

Reproducing kernel Hilbert spaces in Machine Learning

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Gatsby Computational Neuroscience Unit,
University College London

Advanced topics in Machine Learning, 2025

Overview

The course has two parts:

- Kernel methods (Arthur Gretton)
- Convex optimization (Massimiliano Pontil)

The **kernel part** of the course has the following assessment components:

- Exam (50%)
- Coursework (50%)

For **non-Gatsby** students: only the first part of the coursework is mandatory - the group parts are optional.

For **Gatsby** students: the full coursework is required

Course times, locations

Lecture times:

- Kernel lectures are Wednesday, 14:00 -15:30
- Optimization lectures will be on Friday 15:00 -16:30

There will be lectures during reading week, due to clash with NeurIPS conference.

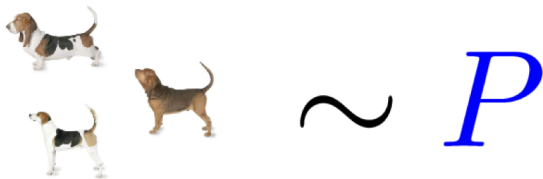
The tutor for the kernels part is Bariscan Bozkurt.

Lecture notes are online:

<http://www.gatsby.ucl.ac.uk/~gretton/rkhscourse.html>

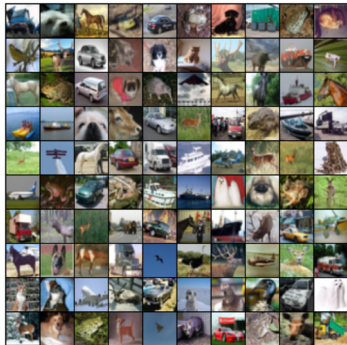
A motivation: comparing two samples

- Given: Samples from unknown distributions P and Q .
- Goal: do P and Q differ?

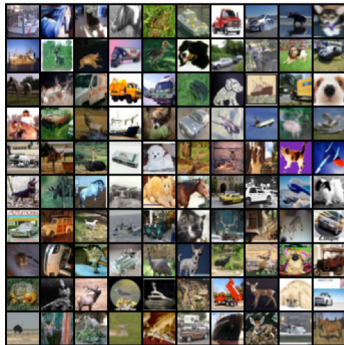


A real-life example: two-sample tests

- Goal: do P and Q differ?



CIFAR 10 samples



Cifar 10.1 samples

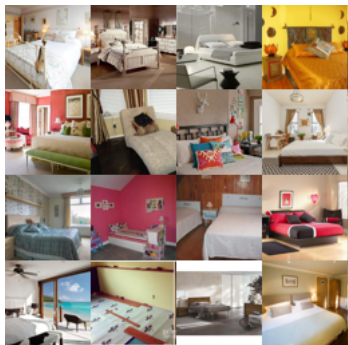
Significant difference?

Feng, Xu, Lu, Zhang, G., Sutherland, Learning Deep Kernels for Non-Parametric Two-Sample Tests, ICML 2020

Sutherland, Tung, Strathmann, De, Ramdas, Smola, G., ICLR 2017.

Training generative models

- Have: One collection of samples X from unknown distribution P .
- Goal: **generate** samples Q that look like P



LSUN bedroom samples P



Generated Q , MMD GAN

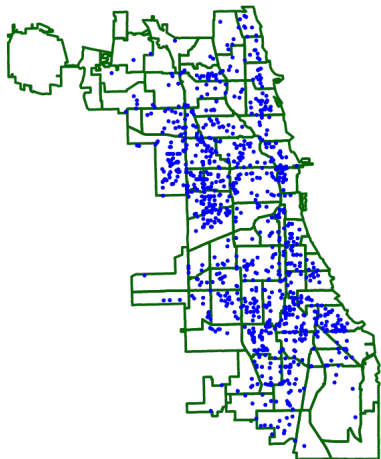
Training a Generative Adversarial Network

(Binkowski, Sutherland, Arbel, G., ICLR 2018),
(Arbel, Sutherland, Binkowski, G., NeurIPS 2018)

Testing goodness of fit

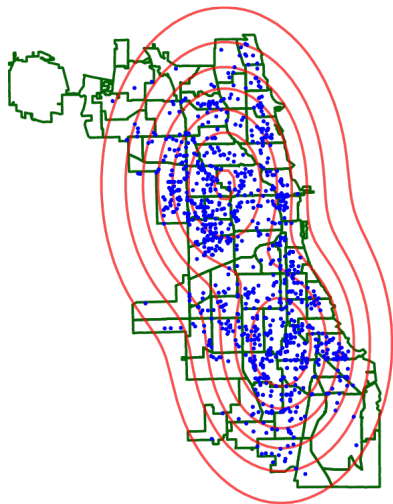
- Given: a model P and samples Q .
- Goal: is P a good fit for Q ?

