

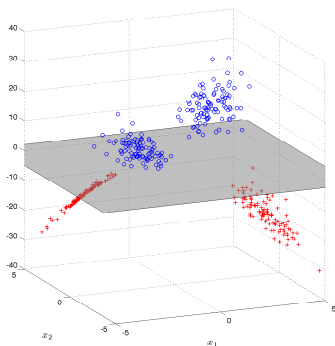
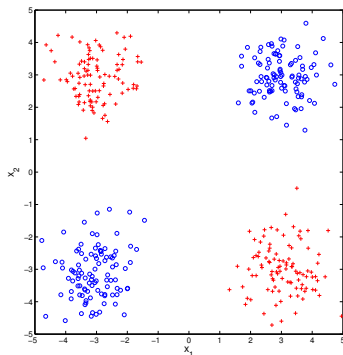
Lecture 1: Introduction to RKHS

MLSS Arequipa, 2016

Gatsby Unit, CSML, UCL

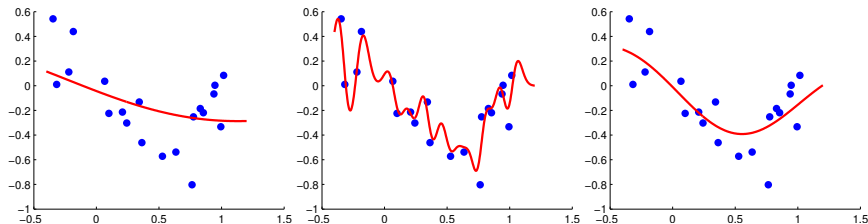
August 4, 2016

Kernels and feature space (1): XOR example



- No linear classifier separates red from blue
- Map points to **higher dimensional feature space**:
$$\phi(x) = \begin{bmatrix} x_1 & x_2 & x_1 x_2 \end{bmatrix} \in \mathbb{R}^3$$

Kernels and feature space (2): smoothing



Kernel methods can control **smoothness** and **avoid overfitting/underfitting**.

Outline: reproducing kernel Hilbert space

We will describe in order:

- 1 Hilbert space
- 2 Kernel (lots of examples: e.g. you can build kernels from simpler kernels)
- 3 Reproducing property

Hilbert space

Definition (Inner product)

Let $\mathcal{H}$ be a vector space over $\mathbb{R}$. A function $\langle \cdot, \cdot \rangle_{\mathcal{H}} : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{R}$ is an **inner product** on $\mathcal{H}$ if

- 1 Linear: $\langle \alpha_1 f_1 + \alpha_2 f_2, g \rangle_{\mathcal{H}} = \alpha_1 \langle f_1, g \rangle_{\mathcal{H}} + \alpha_2 \langle f_2, g \rangle_{\mathcal{H}}$
- 2 Symmetric: $\langle f, g \rangle_{\mathcal{H}} = \langle g, f \rangle_{\mathcal{H}}$
- 3 $\langle f, f \rangle_{\mathcal{H}} \geq 0$ and $\langle f, f \rangle_{\mathcal{H}} = 0$ if and only if $f = 0$.

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Norm induced by the inner product: $\|f\|_{\mathcal{H}} := \sqrt{\langle f, f \rangle_{\mathcal{H}}}$

Definition (Hilbert space)

Inner product space containing Cauchy sequence limits.

Kernel

Definition

Let $\mathcal{X}$ be a non-empty set. A function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a **kernel** if there exists an $\mathbb{R}$ -Hilbert space and a map $\phi : \mathcal{X} \rightarrow \mathcal{H}$ such that $\forall x, x' \in \mathcal{X}$,

$$k(x, x') := \langle \phi(x), \phi(x') \rangle_{\mathcal{H}}.$$

- Almost no conditions on $\mathcal{X}$ (eg, $\mathcal{X}$ itself doesn't need an inner product, eg. documents).
- A single kernel can correspond to several possible features. A trivial example for $\mathcal{X} := \mathbb{R}$:

$$\phi_1(x) = x \quad \text{and} \quad \phi_2(x) = \begin{bmatrix} x/\sqrt{2} \\ x/\sqrt{2} \end{bmatrix}$$

New kernels from old: sums, transformations

Theorem (Sums of kernels are kernels)

Given $\alpha > 0$ and k, k_1 and k_2 all kernels on $\mathcal{X}$, then αk and $k_1 + k_2$ are kernels on $\mathcal{X}$.

(Proof via positive definiteness: **later!**) A difference of kernels may not be a kernel (**why?**)

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Theorem (Mappings between spaces)

Let $\mathcal{X}$ and $\tilde{\mathcal{X}}$ be sets, and define a map $A : \mathcal{X} \rightarrow \tilde{\mathcal{X}}$. Define the kernel k on $\tilde{\mathcal{X}}$. Then the kernel $k(A(x), A(x'))$ is a kernel on $\mathcal{X}$.

Example: $k(x, x') = x^2 (x')^2$.

New kernels from old: products

Theorem (Products of kernels are kernels)

*Given k_1 on $\mathcal{X}_1$ and k_2 on $\mathcal{X}_2$, then $k_1 \times k_2$ is a kernel on $\mathcal{X}_1 \times \mathcal{X}_2$.
 If $\mathcal{X}_1 = \mathcal{X}_2 = \mathcal{X}$, then $k := k_1 \times k_2$ is a kernel on $\mathcal{X}$.*

Proof: Main idea only!

$\mathcal{H}_1$ space of kernels between **shapes**,

$$\phi_1(x) = \begin{bmatrix} \mathbb{I}_{\square} \\ \mathbb{I}_{\triangle} \end{bmatrix} \quad \phi_1(\square) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad k_1(\square, \triangle) = 0.$$

$\mathcal{H}_2$ space of kernels between **colors**,

$$\phi_2(x) = \begin{bmatrix} \mathbb{I}_{\bullet} \\ \mathbb{I}_{\circ} \end{bmatrix} \quad \phi_2(\bullet) = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad k_2(\bullet, \bullet) = 1.$$

New kernels from old: products

“Natural” feature space for **colored shapes**:

$$\Phi(x) = \begin{bmatrix} \mathbb{I}_{\square} & \mathbb{I}_{\triangle} \\ \mathbb{I}_{\square} & \mathbb{I}_{\triangle} \end{bmatrix} = \begin{bmatrix} \mathbb{I} \\ \mathbb{I} \end{bmatrix} \begin{bmatrix} \mathbb{I}_{\square} & \mathbb{I}_{\triangle} \end{bmatrix} = \phi_2(x)\phi_1^T(x)$$

New kernels from old: products

“Natural” feature space for **colored shapes**:

$$\Phi(x) = \begin{bmatrix} \mathbb{I}_{\square} & \mathbb{I}_{\triangle} \\ \mathbb{I}_{\square} & \mathbb{I}_{\triangle} \end{bmatrix} = \begin{bmatrix} \mathbb{I}_{\bullet} \\ \mathbb{I}_{\bullet} \end{bmatrix} \begin{bmatrix} \mathbb{I}_{\square} & \mathbb{I}_{\triangle} \end{bmatrix} = \phi_2(x)\phi_1^\top(x)$$

Kernel is:

$$\begin{aligned} k(x, x') &= \sum_{i \in \{\bullet, \bullet\}} \sum_{j \in \{\square, \triangle\}} \Phi_{ij}(x) \Phi_{ij}(x') = \text{tr} \left(\phi_1(x) \underbrace{\phi_2^\top(x) \phi_2(x') \phi_1^\top(x')}_{k_2(x, x')} \right) \\ &= \text{tr} \left(\underbrace{\phi_1^\top(x') \phi_1(x)}_{k_1(x, x')} \right) k_2(x, x') = k_1(x, x') k_2(x, x') \end{aligned}$$

Sums and products $\implies$ polynomials

Theorem (Polynomial kernels)

Let $x, x' \in \mathbb{R}^d$ for $d \geq 1$, and let $m \geq 1$ be an integer and $c \geq 0$ be a positive real. Then

$$k(x, x') := (\langle x, x' \rangle + c)^m$$

is a valid kernel.

