

Learning with Positive Definite Kernels: Theory, Algorithms and Applications

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Course Outline

- ▶ **Introduction: Positive definite kernels and RKHS** (Lecture 1)
 - ▶ Feature space vs. Function space
 - ▶ Kernel trick
 - ▶ Applications: Ridge regression, Principal component analysis
- ▶ **Generalization of kernel trick to probabilities** (Lecture 2)
 - ▶ Hilbert space embedding of probabilities
 - ▶ Mean element and covariance operator
 - ▶ Applications: Two-sample testing, GAN
- ▶ **Approximate Kernel Methods** (Lecture 3)
 - ▶ Computational vs. Statistical trade-off
 - ▶ Applications: Ridge regression, Principal component analysis

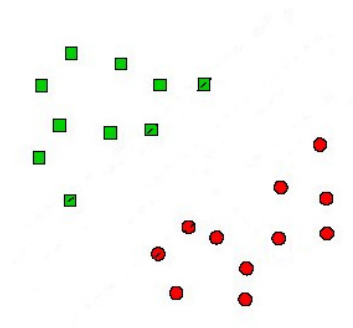
Lecture-1 Outline

- ▶ **Motivating Examples**
 - ▶ Nonlinear classification
 - ▶ Statistical learning
- ▶ **Feature space vs. Function space**
 - ▶ Kernels and properties
 - ▶ RKHS and properties
- ▶ **Applications: Ridge regression, Principal component analysis**
 - ▶ Kernel trick
 - ▶ Representer theorem

Motivating Example: Binary Classification

- ▶ Given: $D := \{(x_j, y_j)\}_{j=1}^n$, $x_j \in \mathcal{X}$, $y_j \in \{-1, +1\}$
- ▶ Goal: Learn a function $f : \mathcal{X} \rightarrow \mathbb{R}$ such that

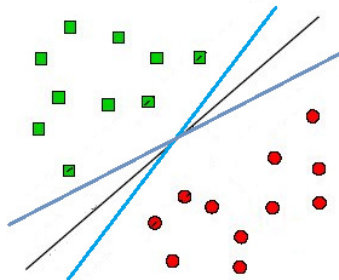
$$y_j = \text{sign}(f(x_j)), \forall j = 1, \dots, n.$$



Linear Classifiers

- ▶ Linear classifier: $f_{w,b}(x) = \langle w, x \rangle_2 + b$, $w, x \in \mathbb{R}^d$, $b \in \mathbb{R}$
- ▶ Find $w \in \mathbb{R}^d$ and $b \in \mathbb{R}$ such that

$$y_j (\langle w, x_j \rangle_2 + b) \geq 0, \forall j = 1, \dots, n.$$



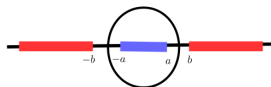
- ▶ Fisher discriminant analysis, Support vector machine, Perceptron, ...

Nonlinear Classification: 1



- ▶ There is no linear classifier that separates red and blue regions.

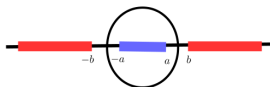
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- ▶ There is no linear classifier that separates red and blue regions.
- ▶ However, the following function perfectly separates red and blue regions

$$f(x) = x^2 - r = \left\langle \underbrace{(1, -r)}_w, \underbrace{(x^2, 1)}_{\Phi(x)} \right\rangle_2, \quad a < r < b.$$

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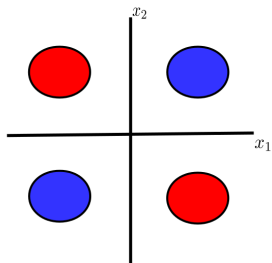


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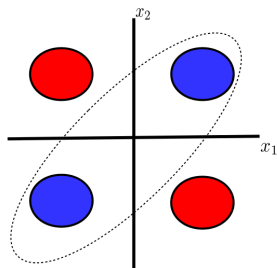
- ▶ By mapping $x \in \mathbb{R}$ to $\Phi(x) = (x^2, 1) \in \mathbb{R}^2$, the nonlinear classification problem is turned into a linear problem.
- ▶ We call Φ as the feature map (starting point of kernel trick)

Nonlinear Classification: 2



- ▶ There is no linear classifier that separates red and blue regions.

Nonlinear Classification: 2



- ▶ There is no linear classifier that separates red and blue regions.
- ▶ A conic section, however, perfectly separates them

$$\begin{aligned} f(x) &= ax_1^2 + bx_1x_2 + cx_2^2 + dx_1 + ex_2 + g \\ &= \left\langle \underbrace{(a, b, c, d, e, g)}_w, \underbrace{(x_1^2, x_1x_2, x_2^2, x_1, x_2, 1)}_{\Phi(x)} \right\rangle_2. \end{aligned}$$

- ▶ $\Phi(x) \in \mathbb{R}^6$.

Motivating Example: Statistical Learning

- ▶ **Given:** A set $D := \{(x_1, y_1), \dots, (x_n, y_n)\}$ of input/output pairs drawn **independently** from an **unknown** probability distribution \mathbf{P} on $X \times Y$.
- ▶ **Goal:** “**Learn**” a function $f : X \rightarrow Y$ such that $f(x)$ is a good approximation of the possible response y for an arbitrary x .
- ▶ We need a means to **assess the quality of an estimated response** $f(x)$ when the true input and output pair is (x, y) .
- ▶ **Loss function:** $L : Y \times Y \rightarrow [0, \infty)$
 - ▶ Squared-loss: $L(y, f(x)) = (y - f(x))^2$
 - ▶ Hinge-loss: $L(y, f(x)) = \max(0, 1 - yf(x))$
- ▶ One common quality measure is the **average loss** or **expected loss** of f , called the **risk functional** i.e.,

$$\mathcal{R}_{L, \mathbf{P}}(f) := \int_{X \times Y} L(y, f(x)) d\mathbf{P}(x, y).$$

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Bayes Risk and Bayes Function

- ▶ Idea: Choose f that has the **smallest risk**.

$$f^* := \arg \inf_{f: X \rightarrow \mathbb{R}} \mathcal{R}_{L, \mathbf{P}}(f),$$

where the infimum is taken over the set of **all** measurable functions.

- ▶ f^* is called the **Bayes function** and $\mathcal{R}_{L, \mathbf{P}}(f^*)$ is called the **Bayes risk**.
- ▶ If \mathbf{P} is known, finding f^* is often a relatively easy task and there is nothing to learn.
 - ▶ **Example:** $L(y, f(x)) = (y - f(x))^2$ and $L(y, f(x)) = |y - f(x)|$
 - ▶ **Exercise:** What is f^* for the above losses?

