$.
- Gaussian kernel: the norm can be written as

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

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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Linear Case

Our function space is 1-dimensional lines

$$f(x) = w\,x \text{ and } K(x, x_i) \equiv x\,x_i$$

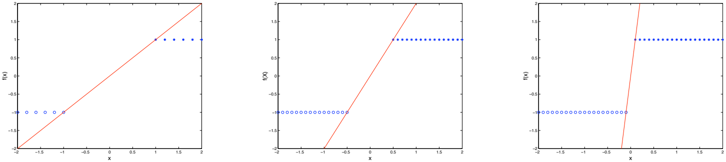
where the RKHS norm is simply

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

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.



Again Tikhonov Regularization

The algorithms (*Regularization Networks*) that we want to study are defined by an optimization problem over RKHS,

$$f_S^\lambda = \arg\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} V(f(x_i), y_i) + \lambda \|f\|_{\mathcal{H}}^2$$

where the *regularization parameter* λ is a positive number, $\mathcal{H}$ is the RKHS as defined by the *pd kernel* $K(\cdot,\cdot)$, and $V(\cdot,\cdot)$ is a **loss function.**

Note that $\mathcal{H}$ is possibly infinite dimensional!

Existence and uniqueness of minimum

If the positive loss function $V(\cdot, \cdot)$ is convex with respect to its first entry, the functional

$$\Phi[f] = \frac{1}{n} \sum_{i=1}^{n} V(f(x_i), y_i) + \lambda \|f\|_{\mathcal{H}}^2$$

is *strictly convex* and *coercive*, hence it has exactly one local (global) minimum.
Both the squared loss and the hinge loss are convex.
On the contrary the 0-1 loss

$$V = \Theta(-f(x)y),$$

where $\Theta(\cdot)$ is the Heaviside step function, is **not** convex.

The Representer Theorem

An important result

The minimizer over the RKHS $\mathcal{H}$, f_S, of the regularized empirical functional

$$I_S[f] + \lambda \|f\|_{\mathcal{H}}^2,$$

can be represented by the expression

$$f_S^\lambda(x) = \sum_{i=1}^{n} c_i K(x_i, x),$$

for some n-tuple $(c_1, \ldots, c_n) \in \mathbb{R}^n$.
Hence, minimizing over the (possibly infinite dimensional) Hilbert space, *boils down to minimizing over* $\mathbb{R}^n$.

Sketch of proof

Define the linear subspace of $\mathcal{H}$,

$$\mathcal{H}_0 = \mathrm{span}(\{K_{x_i}\}_{i=1,\dots,n})$$

Let $\mathcal{H}_0^\perp$ be the linear subspace of $\mathcal{H}$,

$$\mathcal{H}_0^\perp = \{f \in \mathcal{H} | f(x_i) = 0,\ i = 1, \dots, n\}.$$

From the reproducing property of $\mathcal{H}$, $\forall f \in \mathcal{H}_0^\perp$

$$\langle f, \sum_i c_i K_{x_i} \rangle_{\mathcal{H}} = \sum_i c_i \langle f, K_{x_i} \rangle_{\mathcal{H}} = \sum_i c_i f(x_i) = 0.$$

$\mathcal{H}_0^\perp$ is the orthogonal complement of $\mathcal{H}_0$.

Sketch of proof (cont.)

Every $f \in \mathcal{H}$ can be uniquely decomposed in components along and perpendicular to $\mathcal{H}_0$: $f = f_0 + f_0^\perp$.
Since by orthogonality

$$\|f_0 + f_0^\perp\|^2 = \|f_0\|^2 + \|f_0^\perp\|^2,$$

and by the reproducing property

$$I_S[f_0 + f_0^\perp] = I_S[f_0],$$

then

$$I_S[f_0] + \lambda\|f_0\|_{\mathcal{H}}^2 \leq I_S[f_0 + f_0^\perp] + \lambda\|f_0 + f_0^\perp\|_{\mathcal{H}}^2.$$

Hence the minimum $f_S^\lambda = f_0$ *must belong to the linear space* $\mathcal{H}_0$.

Common Loss Functions

The following two important learning techniques are implemented by different choices for the loss function $V(\cdot, \cdot)$

- **Regularized least squares** (RLS)

$$V = (y - f(x))^2$$

- **Support vector machines for classification** (SVMC)