To prove: expand into a sum (with non-negative scalars) of kernels $\langle x, x' \rangle$ raised to integer powers. These individual terms are valid kernels by the product rule.

Infinite sequences

The kernels we've seen so far are dot products between **finitely** many features. E.g.

$$k(x, y) = \begin{bmatrix} \sin(x) & x^3 & \log x \end{bmatrix}^\top \begin{bmatrix} \sin(y) & y^3 & \log y \end{bmatrix}$$

where $\phi(x) = \begin{bmatrix} \sin(x) & x^3 & \log x \end{bmatrix}$

Can a kernel be a dot product between **infinitely many features**?

Infinite sequences

Definition

The space ℓ_2 (**square** summable sequences) comprises all sequences $a := (a_i)_{i \geq 1}$ for which

$$\|a\|_{\ell_2}^2 = \sum_{i=1}^{\infty} a_i^2 < \infty.$$

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Definition

Given sequence of functions $(\phi_i(x))_{i \geq 1}$ in ℓ_2 where $\phi_i : \mathcal{X} \rightarrow \mathbb{R}$ is the i th coordinate of $\phi(x)$. Then

$$k(x, x') := \sum_{i=1}^{\infty} \phi_i(x) \phi_i(x') \quad (1)$$

Infinite sequences (proof)

Why square summable? By Cauchy-Schwarz,

$$\left| \sum_{i=1}^{\infty} \phi_i(x) \phi_i(x') \right| \leq \|\phi(x)\|_{\ell_2} \|\phi(x')\|_{\ell_2},$$

so the sequence defining the inner product converges for all $x, x' \in \mathcal{X}$

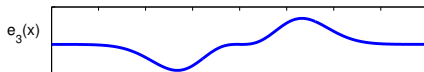
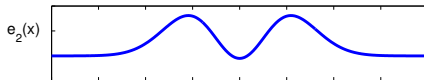
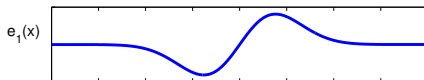
A famous infinite feature space kernel

exponentiated quadratic kernel,

$$k(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right) = \sum_{i=1}^{\infty} \underbrace{\left(\sqrt{\lambda_i} e_i(x)\right)}_{\phi_i(x)} \underbrace{\left(\sqrt{\lambda_i} e_i(x')\right)}_{\phi_i(x')}$$

$$\lambda_k \propto b^k \quad b < 1$$

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



$$\lambda_i e_i(x) = \int k(x, x') e_i(x') p(x') dx',$$

$$p(x) = \mathcal{N}(0, \sigma^2).$$

a, b, c are functions of σ ,
and H_k is k th order Hermite polynomial.

Positive definite functions

If we are given a function of two arguments, $k(x, x')$, how can we determine if it is a valid kernel?

- ① Find a feature map?
 - ① Sometimes this is not obvious (eg if the feature vector is infinite dimensional, e.g. the exponentiated quadratic kernel in the last slide)
 - ② The feature map is not unique.
- ② A direct property of the function: **positive definiteness**.

Positive definite functions

Definition (Positive definite functions)

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

$$\sum_{i=1}^n \sum_{j=1}^n a_i a_j k(x_i, x_j) \geq 0.$$

The function $k(\cdot, \cdot)$ 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

Theorem

Let $\mathcal{H}$ be a Hilbert space, $\mathcal{X}$ a non-empty set and $\phi : \mathcal{X} \rightarrow \mathcal{H}$.
Then $\langle \phi(x), \phi(y) \rangle_{\mathcal{H}} =: k(x, y)$ is positive definite.

Proof.

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

Reverse also holds: positive definite $k(x, x')$ is inner product in a unique $\mathcal{H}$ (**Moore-Aronsjajn**: coming later!).

Sum of kernels is a kernel

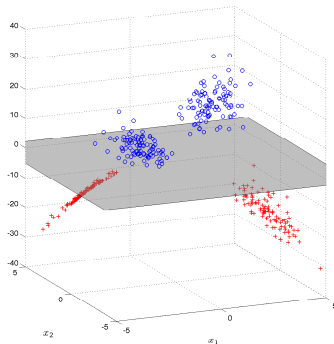
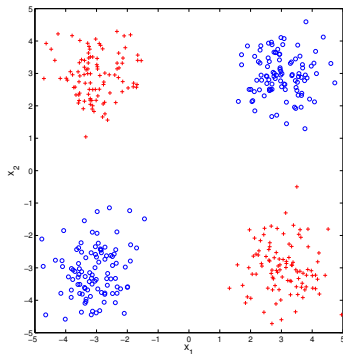
Consider two kernels $k_1(x, x')$ and $k_2(x, x')$. Then

$$\begin{aligned} & \sum_{i=1}^n \sum_{j=1}^n a_i a_j [k_1(x_i, x_j) + k_2(x_i, x_j)] \\ &= \sum_{i=1}^n \sum_{j=1}^n a_i a_j k_1(x_i, x_j) + \sum_{i=1}^n \sum_{j=1}^n a_i a_j k_2(x_i, x_j) \\ &\geq 0 \end{aligned}$$

The reproducing kernel Hilbert space

First example: finite space, polynomial features

Reminder: XOR example:



First example: finite space, polynomial features

Reminder: Feature space from XOR motivating example:

$$\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \mapsto \phi(x) = \begin{bmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{bmatrix},$$

with kernel

$$k(x, y) = \begin{bmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{bmatrix}^\top \begin{bmatrix} y_1 \\ y_2 \\ y_1 y_2 \end{bmatrix}$$

(the standard inner product in $\mathbb{R}^3$ between features). Denote this feature space by $\mathcal{H}$.

First example: finite space, polynomial features

Define a **linear function** of the inputs x_1, x_2 , and their product $x_1 x_2$,

$$f(x) = f_1 x_1 + f_2 x_2 + f_3 x_1 x_2.$$

f in a space of functions mapping from $\mathcal{X} = \mathbb{R}^2$ to $\mathbb{R}$. Equivalent representation for f ,

$$f(\cdot) = \begin{bmatrix} f_1 & f_2 & f_3 \end{bmatrix}^\top.$$

$f(\cdot)$ refers to the function as an object (here as a **vector** in $\mathbb{R}^3$)
 $f(x) \in \mathbb{R}$ is function evaluated at a point (a **real number**).