Chicago crime data



Testing goodness of fit

- Given: a model P and samples Q .
- Goal: is P a good fit for Q ?






Chicago crime data

Model is Gaussian mixture with **two** components. Is this a good model?

Testing independence

- Given: Samples from a distribution P_{XY}
- Goal: Are X and Y independent?

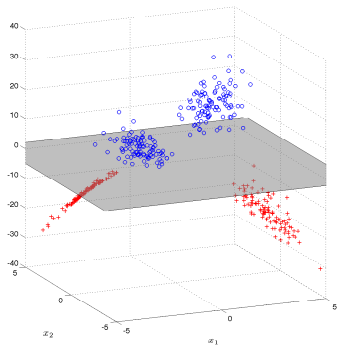
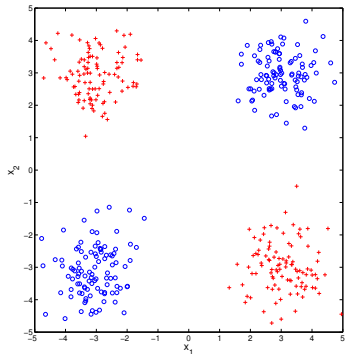
X	Y
	A large animal who slings slobber, exudes a distinctive houndy odor, and wants nothing more than to follow his nose.
	Their noses guide them through life, and they're never happier than when following an interesting scent.
	A responsive, interactive pet, one that will blow in your ear and follow you everywhere.

Course overview (kernels part)

- 1 Construction of RKHS,
- 2 Simple linear algorithms in RKHS (e.g. PCA, ridge regression)
- 3 Kernel methods for hypothesis testing (two-sample, independence, goodness-of-fit)
- 4 Further applications of kernels (feature selection, clustering,...)
- 5 Support vector machines for classification, regression
- 6 Cutting-edge kernel algorithms (to be a surprise)

Reproducing Kernel Hilbert Spaces

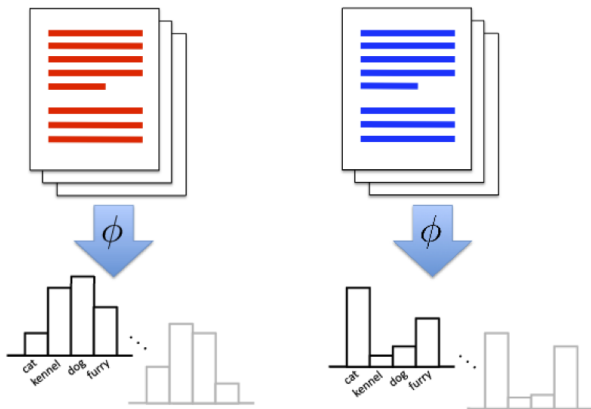
Kernels and feature space (1): XOR example



- No linear classifier separates red from blue
- Map points to higher dimensional feature space:

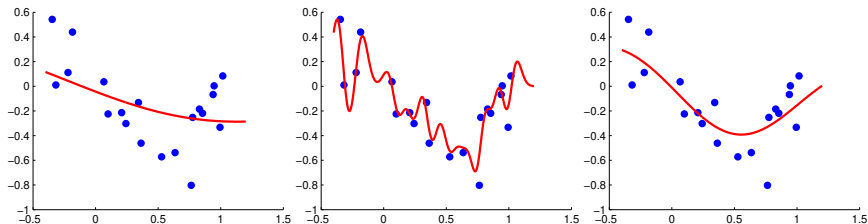
$$\phi(x) = \begin{bmatrix} x_1 & x_2 & x_1 x_2 \end{bmatrix} \in \mathbb{R}^3$$

Kernels and feature space (2): document classification



Kernels let us compare objects on the basis of features

Kernels and feature space (3): smoothing



Kernel methods can control smoothness and avoid overfitting/underfitting.

Outline: reproducing kernel Hilbert space

We will describe in order:

- 1 Hilbert space (very simple)
- 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 $f = 0$.

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.

Hilbert space

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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 a Hilbert space \mathcal{H} and a **feature** 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?)