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Universal Consistency

- ▶ But \mathbf{P} is **unknown**.
- ▶ However “partially known” from the **training set**,
 $D := \{(x_1, y_1), \dots, (x_n, y_n)\}$.
- ▶ Given D , the goal is to construct $f_D : X \rightarrow \mathbb{R}$ such that

$$\mathcal{R}_{L, \mathbf{P}}(f_D) \approx \mathcal{R}_{L, \mathbf{P}}(f^*).$$

- ▶ **Universally consistent learning algorithm**: for **all** \mathbf{P} on $X \times Y$, we have

$$\mathcal{R}_{L, \mathbf{P}}(f_D) \rightarrow \mathcal{R}_{L, \mathbf{P}}(f^*), \quad n \rightarrow \infty$$

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Empirical Risk Minimization

- ▶ Since \mathbf{P} is unknown but is known through D , it is tempting to **replace** $\mathcal{R}_{L,\mathbf{P}}(f)$ by

$$\mathcal{R}_{L,D}(f) := \frac{1}{n} \sum_{i=1}^n L(y_i, f(x_i)),$$

called the **empirical risk** and find f_D by

$$f_D := \arg \min_{f: X \rightarrow \mathbb{R}} \mathcal{R}_{L,D}(f)$$

- ▶ Is it a good idea?
- ▶ **No!** Choose f_D such that $f_D(x) = y_i$, $x = x_i$, $\forall i$ and $f_D(x) = 0$, *otherwise*.
- ▶ $\mathcal{R}_{L,D}(f_D) = 0$ but can be very far from $\mathcal{R}_{L,\mathbf{P}}(f^*)$.

Overfitting!!

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Overfitting!!

Method of Sieves (Structural Risk Minimization)

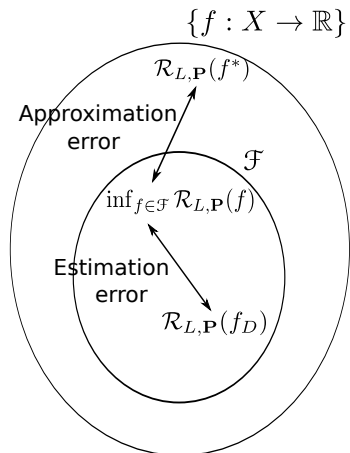
- ▶ **How to avoid overfitting:** Perform ERM on a small set \mathcal{F} of functions $f : X \rightarrow Y$ (**class of smooth functions**) where the size of \mathcal{F} grows appropriately with n .
- ▶ Do minimization over \mathcal{F} :

$$f_D := \arg \inf_{f \in \mathcal{F}} \mathcal{R}_{L,D}(f)$$

- ▶ Total error: Define $\mathcal{R}_{L,\mathbf{P},\mathcal{F}}^* := \inf_{f \in \mathcal{F}} \mathcal{R}_{L,\mathbf{P}}(f)$

$$\begin{aligned} \mathcal{R}_{L,\mathbf{P}}(f_D) - \mathcal{R}_{L,\mathbf{P}}^* &= \overbrace{\mathcal{R}_{L,\mathbf{P}}(f_D) - \mathcal{R}_{L,\mathbf{P},\mathcal{F}}^*}^{\text{Estimation error}} \\ &\quad + \overbrace{\mathcal{R}_{L,\mathbf{P},\mathcal{F}}^* - \mathcal{R}_{L,\mathbf{P}}^*}^{\text{Approximation error}} \end{aligned}$$

Approximation and Estimation Errors



How to choose \mathcal{F} ?

$$f_D = \arg \inf_{f \in \mathcal{F}} \mathcal{R}_{L,D}(f) = \arg \inf_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n L(y_i, \underbrace{f(x_i)}_{\delta_{x_i}(f)})$$

- ▶ An evaluation functional is a linear functional δ_x that **evaluates** each function in the space at the point x , i.e.,

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

- ▶ **Bounded evaluation functional:** An evaluation functional is bounded if there exists a M such that

$$|\delta_x(f)| = |f(x)| \leq M_x \|f\|_{\mathcal{F}}, \quad \forall x \in \mathcal{X}, f \in \mathcal{F}$$

where \mathcal{F} is a normed vector space (**continuity of δ_x**).

- ▶ Evaluation functionals **are not** always bounded.
- ▶ **Example:** $L^2[a, b]$
 - ▶ $\|f\|_2$ remains the same if f is changed at a countable set of points.

Choice of \mathcal{F}

- ▶ Various choices for \mathcal{F} (with evaluation functional bounded):
 - ▶ Lipschitz functions
 - ▶ Bounded Lipschitz functions
 - ▶ Bounded continuous functions
- ▶ If \mathcal{F} is a Hilbert space of functions with bounded evaluation functionals for all $x \in \mathcal{X}$, computationally efficient estimators can be obtained.

Reproducing Kernel Hilbert Space

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Reproducing Kernel Hilbert Space

Summary

Points of view:

- ▶ Feature map, Φ : trick to achieve non-linear methods from linear ones
- ▶ Function space, \mathcal{F} : statistical generalization and computational efficiency

History

- ▶ **Mathematics (Functional analysis):** Introduced in 1907 by Stanisław Zaremba for studying boundary value problems; developed by Mercer, Szegő, Bergman, Bochner, Moore, Aronszajn; reached maturity by late 1950's.
- ▶ **Statistics:** Started by Emmanuel Parzen (early 1960's) and pursued by Wahba (between 1970 and 1990).
- ▶ **Pattern recognition/Machine learning:** Started by Aizerman, Braverman and Rozonoer (1964) but burst of activity following the work of Boser, Guyon and Vapnik (1992).

Other areas: Signal processing, control, probability theory, stochastic processes, numerical analysis

Kernels

(Feature space view point)

Hilbert Space

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

- ▶ **Linear in the first argument:** for any $f_1, f_2, g \in \mathcal{H}$ and $\alpha, \beta \in \mathbb{R}$

$$\langle \alpha f_1 + \beta f_2, g \rangle_{\mathcal{H}} = \alpha \langle f_1, g \rangle_{\mathcal{H}} + \beta \langle f_2, g \rangle_{\mathcal{H}};$$

- ▶ **Symmetric:** for any $f, g \in \mathcal{H}$,

$$\langle f, g \rangle_{\mathcal{H}} = \langle g, f \rangle_{\mathcal{H}};$$

- ▶ **Positive definiteness:** for any $f \in \mathcal{H}$,

$$\langle f, f \rangle_{\mathcal{H}} \geq 0 \quad \text{and} \quad \langle f, f \rangle_{\mathcal{H}} = 0 \Leftrightarrow f = 0.$$

Define $\| \cdot \|_{\mathcal{H}} := \langle \cdot, \cdot \rangle_{\mathcal{H}}$ as the norm on \mathcal{H} induced by the inner product.

A complete (by adding the limits of all Cauchy sequences w.r.t. $\| \cdot \|_{\mathcal{H}}$) inner product space is defined as a **Hilbert space**.

Measure of similarity

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Kernel

(Steinwart and Christmann, 2008)

Throughout, we assume that \mathcal{X} is a non-empty set (input space)

Kernel: A function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is called a kernel if there exists a Hilbert space \mathcal{H} and a map $\Phi : \mathcal{X} \rightarrow \mathcal{H}$ such that

$$k(x, x') := \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}, \quad \forall x, x' \in \mathcal{X}.$$

Φ : **Feature map** and \mathcal{H} : **Feature space**

Non-uniqueness of Φ and \mathcal{H} : Suppose $k(x, x') = xx'$, $x, x' \in \mathbb{R}$. Then

$$\Phi_1(x) = x \quad \text{and} \quad \Phi_2(x) = \frac{1}{2}(x, x)$$

are feature maps with corresponding feature spaces being \mathbb{R} and \mathbb{R}^2 .