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$$f(x) = f(\cdot)^\top \phi(x) = \langle f(\cdot), \phi(x) \rangle_{\mathcal{H}}$$

Evaluation of f at x is an **inner product in feature space** (here standard inner product in $\mathbb{R}^3$)

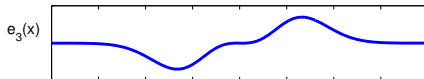
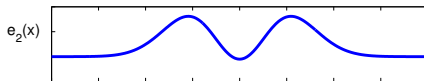
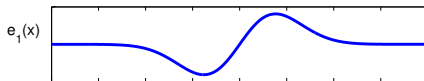
$\mathcal{H}$ is a space of functions mapping $\mathbb{R}^2$ to $\mathbb{R}$.

What if we have infinitely many features?

exponentiated quadratic kernel,

$$k(x, y) = \exp\left(-\frac{\|x - y\|^2}{2\sigma^2}\right) = \sum_{i=1}^{\infty} \phi_i(x)\phi_i(x')$$

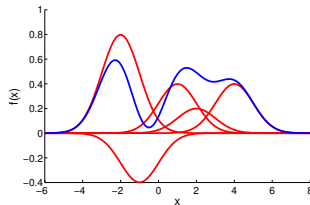
$$f(x) = \sum_{i=1}^{\infty} f_i \phi_i(x) \quad \sum_{i=1}^{\infty} f_i^2 < \infty.$$



What if we have infinitely many features?

Function with **exponentiated quadratic kernel**:

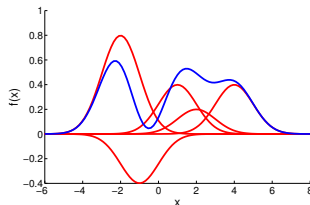
$$\begin{aligned} f(x) &:= \sum_{i=1}^m \alpha_i k(x_i, x) \\ &= \sum_{i=1}^m \alpha_i \langle \phi(x_i), \phi(x) \rangle_{\mathcal{H}} \\ &= \left\langle \sum_{i=1}^m \alpha_i \phi(x_i), \phi(x) \right\rangle_{\mathcal{H}} \end{aligned}$$



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 &= \left\langle \sum_{i=1}^m \alpha_i \phi(x_i), \phi(x) \right\rangle_{\mathcal{H}} \\
 &= \sum_{\ell=1}^{\infty} f_{\ell} \phi_{\ell}(x) \\
 &= \langle f(\cdot), \phi(x) \rangle_{\mathcal{H}}
 \end{aligned}$$



$$f_{\ell} := \sum_{i=1}^m \alpha_i \phi_{\ell}(x_i)$$

Possible to write functions of **infinitely many features!**

The feature map is *also* a function

On previous page,

$$f(x) := \sum_{i=1}^m \alpha_i k(x_i, x) = \langle f(\cdot), \phi(x) \rangle_{\mathcal{H}} \quad \text{where} \quad f(\cdot) = \sum_{i=1}^m \alpha_i \phi_\ell(x_i).$$

What if $m = 1$ and $\alpha_1 = 1$?

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What if $m = 1$ and $\alpha_1 = 1$?

Then

$$f(x) = k(x_1, x) = \left\langle \underbrace{k(x_1, \cdot)}_{f(\cdot)}, \phi(x) \right\rangle_{\mathcal{H}}$$

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....so the feature map is a (very simple) function!

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....so the feature map is a (very simple) function!

We can write without ambiguity

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

The reproducing property

This example illustrates the two defining features of an RKHS:

- **The reproducing property:** (kernel trick)

$$\forall x \in \mathcal{X}, \forall f(\cdot) \in \mathcal{H}, \langle f(\cdot), k(\cdot, x) \rangle_{\mathcal{H}} = f(x)$$

...or use shorter notation $\langle f, \phi(x) \rangle_{\mathcal{H}}$.

- The feature map of every point is a function:

$k(\cdot, x) = \phi(x) \in \mathcal{H}$ for any $x \in \mathcal{X}$, and

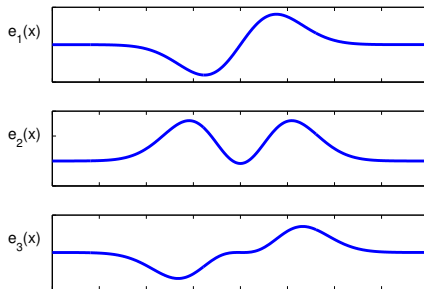
$$k(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{H}} = \langle k(\cdot, x), k(\cdot, x') \rangle_{\mathcal{H}}.$$

A closer look, RKHS with exponentiated quadratic kernel

Reminder, **exponentiated quadratic kernel**,

$$k(x, y) = \exp\left(-\frac{\|x - y\|^2}{2\sigma^2}\right) = \sum_{i=1}^{\infty} \underbrace{\left(\sqrt{\lambda_i} e_i(x)\right)}_{\phi_i(x)} \underbrace{\left(\sqrt{\lambda_i} e_i(x')\right)}_{\phi_i(x')}$$

$$\lambda_k \propto b^k \quad b < 1$$

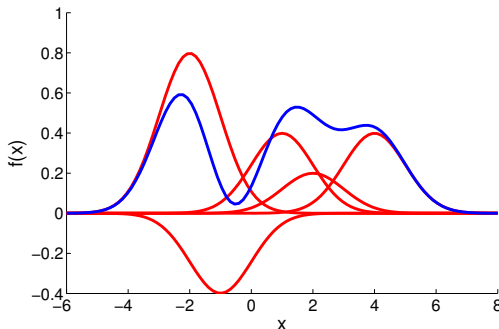


A closer look, RKHS with exponentiated quadratic kernel

RKHS function, exponentiated quadratic kernel:

$$f(x) := \sum_{i=1}^m \alpha_i k(x_i, x) = \sum_{\ell=1}^{\infty} \underbrace{f_{\ell}}_{\phi_{\ell}(x)} \left[\sqrt{\lambda_{\ell}} e_{\ell}(x) \right]$$

where $f_{\ell} = \sum_{i=1}^m \alpha_i \sqrt{\lambda_{\ell}} e_{\ell}(x_i)$.



NOTE that this
enforces
smoothing:

λ_k decay as e_k
become rougher,
 f_j decay since
 $\sum_j f_j^2 < \infty$.