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: sums, transformations

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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,

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

New kernels from old: products

“Natural” feature space for colored shapes:

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

New kernels from old: products

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Kernel is:

$$k(x, x') = \sum_{i \in \{\bullet, \bullet\}} \sum_{j \in \{\square, \triangle\}} \Phi_{ij}(x)\Phi_{ij}(x')$$

New kernels from old: products

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Kernel is:

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

New kernels from old: products

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New kernels from old: products

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New kernels from old: products

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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.

$$k(x, y) = [\sin(x) \quad x^3 \quad \log x]^\top [\sin(y) \quad y^3 \quad \log y]$$

where $\phi(x) = [\sin(x) \quad x^3 \quad \log x]$

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

Taylor series kernels

Definition (Taylor series kernel)

For $r \in (0, \infty]$, with $a_n \geq 0$ for all $n \geq 0$

$$f(z) = \sum_{n=0}^{\infty} a_n z^n \quad |z| < r, z \in \mathbb{R},$$

Define \mathcal{X} to be the \sqrt{r} -ball in \mathbb{R}^d , so $\|x\| < \sqrt{r}$,

$$k(x, x') = f(\langle x, x' \rangle) = \sum_{n=0}^{\infty} a_n \langle x, x' \rangle^n.$$

Exponential kernel:

$$k(x, x') := \exp(\langle x, x' \rangle).$$

Taylor series kernel (proof)

Proof: Non-negative weighted sums of kernels are kernels, and products of kernels are kernels, so the following is a kernel if it converges:

$$k(x, x') = \sum_{n=0}^{\infty} a_n (\langle x, x' \rangle)^n$$

By Cauchy-Schwarz,

$$|\langle x, x' \rangle| \leq \|x\| \|x'\| < r,$$

so the sum converges.

Exponentiated quadratic kernel

Exponentiated quadratic kernel: This kernel on \mathbb{R}^d is defined as

$$k(x, x') := \exp\left(-\gamma^{-2} \|x - x'\|^2\right).$$

Proof: an exercise! Use product rule, mapping rule, exponential kernel.

Infinite sequences

Definition

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

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

Definition

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

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

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Infinite sequences (proof)

Why square summable? By Cauchy-Schwarz,

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

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

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

Proof by positive definiteness:

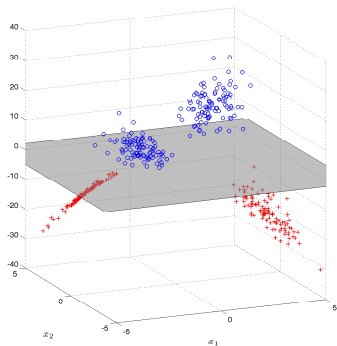
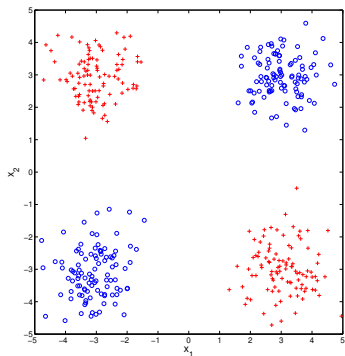
Consider two kernels $k_1(x, x')$ and $k_2(x, x')$. Then

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

The reproducing kernel Hilbert space

First example: finite space, polynomial features

Reminder: XOR example:



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} .

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 ,

$$f(\cdot) = [f_1 \quad f_2 \quad f_3]^\top.$$

$f(\cdot)$ or f 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**).

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

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} .

Example: finite space, polynomial features

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Functions of infinitely many features

Functions are linear combinations of features:

$$f(x) = \langle f, \phi(x) \rangle_{\mathcal{H}} = \sum_{\ell=1}^{\infty} f_{\ell} \phi_{\ell}(x) = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \end{bmatrix}^{\top} \begin{bmatrix} \phi_1(x) \\ \phi_2(x) \\ \phi_3(x) \\ \vdots \end{bmatrix}$$

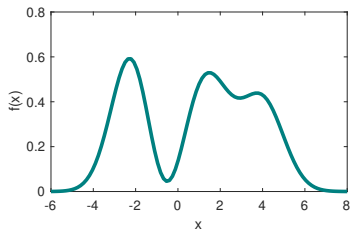
$$k(x, y) = \sum_{\ell=1}^{\infty} \phi_{\ell}(x) \phi_{\ell}(y')$$

$$f(x) = \sum_{\ell=1}^{\infty} f_{\ell} \phi_{\ell}(x) \quad \sum_{\ell=1}^{\infty} f_{\ell}^2 < \infty.$$

Expressing the functions with kernels

Function with **exponentiated quadratic kernel**:

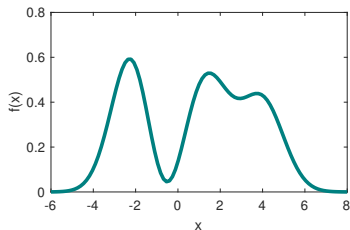
$$\begin{aligned} f(x) &= \sum_{\ell=1}^{\infty} f_{\ell} \phi_{\ell}(x) \\ &= \sum_{\ell=1}^{\infty} \underbrace{\left(\sum_{i=1}^m \alpha_i \phi_{\ell}(x_i) \right)}_{f_{\ell}} \phi_{\ell}(x) \\ &= \left\langle \underbrace{\sum_{i=1}^m \alpha_i \phi(x_i)}_f, \phi(x) \right\rangle_{\mathcal{H}} \\ &=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