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Properties

- ▶ For any $\alpha > 0$, αk is a kernel.

$$\alpha k(x, x') = \alpha \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}} = \langle \sqrt{\alpha} \Phi(x), \sqrt{\alpha} \Phi(x') \rangle_{\mathcal{H}}.$$

- ▶ Conic sum of kernels is a kernel: If $(k_i)_{i=1}^m$ is a collection of kernels, then for any $(\alpha_i)_{i=1}^m \subset \mathbb{R}^+$, $\sum_{i=1}^m \alpha_i k_i$ is a kernel.

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for all $x, x' \in \mathcal{X}$ where

$$\tilde{\Phi}(x) = (\sqrt{\alpha_1} \Phi_1(x), \dots, \sqrt{\alpha_m} \Phi_m(x)) \quad \text{and} \quad \tilde{\mathcal{H}} = \underbrace{\mathcal{H}_1 \oplus \dots \oplus \mathcal{H}_m}_{\text{direct sum}}.$$

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$$(\mathbb{R} \oplus \mathbb{R} = \mathbb{R}^2)$$

Properties

▶ **Difference of kernels is NOT a kernel:**

▶ Suppose $\exists x \in \mathcal{X}$ such that $k_1(x, x) - k_2(x, x) < 0$.

▶ If $k_1 - k_2$ is a kernel, then $\exists \Phi$ and \mathcal{H} such that for all $x, x' \in \mathcal{X}$,

$$k_1(x, x') - k_2(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}.$$

▶ Choose $x = x'$.

▶ **Product of kernels is a kernel:** If k_1 and k_2 are kernels, then $k_1 \cdot k_2$ is a kernel.

$$\begin{aligned} k((x_1, x_2), (x'_1, x'_2)) &= k_1(x_1, x'_1) \cdot k_2(x_2, x'_2) \\ &= \langle \Phi_1(x_1), \Phi_1(x'_1) \rangle_{\mathcal{H}_1} \cdot \langle \Phi_2(x_2), \Phi_2(x'_2) \rangle_{\mathcal{H}_2} \\ &= \langle \Phi_1(x_1) \otimes \Phi_2(x_2), \Phi_1(x'_1) \otimes \Phi_2(x'_2) \rangle_{\mathcal{H}_1 \otimes \mathcal{H}_2} \end{aligned}$$

where \otimes denotes the tensor product.

Properties

▶ Difference of kernels is NOT a kernel:

▶ Suppose $\exists x \in \mathcal{X}$ such that $k_1(x, x) - k_2(x, x) < 0$.

▶ If $k_1 - k_2$ is a kernel, then $\exists \Phi$ and \mathcal{H} such that for all $x, x' \in \mathcal{X}$,

$$k_1(x, x') - k_2(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}.$$

▶ Choose $x = x'$.

▶ Product of kernels is a kernel: If k_1 and k_2 are kernels, then $k_1 \cdot k_2$ is a kernel.

$$\begin{aligned} k((x_1, x_2), (x'_1, x'_2)) &= k_1(x_1, x'_1) \cdot k_2(x_2, x'_2) \\ &= \langle \Phi_1(x_1), \Phi_1(x'_1) \rangle_{\mathcal{H}_1} \cdot \langle \Phi_2(x_2), \Phi_2(x'_2) \rangle_{\mathcal{H}_2} \\ &= \langle \Phi_1(x_1) \otimes \Phi_2(x_2), \Phi_1(x'_1) \otimes \Phi_2(x'_2) \rangle_{\mathcal{H}_1 \otimes \mathcal{H}_2} \end{aligned}$$

where \otimes denotes the tensor product.

Properties

- ▶ Suppose k_1 is defined on $\{0, 1\}$ and k_2 is defined on $\{A, B, C\}$. Then clearly $k_1 \cdot k_2$ is defined on $\{0, 1\} \times \{A, B, C\}$.
- ▶ Suppose for simplicity, we assume $\mathcal{H}_1 = \mathbb{R}^2$ and $\mathcal{H}_2 = \mathbb{R}^5$. Then

$$\begin{aligned}k_1(x_1, x'_1) \cdot k_2(x_2, x'_2) &= \langle \Phi_1(x_1), \Phi_1(x'_1) \rangle_{\mathbb{R}^2} \cdot \langle \Phi_2(x_2), \Phi_2(x'_2) \rangle_{\mathbb{R}^5} \\ &= \Phi_1^\top(x'_1) \Phi_1(x_1) \Phi_2^\top(x_2) \Phi_2(x'_2) \\ &= \text{Tr} \left(\underbrace{\Phi_2(x'_2) \Phi_1^\top(x'_1)}_{\mathbb{R}^2 \rightarrow \mathbb{R}^5} \underbrace{\Phi_1(x_1) \Phi_2^\top(x_2)}_{\mathbb{R}^5 \rightarrow \mathbb{R}^2} \right) \\ &= \langle \Phi_1(x_1) \Phi_2^\top(x_2), \Phi_1(x'_1) \Phi_2^\top(x'_2) \rangle_{\mathbb{R}^2 \otimes \mathbb{R}^5} \\ &=: \langle \Phi_1(x_1) \otimes \Phi_2(x_2), \Phi_1(x'_1) \otimes \Phi_2(x'_2) \rangle_{\mathbb{R}^2 \otimes \mathbb{R}^5}\end{aligned}$$

where $\mathbb{R}^2 \otimes \mathbb{R}^5$ is the space of 2×5 matrices.

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Properties

- ▶ For any arbitrary function $f : \mathcal{X} \rightarrow \mathbb{R}$,

$$\tilde{k}(x, x') = f(x)k(x, x')f(x') \quad (1)$$

is a **kernel**.

$$\begin{aligned} \tilde{k}(x, x') &= f(x)k(x, x')f(x') = f(x)\langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}} f(x') \\ &= \underbrace{\langle f(x)\Phi(x), f(x')\Phi(x') \rangle_{\mathcal{H}}}_{\Phi_f(x) \quad \Phi_f(x')} \end{aligned}$$

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- ▶ Infinite dimensional feature map:

$$k(x, x') = \sum_{i \in I} \phi_i(x) \phi_i(x') \quad \text{is a kernel}$$

if $\|(\phi_i(x))_i\|_{\ell_2(I)}^2 := \sum_{i \in I} \phi_i^2(x) < \infty$ for all $x \in \mathcal{X}$.

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$$k(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$$

where $\Phi(x) = (\phi_i(x))_{i \in I}$ and $\mathcal{H} = \ell_2(I)$, which is the space of square summable sequences on I .