Infinite feature space via Fourier series

Infinite feature space via Fourier series

Function on the torus $\mathbb{T} := [-\pi, \pi]$ with periodic boundary. **Fourier series:**

$$f(x) = \sum_{\ell=-\infty}^{\infty} \hat{f}_{\ell} \exp(i\ell x) = \sum_{\ell=-\infty}^{\infty} \hat{f}_{\ell} (\cos(\ell x) + i \sin(\ell x)).$$

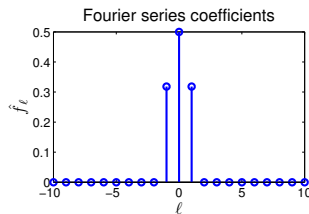
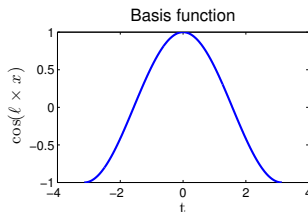
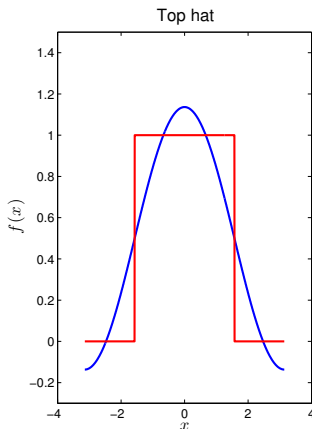
Example: “top hat” function,

$$f(x) = \begin{cases} 1 & |x| < T, \\ 0 & T \leq |x| < \pi. \end{cases}$$

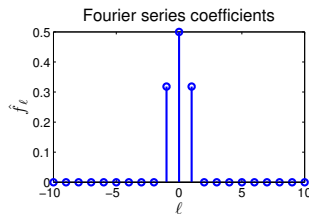
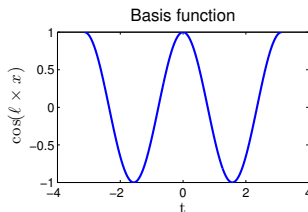
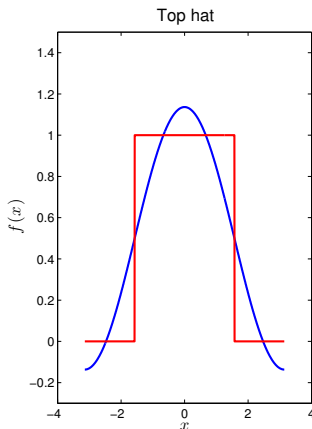
Fourier series:

$$\hat{f}_{\ell} := \frac{\sin(\ell T)}{\ell \pi} \quad f(x) = \sum_{\ell=0}^{\infty} 2\hat{f}_{\ell} \cos(\ell x).$$

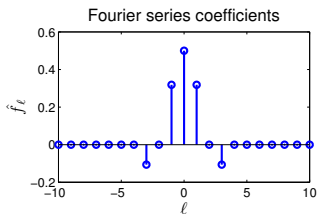
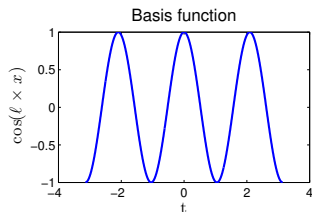
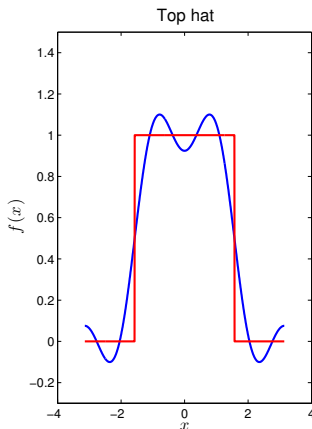
Fourier series for top hat function



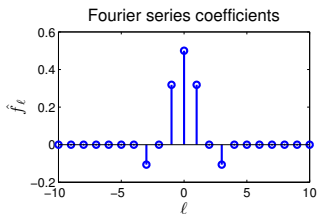
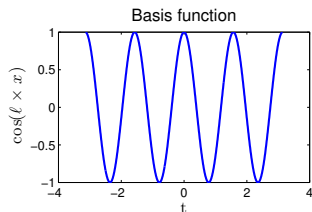
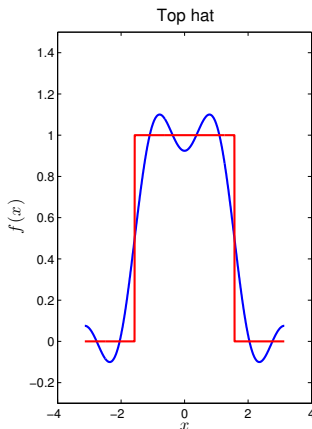
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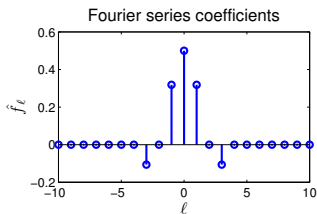
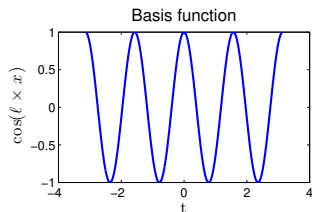
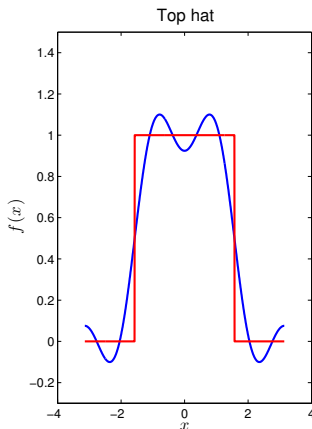
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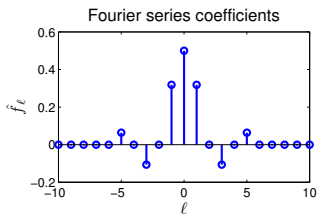
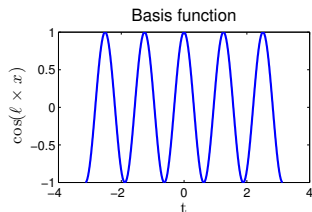
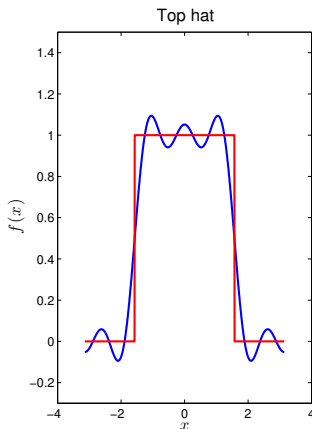
Fourier series for top hat function



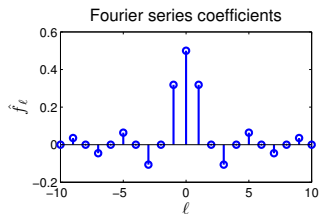
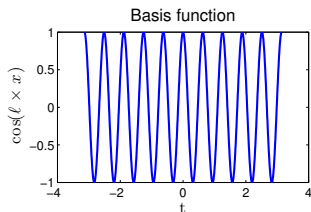
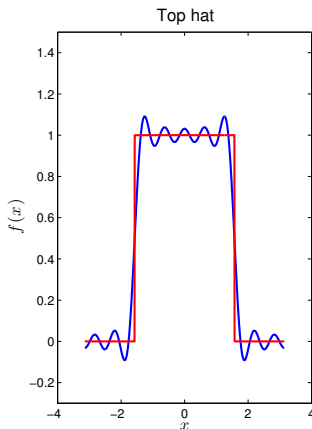
Fourier series for top hat function