Expressing the functions with kernels

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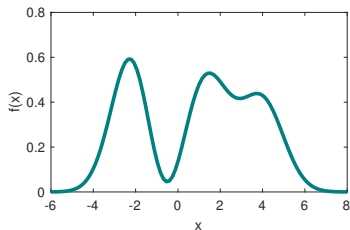


$$f_{\ell} := \sum_{i=1}^m \alpha_i \phi_{\ell}(x_i)$$

Expressing the functions with kernels

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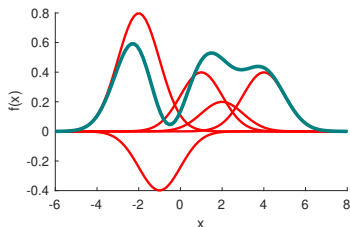


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$$f := \sum_{i=1}^m \alpha_i \phi(x_i)$$

Function of **infinitely many features** expressed using $\{(\alpha_i, x_i)\}_{i=1}^m$.

The feature map is *also* a function

On previous page,

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

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!

We can write without ambiguity

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

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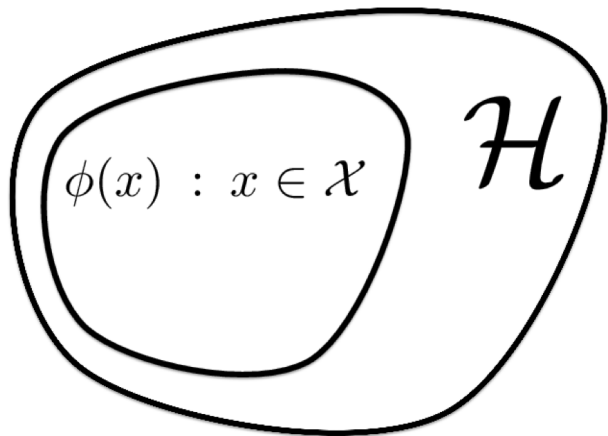
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Features vs functions

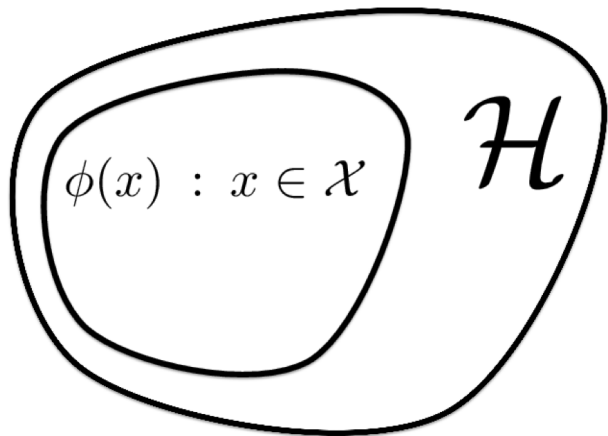
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E.g. $f(\cdot) = [1 \ 1 \ -1] \in \mathcal{H}$ cannot be obtained by $\phi(x) = [x_1 \ x_2 \ (x_1 x_2)]$.

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The reproducing property

This example illustrates the two defining features of an RKHS:

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

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

...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

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

Understanding smoothness in the RKHS

Infinite feature space via fourier series

Function on the interval $[-\pi, \pi]$ with periodic boundary.

Fourier series:

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

using the orthonormal basis on $[-\pi, \pi]$,

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \exp(i l x) \overline{\exp(i m x)} dx = \begin{cases} 1 & l = m, \\ 0 & l \neq m. \end{cases}$$

Example: “top hat” function,

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

$$\hat{f}_l := \frac{\sin(lT)}{l\pi} \quad f(x) = \sum_{l=0}^{\infty} 2\hat{f}_l \cos(lx).$$