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Examples

- ▶ **Polynomial kernel:** $k(x, x') = (c + \langle x, x' \rangle_2)^m$, $x, x' \in \mathbb{R}^d$ for $c \geq 0$ and $m \in \mathbb{N}$. Use binomial theorem to expand, apply sum and product rules.
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- ▶ **Kernels are symmetric and positive definite: EASY**

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Positive Definiteness: Translation Invariant Kernels

Let $\mathcal{X} = \mathbb{R}^d$. A kernel $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^d$ is said to be **translation invariant** if

$$k(x, y) = \psi(x - y), \quad x, y \in \mathbb{R}^d,$$

where ψ is a **positive definite function** on \mathbb{R}^d .

- ▶ **Bochner's theorem** provides a complete characterization for the positive definiteness of ψ .
- ▶ A continuous function $\psi : \mathbb{R}^d \rightarrow \mathbb{R}$ is positive definite if and only if ψ is the Fourier transform of a **finite non-negative Borel measure** Λ , i.e.,

$$\psi(x) = \underbrace{\int_{\mathbb{R}^d} e^{\sqrt{-1}\langle x, \omega \rangle} d\Lambda(\omega)}_{\text{Characteristic function of } \Lambda}.$$

Given a continuous integrable function ψ , i.e., $\int_{\mathbb{R}^d} |\psi(x)| dx < \infty$, compute

$$\hat{\psi}(\omega) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{-\sqrt{-1}\langle \omega, x \rangle} \psi(x) dx.$$

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Exercise

- ▶ Show that

$$\psi(x) = (1 - |x|)1_{[-1,1]}(x), x \in \mathbb{R}$$

is positive definite.

- ▶ Show that

$$\psi(x) = \frac{1}{2}(2 - |x|)^2 1_{\{(2-|x|) \in [0,1]\}} + \left(1 - \frac{x^2}{2}\right) 1_{[-1,1]}(x), x \in \mathbb{R}$$

is NOT positive definite.

So far...

Kernels \Leftrightarrow Symmetric and positive definite functions

Reproducing Kernel Hilbert Space

(Function space view point)

Reproducing Kernel Hilbert Space

- ▶ A Hilbert space \mathcal{H} of real-valued functions on \mathcal{X} is said to be a **reproducing kernel Hilbert space (RKHS)** with $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ as the **reproducing kernel**, if
 - ▶ $\forall x \in \mathcal{X}, k(\cdot, x) \in \mathcal{H}$;
 - ▶ $\forall x \in \mathcal{X}, \forall f \in \mathcal{H}, \langle f, k(\cdot, x) \rangle_{\mathcal{H}} = f(x)$.
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$$k(x, x') = \left\langle \underbrace{k(\cdot, x)}_{\Phi(x)}, \underbrace{k(\cdot, x')}_{\Phi(x')} \right\rangle_{\mathcal{H}}, \quad x, x' \in \mathcal{X}.$$

We refer to $\Phi(x) = k(\cdot, x)$ as the **canonical feature map**.

- ▶ Every r.k. is a **symmetric and positive definite function**.
- ▶ The evaluation functional is **bounded**:

$$\begin{aligned} |\delta_x(f)| &= |f(x)| = |\langle f, k(\cdot, x) \rangle_{\mathcal{H}}| \leq \|k(\cdot, x)\|_{\mathcal{H}} \|f\|_{\mathcal{H}} \\ &= \sqrt{k(x, x)} \|f\|_{\mathcal{H}}, \quad \forall x \in \mathcal{X}, f \in \mathcal{H}. \end{aligned}$$

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- ▶ Every Hilbert function space with a reproducing kernel is an RKHS.
- ▶ The converse is true: **Every RKHS has a unique reproducing kernel.**
- ▶ **(Moore-Aronszajn Theorem)**

If k is a positive definite kernel, then there exists a unique RKHS with k as the reproducing kernel.

(**Proof:** Define $H = \{f : f = \sum_{i=1}^n \alpha_i k(\cdot, x_i), \alpha_i \in \mathbb{R}, x_i \in \mathcal{X}\}$ endowed with the bilinear form

$$\langle f, g \rangle_H = \sum_{i,j=1}^n \alpha_i \beta_j k(x_i, x_j).$$

Verify that $\langle \cdot, \cdot \rangle_H$ is an inner product and $\langle f, k(\cdot, x) \rangle_H = f(x)$ for any $f \in H$. Complete H to obtain an RKHS.)

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- ▶ The converse is true: **Every RKHS has a unique reproducing kernel.**
- ▶ **(Moore-Aronszajn Theorem)**

If k is a positive definite kernel, then there exists a unique RKHS with k as the reproducing kernel.

(Proof: Define $H = \{f : f = \sum_{i=1}^n \alpha_i k(\cdot, x_i), \alpha_i \in \mathbb{R}, x_i \in \mathcal{X}\}$ endowed with the bilinear form

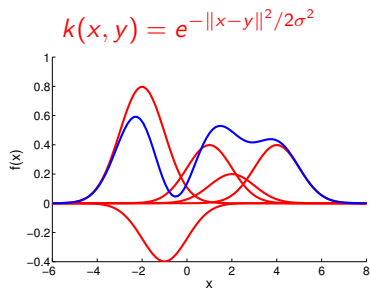
$$\langle f, g \rangle_H = \sum_{i,j=1}^n \alpha_i \beta_j k(x_i, x_j).$$

Verify that $\langle \cdot, \cdot \rangle_H$ is an inner product and $\langle f, k(\cdot, x) \rangle_H = f(x)$ for any $f \in H$.
Complete H to obtain an RKHS.)

Kernels \Leftrightarrow Positive definite & symmetric functions \Leftrightarrow RKHS

Functions in the RKHS

- ▶ $\mathcal{H} = \overline{\text{span}\{k(\cdot, x) : x \in \mathcal{X}\}}$ (linear span of kernel functions)
- ▶ Example: $f(x) = \sum_{i=1}^m \alpha_i k(x, x_i)$ for arbitrary $m \in \mathbb{N}$, $\{\alpha_i\} \subset \mathbb{R}$, $x \in \mathcal{X}$ and $\{x_i\} \subset \mathcal{X}$.



Picture credit: A. Gretton

Properties of RKHS

- ▶ k is **bounded** if and only if every $f \in \mathcal{H}$ is **bounded**.
- ▶ If $\int_{\mathcal{X}} \sqrt{k(x, x)} d\mu(x) < \infty$, then for every $f \in \mathcal{H}$,
 $\int_{\mathcal{X}} f(x) d\mu(x) < \infty$.
- ▶ Every $f \in \mathcal{H}$ is **continuous** if and only if $k(\cdot, x)$ is **continuous** for all $x \in \mathcal{X}$.
- ▶ Every $f \in \mathcal{H}$ is **m -times continuously differentiable** if k is **m -times continuously differentiable**.

k controls the properties of \mathcal{H}

Explicit Realization of RKHS

- ▶ $\mathcal{X} = \mathbb{R}^d$ and $k(x, y) = \psi(x - y)$ where ψ is a positive definite function.
- ▶ Assume ψ satisfies $\int_{\mathbb{R}^d} |\psi(x)| dx < \infty$. Denote $\hat{\psi}$ to be the Fourier transform of ψ .
- ▶ Define $L^2(\mathbb{R}^d) := \{f : \int_{\mathbb{R}^d} |f(x)|^2 dx < \infty\}$. Then

$$\mathcal{H} = \left\{ f \in L^2(\mathbb{R}^d) \mid \int_{\mathbb{R}^d} \frac{|\hat{f}(\omega)|^2}{\hat{\psi}(\omega)} d\omega < \infty \right\}$$

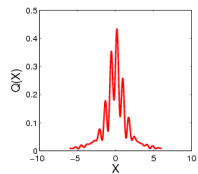
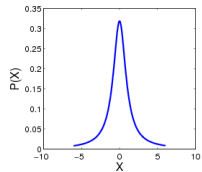
endowed with

$$\langle f, g \rangle_{\mathcal{H}} = (2\pi)^{-d/2} \int \frac{\hat{f}(\omega) \overline{\hat{g}(\omega)}}{\hat{\psi}(\omega)} d\omega$$

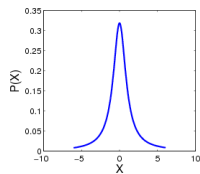
is an RKHS with k as the r.k.