Fourier series for top hat function



Fourier series for top hat function



Fourier series for kernel function

Kernel takes a single argument,

$$k(x, y) = k(x - y),$$

Define the Fourier series representation of k

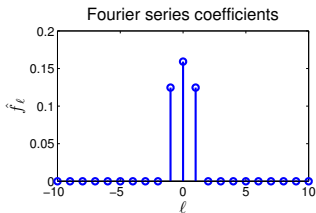
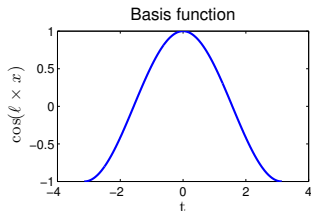
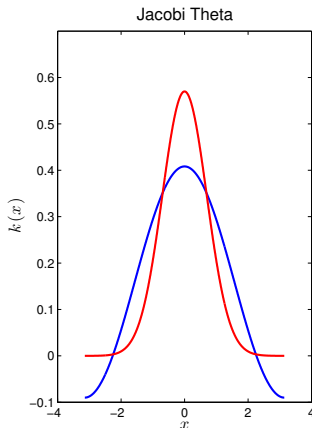
$$k(x) = \sum_{\ell=-\infty}^{\infty} \hat{k}_{\ell} \exp(i\ell x),$$

k and its Fourier transform are real and symmetric. E.g. ,

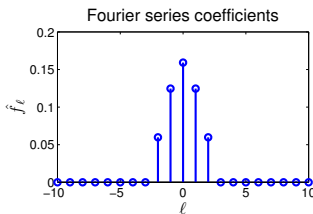
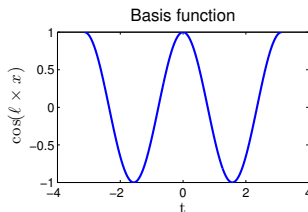
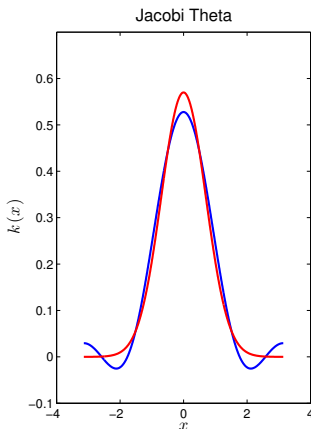
$$k(x) = \frac{1}{2\pi} \vartheta\left(\frac{x}{2\pi}, \frac{\sigma^2}{2\pi}\right), \quad \hat{k}_{\ell} = \frac{1}{2\pi} \exp\left(\frac{-\sigma^2 \ell^2}{2}\right).$$

ϑ is the Jacobi theta function, close to Gaussian when σ^2 sufficiently narrower than $[-\pi, \pi]$.

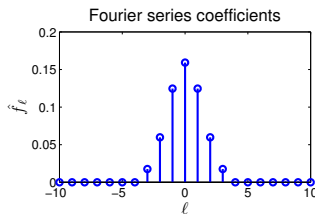
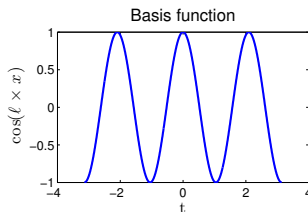
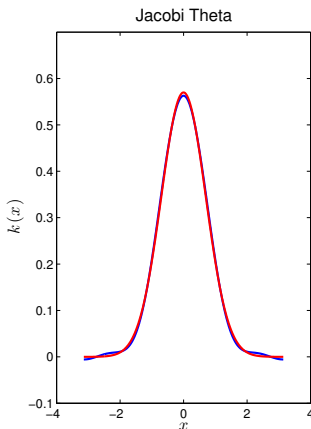
Fourier series for Gaussian-spectrum kernel



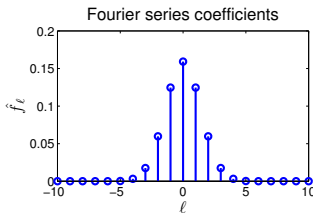
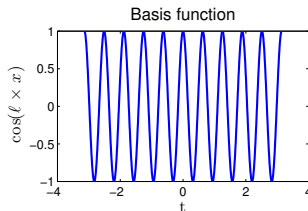
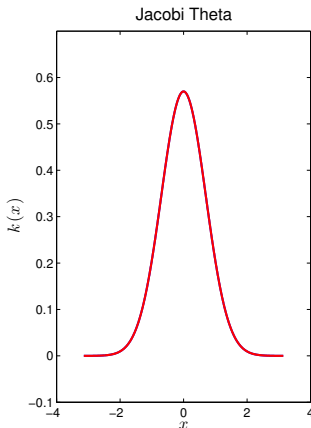
Fourier series for Gaussian-spectrum kernel



Fourier series for Gaussian-spectrum kernel



Fourier series for Gaussian-spectrum kernel



Feature space via fourier series

Define $\mathcal{H}$ to be the space of functions with (infinite) feature space representation

$$f(\cdot) = \left[\dots \quad \hat{f}_\ell / \sqrt{\hat{k}_\ell} \quad \dots \right]^\top.$$

Feature space via fourier series

Define $\mathcal{H}$ to be the space of functions with (infinite) feature space representation

$$f(\cdot) = \left[\dots \hat{f}_\ell / \sqrt{\hat{k}_\ell} \dots \right]^\top.$$

Define the feature map

$$k(\cdot, x) = \phi(x) = \left[\dots \sqrt{\hat{k}_\ell} \exp(-i\ell x) \dots \right]^\top$$

Feature space via fourier series

The reproducing theorem holds,

$$\begin{aligned}\langle f(\cdot), k(\cdot, x) \rangle_{\mathcal{H}} &= \sum_{\ell=-\infty}^{\infty} \left(\frac{\hat{f}_{\ell}}{\sqrt{\hat{k}_{\ell}}} \right) \overline{\sqrt{\hat{k}_{\ell}} \exp(-i\ell x)} \\ &= \sum_{\ell=-\infty}^{\infty} \hat{f}_{\ell} \exp(i\ell x) = f(x),\end{aligned}$$

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...including for the kernel itself,

$$\begin{aligned}\langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}} &= \sum_{\ell=-\infty}^{\infty} \left(\sqrt{\hat{k}_{\ell}} \exp(-i\ell x) \right) \overline{\left(\sqrt{\hat{k}_{\ell}} \exp(-i\ell y) \right)} \\ &= \sum_{\ell=-\infty}^{\infty} \hat{k}_{\ell} \exp(i\ell(y - x)) = k(x - y).\end{aligned}$$

Fourier series and smoothness

The squared norm of a function f in $\mathcal{H}$ is:

$$\|f\|_{\mathcal{H}}^2 = \langle f, f \rangle_{\mathcal{H}} = \sum_{l=-\infty}^{\infty} \frac{\hat{f}_l \overline{\hat{f}_l}}{\hat{k}_l}.$$

If $\hat{k}_l$ decays fast, then so must $\hat{f}_l$ if we want $\|f\|_{\mathcal{H}}^2 < \infty$.

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Recall

$$f(x) = \sum_{l=-\infty}^{\infty} \hat{f}_l (\cos(lx) + i \sin(lx)).$$

Enforces smoothness.

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Enforces smoothness.

Question: is the top hat function in the Gaussian-spectrum RKHS?

Some reproducing kernel Hilbert space theory

Reproducing kernel Hilbert space (1)

Definition

$\mathcal{H}$ a Hilbert space of $\mathbb{R}$ -valued functions on non-empty set $\mathcal{X}$. A function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a **reproducing kernel** of $\mathcal{H}$, and $\mathcal{H}$ is a **reproducing kernel Hilbert space**, if

- $\forall x \in \mathcal{X}, k(\cdot, x) \in \mathcal{H}$,
- $\forall x \in \mathcal{X}, \forall f \in \mathcal{H}, \langle f(\cdot), k(\cdot, x) \rangle_{\mathcal{H}} = f(x)$ (the reproducing property).