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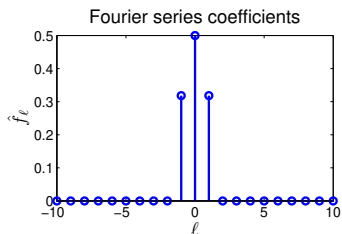
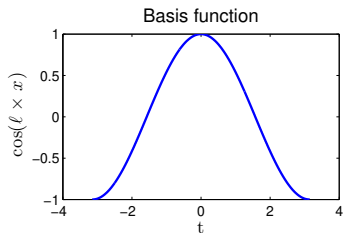
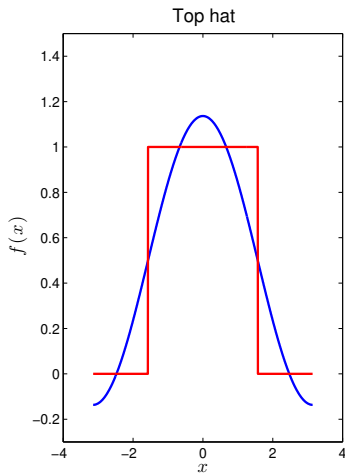
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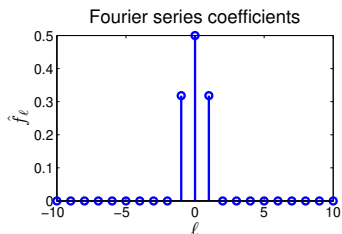
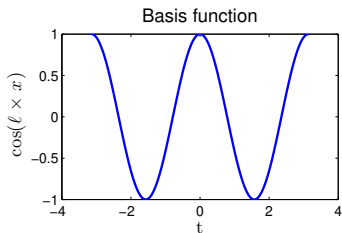
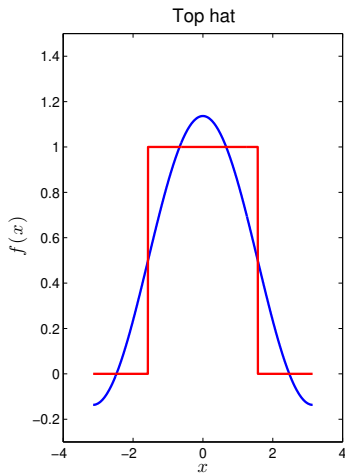
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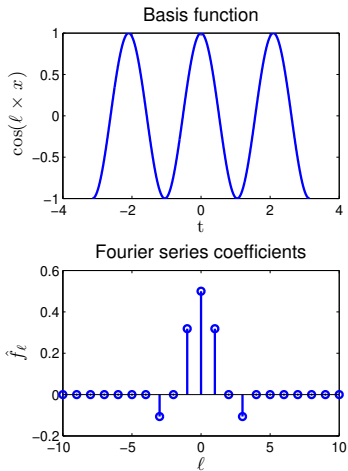
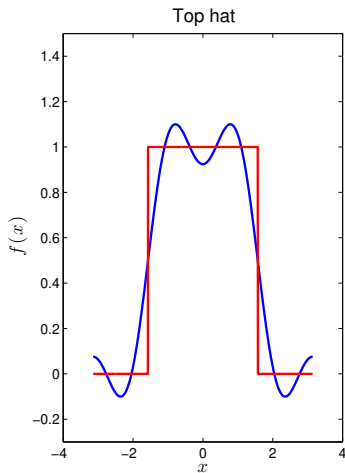
Fourier series for top hat function