(Wendland, 2005)

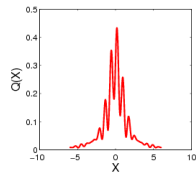
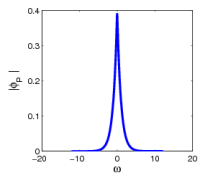
Fourier Transform



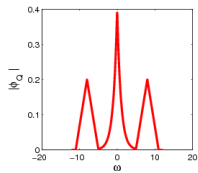
Fourier Transform



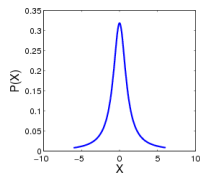
\mathcal{F}
↓



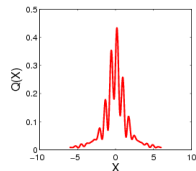
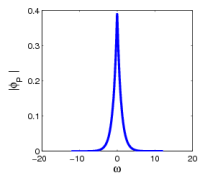
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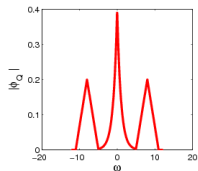
Fourier Transform



\mathcal{F}
→



\mathcal{F}
→



Smooth function



Fast rate of decay of
Fourier transform



Gaussian RKHS

- ▶ Gaussian kernel:

$$k(x, y) = \psi(x - y) = e^{-\|x-y\|_2^2/\gamma^2}, \quad x, y \in \mathbb{R}^d$$

- ▶ Fourier transform:

$$\hat{\psi}(\omega) = \left(\frac{\gamma^2}{2}\right)^{d/2} e^{-\frac{\gamma^2 \|\omega\|_2^2}{4}}, \quad \omega \in \mathbb{R}^d$$

- ▶

$$\mathcal{H}_\gamma(\mathbb{R}^d) := \left\{ f \in L^2(\mathbb{R}^d) : \underbrace{\int_{\mathbb{R}^d} |\hat{f}(\omega)|^2 e^{\frac{\gamma^2 \|\omega\|_2^2}{4}} d\omega}_{\|f\|_{\mathcal{H}_\gamma}^2} < \infty \right\}$$

Fast decay of $\hat{\psi} \Rightarrow$ Smooth \mathcal{H}

Gaussian RKHS

- ▶ Gaussian kernel:

$$k(x, y) = \psi(x - y) = e^{-\|x-y\|_2^2/\gamma^2}, \quad x, y \in \mathbb{R}^d$$

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- ▶ $\{f : \|f\|_{\mathcal{H}_\gamma} \leq \alpha\} \subset \{f : \|f\|_{\mathcal{H}_\gamma} \leq \beta\} \subset \mathcal{H}_\gamma$ for any $\alpha < \beta$.

More smoothness

Sobolev RKHS

- ▶ Laplacian kernel:

$$k(x, y) = \psi(x - y) = \sqrt{\frac{\pi}{2}} e^{-|x-y|}, \quad x, y \in \mathbb{R}$$

- ▶ Fourier transform:

$$\hat{\psi}(\omega) = \frac{1}{1 + |\omega|^2}, \quad \omega \in \mathbb{R}$$



$$\mathcal{H}_1^2(\mathbb{R}) := \left\{ f \in L^2(\mathbb{R}) : \underbrace{\int_{\mathbb{R}} |\hat{f}(\omega)|^2 (1 + |\omega|^2) d\omega}_{\|f\|_{\mathcal{H}_1^2}^2} < \infty \right\}$$

- ▶ $\{f : \|f\|_{\mathcal{H}_1^2} \leq \alpha\} \subset \{f : \|f\|_{\mathcal{H}_1^2} \leq \beta\} \subset \mathcal{H}_1^2$ for any $\alpha < \beta$.

Extension to \mathbb{R}^d : Matérn Kernel

Summing Up

- ▶ **Kernels:** Feature map Φ and feature space \mathcal{H}
- ▶ **Positive definiteness** and Bochner's theorem
- ▶ **RKHS:** Canonical feature map $\Phi(x) = k(\cdot, x)$
- ▶ **Kernels** \Leftrightarrow **Positive definite & symmetric functions** \Leftrightarrow **RKHS**
- ▶ Properties of k control the properties of the RKHS.
- ▶ Smoothness

Application: Ridge Regression

(Kernel Trick: Feature map point of view)

Ridge regression

- ▶ **Given:** $\{(x_i, y_i)\}_{i=1}^n$ where $x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$
- ▶ **Task:** Find a linear regressor $f = \langle w, \cdot \rangle_2$ s.t. $f(x_i) \approx y_i$,

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n (\langle w, x_i \rangle_2 - y_i)^2 + \lambda \|w\|_2^2 \quad (\lambda > 0)$$

- ▶ **Solution:** For $\mathbf{X} := (x_1, \dots, x_n) \in \mathbb{R}^{d \times n}$ and $\mathbf{y} := (y_1, \dots, y_n)^\top \in \mathbb{R}^n$,

$$w = \frac{1}{n} \underbrace{\left(\frac{1}{n} \mathbf{X} \mathbf{X}^\top + \lambda I_d \right)^{-1}}_{\text{primal}} \mathbf{X} \mathbf{y}$$

- ▶ **Easy:**

$$\left(\frac{1}{n} \mathbf{X} \mathbf{X}^\top + \lambda I_d \right) \mathbf{X} = \mathbf{X} \left(\frac{1}{n} \mathbf{X}^\top \mathbf{X} + \lambda I_n \right)$$

$$w = \frac{1}{n} \mathbf{X} \underbrace{\left(\frac{1}{n} \mathbf{X}^\top \mathbf{X} + \lambda I_n \right)^{-1}}_{\text{dual}} \mathbf{y}$$

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Ridge regression

- ▶ **Prediction:** Given $t \in \mathbb{R}^d$

$$\begin{aligned} f(t) &= \langle w, t \rangle_2 = \mathbf{y}^\top \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top + n\lambda I_d)^{-1} t \\ &= \mathbf{y}^\top (\mathbf{X}^\top \mathbf{X} + n\lambda I_n)^{-1} \mathbf{X}^\top t \end{aligned}$$