In particular, for any $x, y \in \mathcal{X}$,

$$k(x, y) = \langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}}. \quad (2)$$

Original definition: kernel an inner product between feature maps.
Then $\phi(x) = k(\cdot, x)$ a valid feature map.

Reproducing kernel Hilbert space (2)

Another RKHS definition:

Define δ_x to be the operator of evaluation at x , i.e.

$$\delta_x f = f(x) \quad \forall f \in \mathcal{H}, x \in \mathcal{X}.$$

Definition (Reproducing kernel Hilbert space)

$\mathcal{H}$ is an RKHS if the evaluation operator δ_x is **bounded**: $\forall x \in \mathcal{X}$ there exists $\lambda_x \geq 0$ such that for all $f \in \mathcal{H}$,

$$|f(x)| = |\delta_x f| \leq \lambda_x \|f\|_{\mathcal{H}}$$

$\implies$ two functions identical in RKHS norm agree at every point:

$$|f(x) - g(x)| = |\delta_x(f - g)| \leq \lambda_x \|f - g\|_{\mathcal{H}} \quad \forall f, g \in \mathcal{H}.$$

RKHS definitions equivalent

Theorem (Reproducing kernel equivalent to bounded δ_x)

$\mathcal{H}$ is a reproducing kernel Hilbert space (i.e., its evaluation operators δ_x are bounded linear operators), if and only if $\mathcal{H}$ has a reproducing kernel.

Proof: If $\mathcal{H}$ has a reproducing kernel $\implies \delta_x$ bounded

$$\begin{aligned} |\delta_x[f]| &= |f(x)| \\ &= |\langle f, k(\cdot, x) \rangle_{\mathcal{H}}| \\ &\leq \|k(\cdot, x)\|_{\mathcal{H}} \|f\|_{\mathcal{H}} \\ &= \langle k(\cdot, x), k(\cdot, x) \rangle_{\mathcal{H}}^{1/2} \|f\|_{\mathcal{H}} \\ &= k(x, x)^{1/2} \|f\|_{\mathcal{H}} \end{aligned}$$

Cauchy-Schwarz in 3rd line . Consequently, $\delta_x : \mathcal{F} \rightarrow \mathbb{R}$ bounded with $\lambda_x = k(x, x)^{1/2}$.

RKHS definitions equivalent

Proof: δ_x bounded $\implies \mathcal{H}$ has a reproducing kernel

We use...

Theorem

(Riesz representation) In a Hilbert space $\mathcal{H}$, all bounded linear functionals are of the form $\langle \cdot, g \rangle_{\mathcal{H}}$, for some $g \in \mathcal{H}$.

If $\delta_x : \mathcal{F} \rightarrow \mathbb{R}$ is a bounded linear functional, by Riesz $\exists f_{\delta_x} \in \mathcal{H}$ such that

$$\delta_x f = \langle f, f_{\delta_x} \rangle_{\mathcal{H}}, \quad \forall f \in \mathcal{H}.$$

Define $k(\cdot, x) = f_{\delta_x}(\cdot)$, $\forall x, x' \in \mathcal{X}$. By its definition, both $k(\cdot, x) = f_{\delta_x}(\cdot) \in \mathcal{H}$ and $\langle f(\cdot), k(\cdot, x) \rangle_{\mathcal{H}} = \delta_x f = f(x)$. Thus, k is the reproducing kernel.

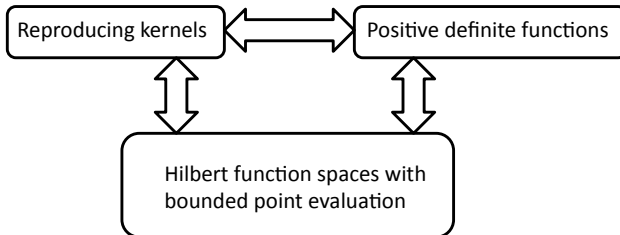
Moore-Aronszajn Theorem

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 .

Recall feature map is *not* unique (as we saw earlier): **only kernel is**.

Main message #1

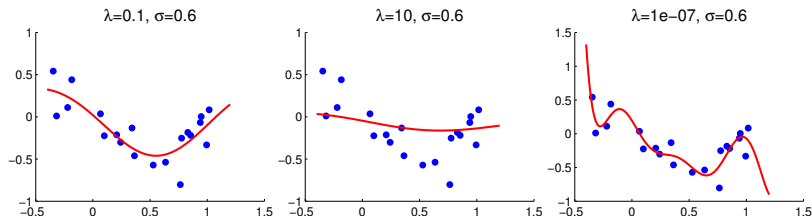


Main message #2

Small RKHS norm results in smooth functions.

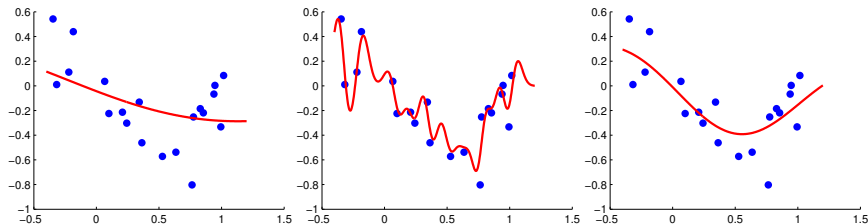
E.g. kernel ridge regression with exponentiated quadratic kernel:

$$f^* = \arg \min_{f \in \mathcal{H}} \left(\sum_{i=1}^n (y_i - \langle f, \phi(x_i) \rangle_{\mathcal{H}})^2 + \lambda \|f\|_{\mathcal{H}}^2 \right).$$



Kernel Ridge Regression

Kernel ridge regression



Very simple to implement, works well when no outliers.

Kernel ridge regression

Use features of $\phi(x_i)$ in the place of x_i :

$$f^* = \arg \min_{f \in \mathcal{H}} \left(\sum_{i=1}^n (y_i - \langle f, \phi(x_i) \rangle_{\mathcal{H}})^2 + \lambda \|f\|_{\mathcal{H}}^2 \right).$$

E.g. for finite dimensional feature spaces,

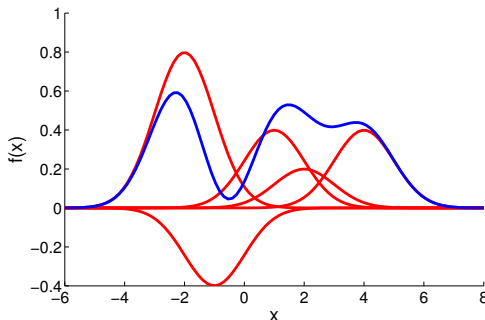
$$\phi_p(x) = \begin{bmatrix} x \\ x^2 \\ \vdots \\ x^\ell \end{bmatrix} \quad \phi_s(x) = \begin{bmatrix} \sin x \\ \cos x \\ \sin 2x \\ \vdots \\ \cos \ell x \end{bmatrix}$$

a is a vector of length ℓ giving weight to each of these features so as to find the mapping between x and y . Feature vectors can also have *infinite* length (more soon).

Kernel ridge regression

Solution easy if we **already know** f is a linear combination of feature space mappings of points: **representer theorem**.