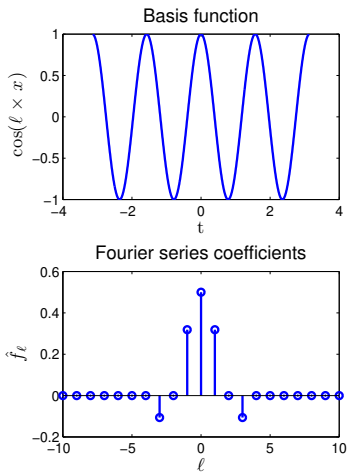
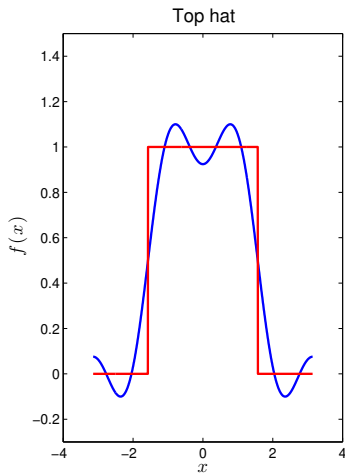
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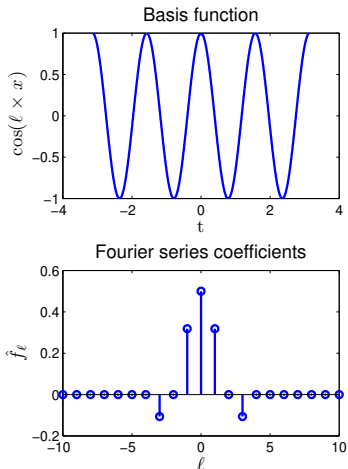
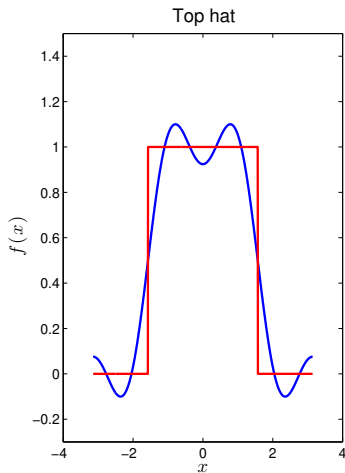
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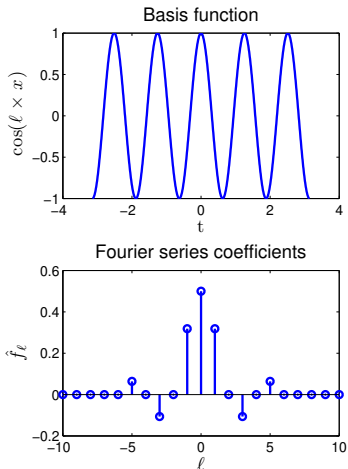
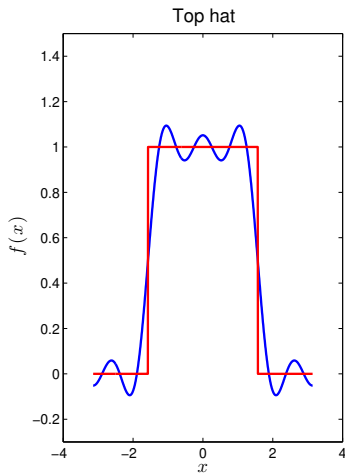
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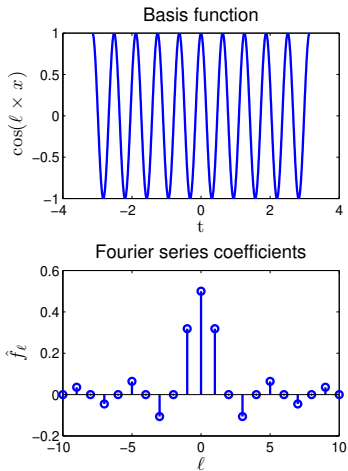
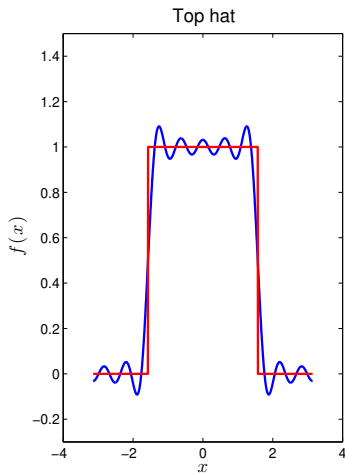
Fourier series for top hat function



Fourier series for top hat function



Fourier series for top hat function



Fourier series for kernel function

Assume kernel translation invariant,

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

Fourier series representation of k

$$\begin{aligned} k(x - y) &= \sum_{\ell=-\infty}^{\infty} \hat{k}_{\ell} \exp(i\ell(x - y)) \\ &= \sum_{\ell=-\infty}^{\infty} \underbrace{\left[\sqrt{\hat{k}_{\ell}} \exp(i\ell x) \right]}_{\phi_{\ell}(x)} \underbrace{\left[\sqrt{\hat{k}_{\ell}} \exp(-i\ell y) \right]}_{\overline{\phi_{\ell}(y)}}. \end{aligned}$$

Example: Jacobi theta kernel:

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

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

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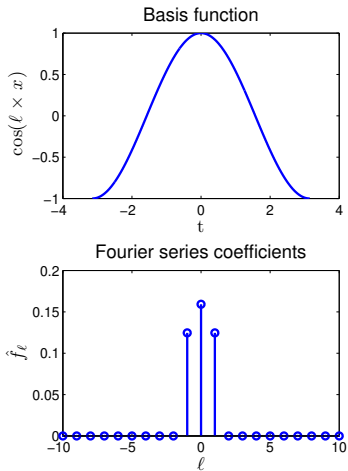
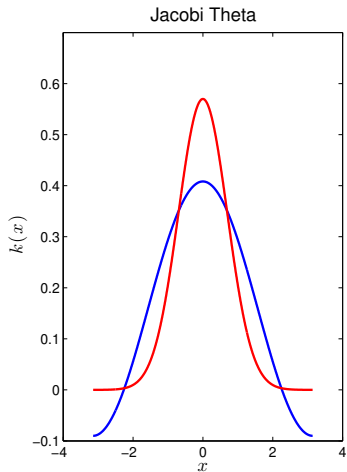
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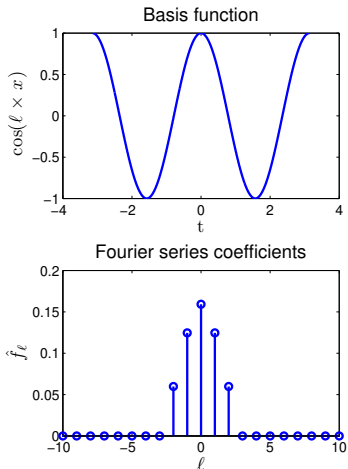
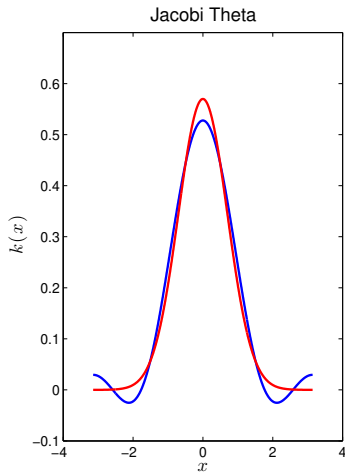
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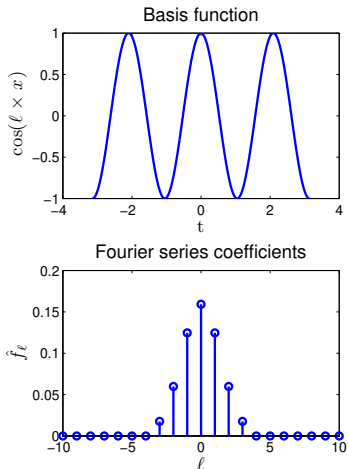
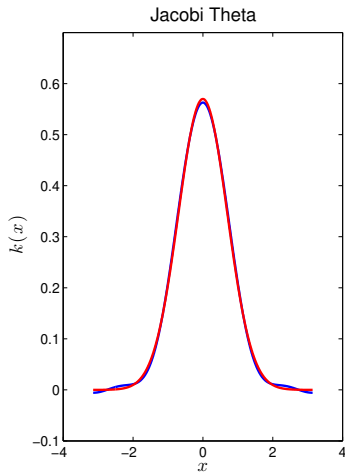
Fourier series for Gaussian-spectrum kernel



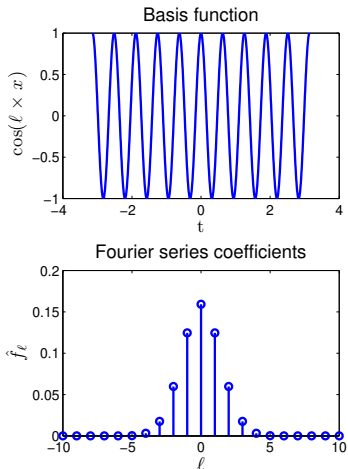
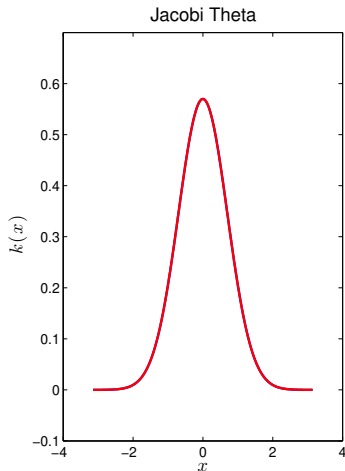
Fourier series for Gaussian-spectrum kernel



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Fourier series for Gaussian-spectrum kernel



RKHS via fourier series

Recall **standard dot product** in L_2 :

$$\begin{aligned}\langle f, g \rangle_{L_2} &= \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) \overline{g(x)} dx \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \left[\sum_{\ell=-\infty}^{\infty} \hat{f}_{\ell} \exp(i\ell x) \right] \left[\sum_{m=-\infty}^{\infty} \overline{\hat{g}_m \exp(imx)} \right] dx \\ &= \sum_{\ell=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \hat{f}_{\ell} \overline{\hat{g}_m} \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp(i\ell x) \exp(-imx) \\ &= \sum_{\ell=-\infty}^{\infty} \hat{f}_{\ell} \overline{\hat{g}_{\ell}}.\end{aligned}$$

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Define the **dot product** in \mathcal{H} to have a **roughness penalty**,

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

Roughness penalty explained

The **squared norm** of a function f in \mathcal{H} **enforces smoothness**:

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

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

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

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

Warning: need stronger conditions on kernel than L_2 convergence: **Mercer's theorem**.