- ▶ How does $\mathbf{X}^\top \mathbf{X}$ look like?

$$\mathbf{X}^\top \mathbf{X} = \begin{bmatrix} \langle x_1, x_1 \rangle_2 & \langle x_1, x_2 \rangle_2 & \cdots & \langle x_1, x_n \rangle_2 \\ \langle x_2, x_1 \rangle_1 & \langle x_2, x_2 \rangle_2 & \cdots & \langle x_2, x_n \rangle_2 \\ \vdots & \langle x_i, x_j \rangle_2 & \ddots & \vdots \\ \langle x_n, x_1 \rangle_1 & \langle x_n, x_2 \rangle_2 & \cdots & \langle x_n, x_n \rangle_2 \end{bmatrix}$$

Matrix of inner products: Gram Matrix

Ridge regression

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Matrix of inner products: **Gram Matrix**

Kernel Ridge regression: Feature Map and Kernel Trick

- ▶ **Given:** $\{(x_i, y_i)\}_{i=1}^n$ where $x_i \in \mathcal{X}$, $y_i \in \mathbb{R}$
- ▶ **Task:** Find a regressor $f \in \mathcal{H}$ (some feature space) s.t. $f(x_i) \approx y_i$.
- ▶ **Idea:** Map x_i to $\Phi(x_i)$ and do linear regression,

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n (\langle f, \Phi(x_i) \rangle_{\mathcal{H}} - y_i)^2 + \lambda \|f\|_{\mathcal{H}}^2 \quad (\lambda > 0)$$

- ▶ **Solution:** For $\Phi(\mathbf{X}) := (\Phi(x_1), \dots, \Phi(x_n)) \in \mathbb{R}^{\dim(\mathcal{H}) \times n}$ and $\mathbf{y} := (y_1, \dots, y_n)^\top \in \mathbb{R}^n$,

$$\begin{aligned} f &= \frac{1}{n} \underbrace{\left(\frac{1}{n} \Phi(\mathbf{X}) \Phi(\mathbf{X})^\top + \lambda I_{\dim(\mathcal{H})} \right)^{-1}}_{\text{primal}} \Phi(\mathbf{X}) \mathbf{y} \\ &= \frac{1}{n} \Phi(\mathbf{X}) \underbrace{\left(\frac{1}{n} \Phi(\mathbf{X})^\top \Phi(\mathbf{X}) + \lambda I_n \right)^{-1}}_{\text{dual}} \mathbf{y} \end{aligned}$$

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Kernel Ridge regression: Feature Map and Kernel Trick

- **Prediction:** Given $t \in \mathcal{X}$

$$\begin{aligned} f(t) &= \langle f, \Phi(t) \rangle_{\mathcal{H}} = \frac{1}{n} \mathbf{y}^\top \Phi(\mathbf{X})^\top \left(\frac{1}{n} \Phi(\mathbf{X}) \Phi(\mathbf{X})^\top + \lambda I_{\dim(\mathcal{H})} \right)^{-1} \Phi(t) \\ &= \frac{1}{n} \mathbf{y}^\top \left(\frac{1}{n} \Phi(\mathbf{X})^\top \Phi(\mathbf{X}) + \lambda I_n \right)^{-1} \Phi(\mathbf{X})^\top \Phi(t) \end{aligned}$$

As before

$$\Phi(\mathbf{X})^\top \Phi(\mathbf{X}) = \underbrace{\begin{bmatrix} \langle \Phi(x_1), \Phi(x_1) \rangle_{\mathcal{H}} & \cdots & \langle \Phi(x_1), \Phi(x_n) \rangle_{\mathcal{H}} \\ \langle \Phi(x_2), \Phi(x_1) \rangle_{\mathcal{H}} & \cdots & \langle \Phi(x_2), \Phi(x_n) \rangle_{\mathcal{H}} \\ \vdots & \ddots & \vdots \\ \langle \Phi(x_n), \Phi(x_1) \rangle_{\mathcal{H}} & \cdots & \langle \Phi(x_n), \Phi(x_n) \rangle_{\mathcal{H}} \end{bmatrix}}_{k(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle_{\mathcal{H}}}$$

and

$$\Phi(\mathbf{X})^\top \Phi(t) = [\langle \Phi(x_1), \Phi(t) \rangle_{\mathcal{H}}, \dots, \langle \Phi(x_n), \Phi(t) \rangle_{\mathcal{H}}]^\top$$

Kernel Ridge regression: Feature Map and Kernel Trick

► **Prediction:** Given $t \in \mathcal{X}$

$$\begin{aligned} f(t) &= \langle f, \Phi(t) \rangle_{\mathcal{H}} = \frac{1}{n} \mathbf{y}^\top \Phi(\mathbf{X})^\top \left(\frac{1}{n} \Phi(\mathbf{X}) \Phi(\mathbf{X})^\top + \lambda I_{\dim(\mathcal{H})} \right)^{-1} \Phi(t) \\ &= \frac{1}{n} \mathbf{y}^\top \left(\frac{1}{n} \Phi(\mathbf{X})^\top \Phi(\mathbf{X}) + \lambda I_n \right)^{-1} \Phi(\mathbf{X})^\top \Phi(t) \end{aligned}$$

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Feature Map and Kernel Trick: Remarks

- ▶ The **primal formulation** requires the knowledge of feature map Φ (and of course \mathcal{H}) and these could be infinite dimensional.
- ▶ Suppose we have access to a **kernel function, k** (**Recall:** not easy to verify that k is a kernel). Then the **dual formulation** is entirely determined by k (**Gram matrix or kernel matrix**).
- ▶ Linear regression in the dual uses a **linear kernel**.

Kernel trick or heuristic

Replace $\langle x_i, x_j \rangle_2$ in your linear method by $k(x_i, x_j)$ where k is your favorite kernel

Application: Principal Component Analysis

(Kernel Trick: Feature map point of view)

Principal Component Analysis

- ▶ Dimensionality reduction
- ▶ **Given:** $\{(x_i)\}_{i=1}^n$ where $x_i \in \mathbb{R}^d$
- ▶ **Task:** Find a low-dimensional representation for (x_i) .

$$\begin{aligned} & \max_{\|w\|_2=1} \text{Var}(\langle w, x_1 \rangle_2, \langle w, x_2 \rangle_2, \dots, \langle w, x_n \rangle_2) \\ & \equiv \max_{\|w\|_2=1} \frac{1}{n} \sum_{i=1}^n \langle w, x_i \rangle_2^2 - \left(\frac{1}{n} \sum_{i=1}^n \langle w, x_i \rangle_2 \right)^2 \\ & \equiv \max_{\|w\|_2=1} w^\top \hat{\Sigma} w \end{aligned}$$

where

$$\begin{aligned} \hat{\Sigma} & := \frac{1}{n} \sum_{i=1}^n x_i x_i^\top - \left(\frac{1}{n} \sum_{i=1}^n x_i \right) \left(\frac{1}{n} \sum_{i=1}^n x_i \right)^\top \\ & = \frac{1}{n} \mathbf{X} \left(I_d - \frac{1}{n} \mathbf{1}\mathbf{1}^\top \right) \mathbf{X}^\top =: \mathbf{X}\mathbf{H}\mathbf{X}^\top. \end{aligned}$$