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



Representer theorem

Given a set of paired observations $(x_1, y_1), \dots, (x_n, y_n)$ (regression or classification).

Find the function f^* in the RKHS $\mathcal{H}$ which satisfies

$$J(f^*) = \min_{f \in \mathcal{H}} J(f), \quad (3)$$

where

$$J(f) = L_y(f(x_1), \dots, f(x_n)) + \Omega \left(\|f\|_{\mathcal{H}}^2 \right),$$

Ω is non-decreasing, and y is the vector of y_i .

- Classification: $L_y(f(x_1), \dots, f(x_n)) = \sum_{i=1}^n \mathbb{I}_{y_i f(x_i) \leq 0}$
- Regression: $L_y(f(x_1), \dots, f(x_n)) = \sum_{i=1}^n (y_i - f(x_i))^2$

Representer theorem

The representer theorem: (simple version) solution to

$$\min_{f \in \mathcal{H}} \left[L_Y(f(x_1), \dots, f(x_n)) + \Omega \left(\|f\|_{\mathcal{H}}^2 \right) \right]$$

takes the form

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

If Ω is strictly increasing, all solutions have this form.

Representer theorem: proof

Proof: Denote f_s projection of f onto the subspace

$$\text{span} \{k(x_i, \cdot) : 1 \leq i \leq n\}, \quad (4)$$

such that

$$f = f_s + f_{\perp},$$

where $f_s = \sum_{i=1}^n \alpha_i k(x_i, \cdot)$.

Regularizer:

$$\|f\|_{\mathcal{H}}^2 = \|f_s\|_{\mathcal{H}}^2 + \|f_{\perp}\|_{\mathcal{H}}^2 \geq \|f_s\|_{\mathcal{H}}^2,$$

then

$$\Omega \left(\|f\|_{\mathcal{H}}^2 \right) \geq \Omega \left(\|f_s\|_{\mathcal{H}}^2 \right),$$

so this term is minimized for $f = f_s$.

Representer theorem: proof

Proof (cont.): Individual terms $f(x_i)$ in the loss:

$$f(x_i) = \langle f, k(x_i, \cdot) \rangle_{\mathcal{H}} = \langle f_s + f_{\perp}, k(x_i, \cdot) \rangle_{\mathcal{H}} = \langle f_s, k(x_i, \cdot) \rangle_{\mathcal{H}},$$

so

$$L_y(f(x_1), \dots, f(x_n)) = L_y(f_s(x_1), \dots, f_s(x_n)).$$

Hence

- Loss $L(\dots)$ only depends on the component of f in the data subspace,
- Regularizer $\Omega(\dots)$ minimized when $f = f_s$.
- If Ω is strictly non-decreasing, then $\|f_{\perp}\|_{\mathcal{H}} = 0$ is required at the minimum.

Kernel ridge regression: proof

We *begin* knowing f is a linear combination of feature space mappings of points (**representer theorem**)

$$f = \sum_{i=1}^n \alpha_i \phi(x_i).$$

Then

$$\sum_{i=1}^n (y_i - \langle f, \phi(x_i) \rangle_{\mathcal{H}})^2 + \lambda \|f\|_{\mathcal{H}}^2 = \|y - K\alpha\|^2 + \lambda \alpha^\top K \alpha$$

Differentiating wrt α and setting this to zero, we get

$$\alpha^* = (K + \lambda I_n)^{-1} y.$$

Reminder: smoothness

What does $\|a\|_{\mathcal{H}}$ have to do with smoothing?

Example 1: The Fourier series representation on torus $\mathbb{T}$:

$$f(x) = \sum_{l=-\infty}^{\infty} \hat{f}_l \exp(2\pi i l x),$$

and

$$\langle f, g \rangle_{\mathcal{H}} = \sum_{l=-\infty}^{\infty} \frac{\hat{f}_l \overline{\hat{g}_l}}{\hat{k}_l}.$$

Thus,

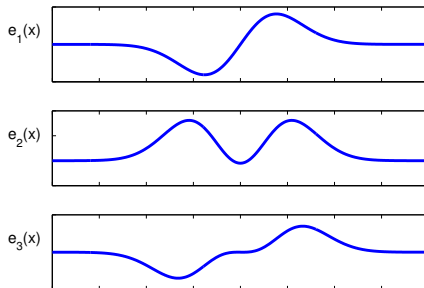
$$\|f\|_{\mathcal{H}}^2 = \langle f, f \rangle_{\mathcal{H}} = \sum_{l=-\infty}^{\infty} \frac{|\hat{f}_l|^2}{\hat{k}_l}.$$

Reminder: smoothness

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Example 2: The exponentiated quadratic kernel on $\mathbb{R}$. Recall

$$f(x) = \sum_{i=1}^{\infty} a_i \sqrt{\lambda_i} e_i(x), \quad \|f\|_{\mathcal{H}}^2 = \sum_{i=1}^{\infty} a_i^2.$$



Parameter selection for KRR

Given the objective

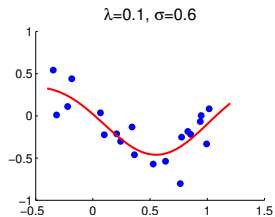
$$f^* = \arg \min_{f \in \mathcal{H}} \left(\sum_{i=1}^n (y_i - \langle f, \phi(x_i) \rangle_{\mathcal{H}})^2 + \lambda \|f\|_{\mathcal{H}}^2 \right).$$

How do we choose

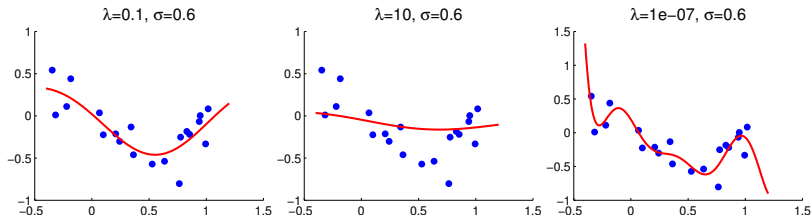
- The regularization parameter λ ?
- The kernel parameter: for exponentiated quadratic kernel, σ in

$$k(x, y) = \exp \left(\frac{-\|x - y\|^2}{\sigma} \right).$$

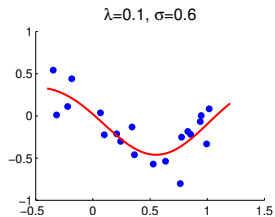
Choice of λ



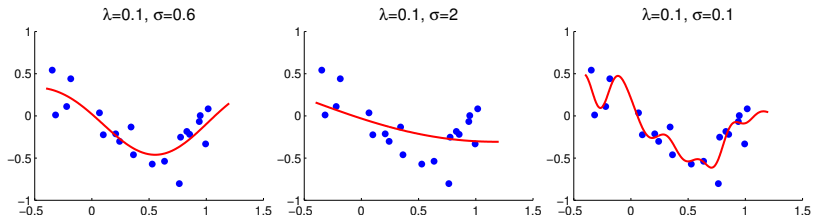
Choice of λ



Choice of σ

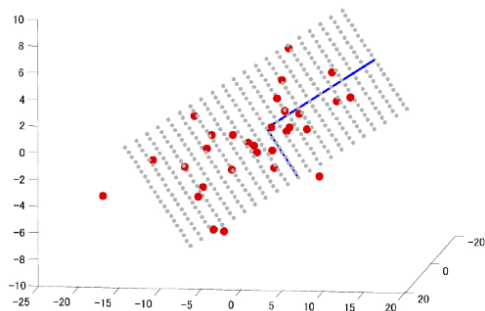


Choice of σ



PCA (1)

Goal of classical PCA: to find a d -dimensional subspace of a higher dimensional space (D -dimensional, $\mathbb{R}^D$) containing the directions of maximum variance.