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Feature map and reproducing property

Reproducing property: define a function

$$g(x) := k(x - z) = \sum_{\ell=-\infty}^{\infty} \exp(i\ell x) \underbrace{\hat{k}_{\ell} \exp(-i\ell z)}_{\hat{g}_{\ell}}$$

Then for a function $f(\cdot) \in \mathcal{H}$,

$$\langle f(\cdot), k(\cdot, z) \rangle_{\mathcal{H}} = \langle f(\cdot), g(\cdot) \rangle_{\mathcal{H}}$$

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Feature map and reproducing property

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Recall kernel definition:

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

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Second infinite feature space (on \mathbb{R})

Define a probability measure on $\mathcal{X} := \mathbb{R}$. We'll use the Gaussian density,

$$p(x) = \frac{1}{\sqrt{2\pi}} \exp(-x^2)$$

Define the eigenexpansion of $k(x, x')$ wrt this measure:

$$\lambda_\ell e_\ell(x) = \int k(x, x') e_\ell(x') p(x') dx' \quad \int e_i(x) e_j(x) p(x) dx = \begin{cases} 1 & i = j \\ 0 & i \neq j. \end{cases}$$

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$$k(x, x') = \sum_{\ell=1}^{\infty} \lambda_\ell e_\ell(x) e_\ell(x'),$$

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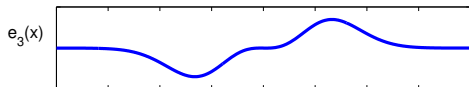
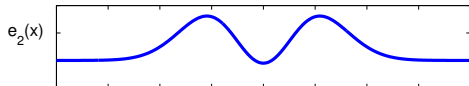
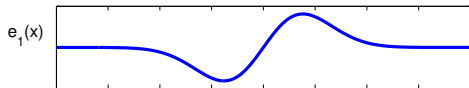
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$$\lambda_{\ell} \propto b^{\ell} \quad b < 1$$

$$e_{\ell}(x) \propto \exp(-(c - a)x^2) H_{\ell}(x\sqrt{2c}),$$

a, b, c are functions of σ ,
and H_{ℓ} is ℓ th order Hermite polynomial.

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Reminder: for two functions f, g in $L_2(p)$,

$$f(x) = \sum_{\ell=1}^{\infty} \hat{f}_{\ell} e_{\ell}(x) \quad g(x) = \sum_{m=1}^{\infty} \hat{g}_m e_m(x),$$

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$$\langle f, g \rangle_{\mathcal{H}} = \sum_{\ell=1}^{\infty} \frac{\hat{f}_{\ell} \hat{g}_{\ell}}{\lambda_{\ell}} \quad \|f\|_{\mathcal{H}}^2 = \sum_{\ell=1}^{\infty} \frac{\hat{f}_{\ell}^2}{\lambda_{\ell}}.$$

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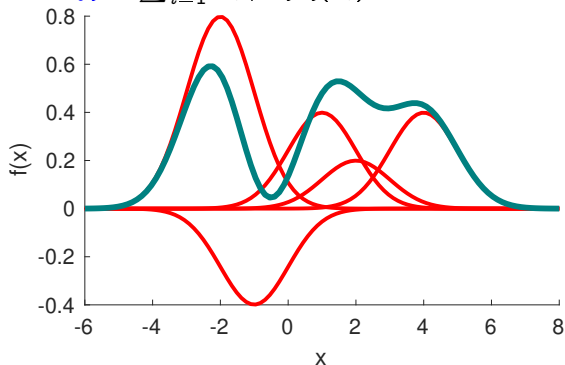
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By inspection: $f_{\ell} = \hat{f}_{\ell} / \sqrt{\lambda_{\ell}}$ $\phi_{\ell}(z) = \sqrt{\lambda_{\ell}} e_{\ell}(z)$.

RKHS function, exponentiated quadratic kernel:

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

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



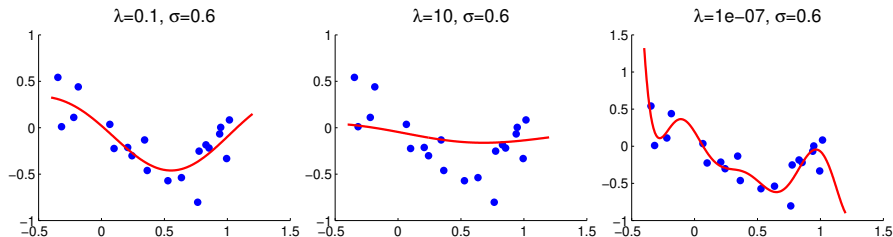
NOTE that this enforces smoothing: λ_{ℓ} decay as e_{ℓ} become rougher, f_{ℓ} decay since $\|f\|_{\mathcal{H}}^2 = \sum_{\ell} f_{\ell}^2 < \infty$.

Main message

Small RKHS norm results in smooth functions.

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

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



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 unique.

Main message