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- ▶ **Given:** $\{(x_i)\}_{i=1}^n$ where $x_i \in \mathbb{R}^d$
- ▶ **Task:** Find a low-dimensional representation for (x_i) .

$$\begin{aligned} & \max_{\|w\|_2=1} \text{Var}(\langle w, x_1 \rangle_2, \langle w, x_2 \rangle_2, \dots, \langle w, x_n \rangle_2) \\ & \equiv \max_{\|w\|_2=1} \frac{1}{n} \sum_{i=1}^n \langle w, x_i \rangle_2^2 - \left(\frac{1}{n} \sum_{i=1}^n \langle w, x_i \rangle_2 \right)^2 \\ & \equiv \max_{\|w\|_2=1} w^T \hat{\Sigma} w \end{aligned}$$

where

$$\begin{aligned} \hat{\Sigma} & := \frac{1}{n} \sum_{i=1}^n x_i x_i^T - \left(\frac{1}{n} \sum_{i=1}^n x_i \right) \left(\frac{1}{n} \sum_{i=1}^n x_i \right)^T \\ & = \frac{1}{n} \mathbf{X} \left(I_d - \frac{1}{n} \mathbf{1}\mathbf{1}^T \right) \mathbf{X}^T =: \mathbf{X}\mathbf{H}\mathbf{X}^T. \end{aligned}$$

Principal Component Analysis

- ▶ Dimensionality reduction
- ▶ Given: $\{(x_i)\}_{i=1}^n$ where $x_i \in \mathbb{R}^d$
- ▶ Task: Find a low-dimensional representation for (x_i) .

$$\begin{aligned} & \max_{\|w\|_2=1} \text{Var}(\langle w, x_1 \rangle_2, \langle w, x_2 \rangle_2, \dots, \langle w, x_n \rangle_2) \\ & \equiv \max_{\|w\|_2=1} \frac{1}{n} \sum_{i=1}^n \langle w, x_i \rangle_2^2 - \left(\frac{1}{n} \sum_{i=1}^n \langle w, x_i \rangle_2 \right)^2 \\ & \equiv \max_{\|w\|_2=1} w^T \hat{\Sigma} w \end{aligned}$$

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Principal Component Analysis

- **Solution:** Find the eigenvector corresponding to the maximum eigenvalue of $\hat{\Sigma}$,

$$\begin{aligned}\hat{\Sigma}w &= \lambda_1 w \\ \mathbf{XHX}^T w &= \lambda_1 w \\ \underbrace{\mathbf{X}^T \mathbf{X}}_K \mathbf{H} \underbrace{\mathbf{X}^T w}_\alpha &= \lambda_1 \mathbf{X}^T w \\ \mathbf{KH}\alpha &= \lambda_1 \alpha\end{aligned}$$

- The eigenvalues of \mathbf{KH} are the same as that of $\hat{\Sigma}$
-

$$\alpha = \mathbf{X}^T w \implies \mathbf{XH}\alpha = \mathbf{XHX}^T w = \hat{\Sigma}w = \lambda_1 w$$

The eigenvector of $\hat{\Sigma}$ can be computed from the eigenvector of \mathbf{KH} as

$$w = \frac{1}{\lambda_1} \mathbf{XH}\alpha$$

- Kernel PCA (Schölkopf et al., 1998):

$$w = \frac{1}{\lambda_1} \Phi(\mathbf{X})\mathbf{H}\alpha = \sum_{i=1}^n (\mathbf{H}\alpha)_i \Phi(x_i)$$

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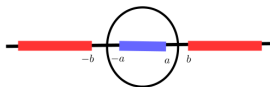
Feature Map and Kernel Trick

Same idea yields: (Schölkopf and Smola, 2002)

- ▶ Linear SVM \rightarrow Kernel SVM
- ▶ Fisher discriminant analysis (FDA) \rightarrow Kernel FDA
- ▶ Canonical correlation analysis (CCA) \rightarrow Kernel CCA

many more ...

Revisiting Nonlinear Classification: 1

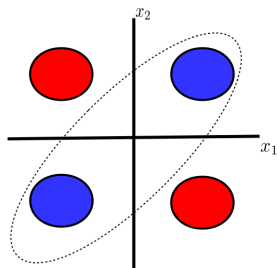


- ▶ The following function perfectly separates red and blue regions

$$f(x) = x^2 - r = \left\langle \underbrace{(1, -r)}_w, \underbrace{(x^2, 1)}_{\Phi(x)} \right\rangle_2, \quad a < r < b.$$

- ▶ Apply kernel trick with $k(x, y) = x^2y^2 + 1$.

Revisiting Nonlinear Classification: 2



- ▶ A conic section, however, perfectly separates them

$$\begin{aligned} f(x_1, x_2) &= ax_1^2 + bx_1x_2 + cx_2^2 + dx_1 + ex_2 + g \\ &= \left\langle \underbrace{(a, b, c, d, e, g)}_w, \underbrace{(x_1^2, x_1x_2, x_2^2, x_1, x_2, 1)}_{\Phi(x)} \right\rangle_2. \end{aligned}$$

- ▶ Apply kernel trick with $k(x, y)$. **Exercise:** Find the kernel $k(x, y)$.

Application: Ridge Regression

(Representer Theorem: Function space point of view)

Learning Theory: Revisit

- ▶ **Empirical risk:** $\mathcal{R}_{L,D}(f) := \frac{1}{n} \sum_{i=1}^n L(y_i, f(x_i))$

$$f_D := \arg \min_{f: X \rightarrow \mathbb{R}} \mathcal{R}_{L,D}(f)$$

- ▶ **To avoid overfitting:** Perform ERM on a small set \mathcal{F} of functions (class of smooth functions)

$$f_D := \arg \inf_{f \in \mathcal{F}} \mathcal{R}_{L,D}(f)$$

- ▶ **Choice of \mathcal{F} :** Evaluation functionals are bounded.

$$|\delta_x(f)| = |f(x)| \leq M_x \|f\|_{\mathcal{F}}, \quad \forall x \in \mathcal{X}, f \in \mathcal{F}$$

Pick $\mathcal{F} = \{f : \|f\|_{\mathcal{H}} \leq \alpha\}$; \mathcal{H} is an RKHS

Penalized Estimation

- ▶ We have

$$\begin{aligned}f_D &= \arg \inf_{\|f\|_{\mathcal{H}} \leq \alpha} R_{L,D}(f) \\ &= \arg \inf_{\|f\|_{\mathcal{H}} \leq \alpha} \frac{1}{n} \sum_{i=1}^n L(y_i, f(x_i))\end{aligned}$$

- ▶ In the Lagrangian formulation, we have

$$\begin{aligned}f_D &= \arg \inf_{f \in \mathcal{H}} R_{L,D}(f) + \lambda \|f\|_{\mathcal{H}}^2 \\ &= \arg \inf_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n L(y_i, f(x_i)) + \lambda \|f\|_{\mathcal{H}}^2\end{aligned}$$

where $\lambda > 0$.