(Figure from Kenji Fukumizu)

Application of kPCA: image denoising

What is the purpose of kernel PCA?

We consider the problem of **denoising** hand-written digits.

Application of kPCA: image denoising

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We consider the problem of **denoising** hand-written digits.

We are given a noisy digit x^* .

$$P_d \phi(x^*) = P_{f_1} \phi(x^*) + \dots + P_{f_d} \phi(x^*)$$

is the projection of $\phi(x^*)$ onto one of the first d eigenvectors from kernel PCA (these are orthogonal).

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Define the nearest point $y^* \in \mathcal{X}$ to this feature space projection as

$$y^* = \arg \min_{y \in \mathcal{X}} \|\phi(y) - P_d \phi(x^*)\|_{\mathcal{H}}^2.$$

In many cases, not possible to reduce the squared error to zero, as no single y^* corresponds to exact solution.

Application of kPCA: image denoising

Projection onto PCA subspace for denoising. **kPCA**: data may not be Gaussian distributed, but can lie in a submanifold in input space.

USPS hand-written digits data:

7191 images of hand-written digits of 16×16 pixels.



Sample of original images (not used for experiments)



Sample of noisy images



Sample of denoised images (**linear PCA**)



Sample of denoised images (**kernel PCA, Gaussian kernel**)

What is PCA?

First principal component (max. variance)

$$\begin{aligned} u_1 &= \arg \max_{\|u\| \leq 1} \frac{1}{n} \sum_{i=1}^n \left(u^\top \left(x_i - \frac{1}{n} \sum_{j=1}^n x_j \right) \right)^2 \\ &= \arg \max_{\|u\| \leq 1} u^\top C u \end{aligned}$$

where

$$C = \frac{1}{n} \sum_{i=1}^n \left(x_i - \frac{1}{n} \sum_{j=1}^n x_j \right) \left(x_i - \frac{1}{n} \sum_{j=1}^n x_j \right)^\top = \frac{1}{n} X H X^\top,$$

$X = \begin{bmatrix} x_1 & \dots & x_n \end{bmatrix}$, $H = I_n - n^{-1} \mathbf{1}_{n \times n}$, $\mathbf{1}_{n \times n}$ a matrix of ones.

Definition (Principal components)

The pairs (λ_i, u_i) are the eigensystem of $n\lambda_i u_i = C u_i$.

PCA in feature space

Kernel version, first principal component:

$$\begin{aligned} f_1 &= \arg \max_{\|f\|_{\mathcal{H}} \leq 1} \frac{1}{n} \sum_{i=1}^n \left(\left\langle f, \phi(x_i) - \frac{1}{n} \sum_{j=1}^n \phi(x_j) \right\rangle_{\mathcal{H}} \right)^2 \\ &= \arg \max_{\|f\|_{\mathcal{H}} \leq 1} \text{var}(f). \end{aligned}$$

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We can write

$$f = \sum_{i=1}^n \alpha_i \left(\phi(x_i) - \frac{1}{n} \sum_{j=1}^n \phi(x_j) \right) = \sum_{i=1}^n \alpha_i \tilde{\phi}(x_i),$$

since any component orthogonal to the span of $\tilde{\phi}(x_i) := \phi(x_i) - \frac{1}{n} \sum_{j=1}^n \phi(x_j)$ vanishes.

How to solve kernel PCA

We can also define an infinite dimensional analog of the covariance:

$$\begin{aligned} C &= \frac{1}{n} \sum_{i=1}^n \left(\phi(x_i) - \frac{1}{n} \sum_{j=1}^n \phi(x_j) \right) \otimes \left(\phi(x_i) - \frac{1}{n} \sum_{j=1}^n \phi(x_j) \right), \\ &= \frac{1}{n} \sum_{i=1}^n \tilde{\phi}(x_i) \otimes \tilde{\phi}(x_i) \end{aligned}$$

where we use the definition

$$(a \otimes b)c := a \langle b, c \rangle_{\mathcal{H}} \quad (5)$$

this is analogous to the case of finite dimensional vectors,
 $(ab^{\top})c = a(b^{\top}c)$.

How to solve kernel PCA (1)

Eigenfunctions of kernel covariance:

$$\begin{aligned}
 f_\ell \lambda_\ell &= C f_\ell \\
 &= \left(\frac{1}{n} \sum_{i=1}^n \tilde{\phi}(x_i) \otimes \tilde{\phi}(x_i) \right) f_\ell \\
 &= \frac{1}{n} \sum_{i=1}^n \tilde{\phi}(x_i) \left\langle \tilde{\phi}(x_i), \sum_{j=1}^n \alpha_{\ell j} \tilde{\phi}(x_j) \right\rangle_{\mathcal{H}}
 \end{aligned}$$

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 &= \frac{1}{n} \sum_{i=1}^n \tilde{\phi}(x_i) \left(\sum_{j=1}^n \alpha_{\ell j} \tilde{k}(x_i, x_j) \right)
 \end{aligned}$$

$\tilde{k}(x_i, x_j)$ is the (i, j) th entry of the matrix $\tilde{K} := HKH$ (exercise!).

How to solve kernel PCA (2)

We can now project both sides of

$$f_\ell \lambda_\ell = C f_\ell$$

onto all of the $\tilde{\phi}(x_q)$:

$$\left\langle \tilde{\phi}(x_q), \text{LHS} \right\rangle_{\mathcal{H}} = \lambda_\ell \left\langle \tilde{\phi}(x_q), f_\ell \right\rangle = \lambda_\ell \sum_{i=1}^n \alpha_{\ell i} \tilde{k}(x_q, x_i) \quad \forall q \in \{1 \dots n\}$$

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$$\langle \tilde{\phi}(x_q), \text{RHS} \rangle_{\mathcal{H}} = \langle \tilde{\phi}(x_q), C f_\ell \rangle_{\mathcal{H}} = \frac{1}{n} \sum_{i=1}^n \tilde{k}(x_q, x_i) \left(\sum_{j=1}^n \alpha_{\ell j} \tilde{k}(x_i, x_j) \right)$$

Writing this as a matrix equation,

$$n \lambda_\ell \tilde{K} \alpha_\ell = \tilde{K}^2 \alpha_\ell \quad n \lambda_\ell \alpha_\ell = \tilde{K} \alpha_\ell.$$

Projection onto kernel PC

How do you project a new point x^* onto the principal component f ?
 Assuming f is properly normalised, the projection is

$$\begin{aligned} P_f \tilde{\phi}(x^*) &= \left\langle \tilde{\phi}(x^*), f \right\rangle_{\mathcal{H}} f \\ &= \sum_{i=1}^n \alpha_i \left(\sum_{j=1}^n \alpha_j \tilde{k}(x_j, x^*) \right) \tilde{\phi}(x_i). \end{aligned}$$