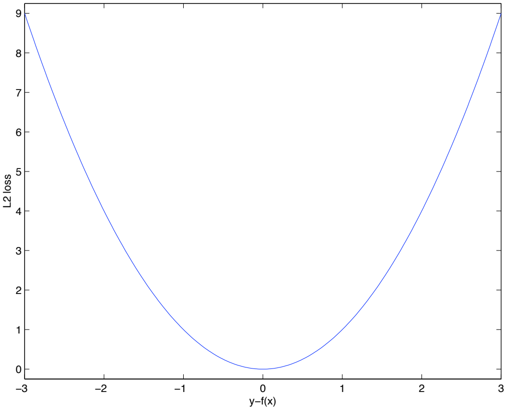
$$V = |1 - yf(x)|_+$$

where

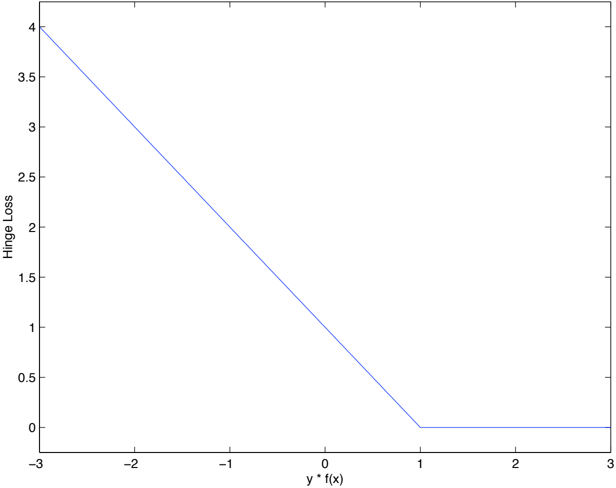
$$(k)_+ \equiv \max(k, 0).$$

The Square Loss

For regression, a natural choice of loss function is the square loss $V(f(x), y) = (f(x) - y)^2$.



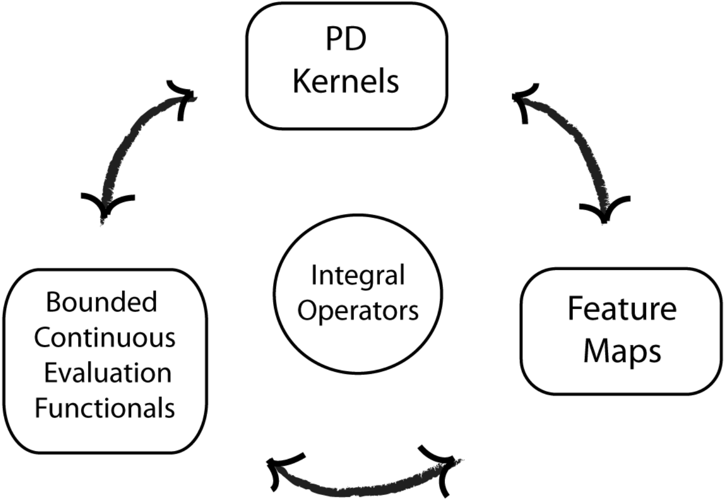
The Hinge Loss



Tikhonov Regularization for RLS and SVMs

In the next two classes we will study Tikhonov regularization with different loss functions for both regression and classification. We will start with the square loss and then consider SVM loss functions.

Some Other Facts on RKH Spaces



Integral Operator

RKH space can be characterized via the integral operator

$$L_K f(x) = \int_X K(x,s) f(s) p(x) dx$$

where $p(x)$ is the probability density on X.

The operator has domain and range in $L^2(X, p(x)dx)$ the space of functions $f : X \to \mathbb{R}$ such that

$$< f, f >= \int_X |f(x)|^2 p(x) dx < \infty$$

Mercer Theorem

If X is a compact subset in $\mathbb{R}^d$ and K continuous, symmetric (and PD) then L_K is a **compact, positive** and **self-adjoint** operator.

- There is a decreasing sequence $(\sigma_i)_i \geq 0$ such that $\lim_{i \to \infty} \sigma_i = 0$ and

  $$L_K \phi_i(x) = \int_X K(x,s) \phi_i(s) p(s) ds = \sigma_i \phi_i(x),$$

  where ϕ_i is an orthonormal basis in $L^2(X, p(x)dx)$.
- The action of L_K can be written as

  $$L_K f = \sum_{i \geq 1} \sigma_i < f, \phi_i > \phi_i.$$

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Mercer Theorem (cont.)

- The kernel function have the following representation

$$K(x,s) = \sum_{i \geq 1} \sigma_i \phi_i(x) \phi_i(s).$$

A symmetric, positive definite *and* continuous Kernel is called a *Mercer* kernel.

- The above decomposition allows to look at the kernel as a dot product in some *feature space*. **(more in the problem sets.)**

Different Definition of RKHS

It is possible to prove that:

- $$\mathcal{H} = \{f \in L^2(X, p(x)dx) | \sum_{i \geq 1} \frac{< f, \phi_i >^2}{\sigma_i^2} < \infty\}.$$
- The scalar product in $\mathcal{H}$ is
$$< f, g >_{\mathcal{H}} = \sum_{i \geq 1} \frac{< f, \phi_i >< g, \phi_i >}{\sigma_i}.$$

A different proof of the representer theorem can be given using Mercer theorem.

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