Optimization over (possibly infinite dimensional) function space

Representer Theorem

Consider the penalized estimation problem,

$$\inf_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n L(y_i, f(x_i)) + \lambda \theta(\|f\|_{\mathcal{H}})$$

where $\theta : [0, \infty) \rightarrow \mathbb{R}$ is a non-decreasing function.

- ▶ (Kimeldorf and Wahba, 1971; Schölkopf et al., ALT 2001) The solution to the above minimization problem is achieved by a function of the form

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

where $(\alpha_i)_{i=1}^n \subset \mathbb{R}$.

The infinite dimensional optimization problem reduces to a finite dimensional optimization problem in \mathbb{R}^n .

Proof

- ▶ **Decomposition:**

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_0^\perp,$$

where $\mathcal{H}_0 = \text{span}\{k(\cdot, x_1), \dots, k(\cdot, x_n)\}$, \mathcal{H}_0^\perp : orthogonal complement. Decompose

$$f = f_0 + f^\perp$$

accordingly.

- ▶ The loss function L does not change by replacing f with f_0 because

$$f(x_i) = \langle f, k(\cdot, x_i) \rangle_{\mathcal{H}} = \langle f_0, k(\cdot, x_i) \rangle_{\mathcal{H}} + \underbrace{\langle f^\perp, k(\cdot, x_i) \rangle_{\mathcal{H}}}_{=0}.$$

- ▶ **Penalty term:**

$$\|f_0\|_{\mathcal{H}} \leq \|f\|_{\mathcal{H}} \quad \Rightarrow \quad \theta(\|f_0\|_{\mathcal{H}}) \leq \theta(\|f\|_{\mathcal{H}}).$$

- ▶ Thus the optimum lies in \mathcal{H}_0 .

Kernel Ridge Regression

- ▶ $f : \mathcal{X} \rightarrow \mathbb{R}$ and $L(y, f(x)) = (y - f(x))^2$ (Squared loss)

$$\inf_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n (y_i - \langle f, k(\cdot, x_i) \rangle_{\mathcal{H}})^2 + \lambda \|f\|_{\mathcal{H}}^2$$

- ▶ By representer theorem, the solution is of the form $f = \sum_{i=1}^n \alpha_i k(\cdot, x_i)$ which on substitution yields

$$\inf_{\alpha} \frac{1}{n} \|\mathbf{Y} - \mathbf{K}\alpha\|^2 + \lambda \alpha^\top \mathbf{K}\alpha$$

where \mathbf{K} is the Gram matrix with $\mathbf{K}_{ij} = k(x_i, x_j)$.

- ▶ **Solution:** $\hat{\alpha} = (\mathbf{K} + n\lambda I_n)^{-1} \mathbf{Y}$ (assuming \mathbf{K} is invertible). For any $t \in \mathcal{X}$,

$$\hat{f}(t) = \sum_{i=1}^n \hat{\alpha}_i k(t, x_i) = \mathbf{Y}^\top (\mathbf{K} + n\lambda I_n)^{-1} \mathbf{k}_t,$$

where $(\mathbf{k}_t)_i := k(t, x_i)$. (Same solution as the feature map view point)

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Application: Principal Component Analysis

(Representer Theorem: Function space point of view)

Principal Component Analysis

- ▶ **Given:** $\{(x_i)\}_{i=1}^n$ where $x_i \in \mathcal{X}$.



$$\begin{aligned} & \min_{\|f\|_{\mathcal{H}}=1} \text{Var}(f(x_1), \dots, f(x_n)) \\ &= \min_{\|f\|_{\mathcal{H}}=1} \text{Var}(\langle f, k(\cdot, x_1) \rangle_{\mathcal{H}}, \dots, \langle f, k(\cdot, x_n) \rangle_{\mathcal{H}}) \\ &= \min_{\|f\|_{\mathcal{H}}=1} \frac{1}{n} \sum_{i=1}^n \langle f, k(\cdot, x_i) \rangle_{\mathcal{H}}^2 - \left\langle f, \frac{1}{n} \sum_{i=1}^n k(\cdot, x_i) \right\rangle_{\mathcal{H}}^2 \\ &= \min_{\|f\|_{\mathcal{H}}=1} \langle f, \hat{\Sigma} f \rangle_{\mathcal{H}} \end{aligned}$$

where

$$\hat{\Sigma} := \frac{1}{n} \sum_{i=1}^n k(\cdot, x_i) \otimes k(\cdot, x_i) - \left(\frac{1}{n} \sum_{i=1}^n k(\cdot, x_i) \right) \otimes \left(\frac{1}{n} \sum_{i=1}^n k(\cdot, x_i) \right)$$

is the **covariance operator**.

- ▶ The solution to the above problem is the eigenfunction of $\hat{\Sigma}$ corresponding to the **maximum eigenvalue**. (CAUTION!!)

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$$\begin{aligned} & \min_{\|f\|_{\mathcal{H}}=1} \text{Var}(f(x_1), \dots, f(x_n)) \\ &= \min_{\|f\|_{\mathcal{H}}=1} \text{Var}(\langle f, k(\cdot, x_1) \rangle_{\mathcal{H}}, \dots, \langle f, k(\cdot, x_n) \rangle_{\mathcal{H}}) \\ &= \min_{\|f\|_{\mathcal{H}}=1} \frac{1}{n} \sum_{i=1}^n \langle f, k(\cdot, x_i) \rangle_{\mathcal{H}}^2 - \left\langle f, \frac{1}{n} \sum_{i=1}^n k(\cdot, x_i) \right\rangle_{\mathcal{H}}^2 \\ &= \min_{\|f\|_{\mathcal{H}}=1} \langle f, \hat{\Sigma} f \rangle_{\mathcal{H}} \end{aligned}$$

where

$$\hat{\Sigma} := \frac{1}{n} \sum_{i=1}^n k(\cdot, x_i) \otimes k(\cdot, x_i) - \left(\frac{1}{n} \sum_{i=1}^n k(\cdot, x_i) \right) \otimes \left(\frac{1}{n} \sum_{i=1}^n k(\cdot, x_i) \right)$$

is the **covariance operator**.

- ▶ The solution to the above problem is the eigenfunction of $\hat{\Sigma}$ corresponding to the **maximum eigenvalue**. (CAUTION!!)

Principal Component Analysis (Schölkopf et al., 1998)

- ▶ By the **representer theorem**, the solution to the optimization problem is of the form

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

- ▶ This yields

$$\min_{\alpha^T \mathbf{K} \alpha = 1} \alpha^T \mathbf{K} \mathbf{H} \mathbf{K} \alpha$$

and therefore α satisfies

$$\mathbf{K} \mathbf{H} \mathbf{K} \alpha = \lambda_1 \mathbf{K} \alpha.$$

- ▶ If \mathbf{K} is invertible, then α is an eigenvector to $\mathbf{K} \mathbf{H}$ (same solution as the feature map view point)

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How to choose \mathcal{H} ?

Large RKHS: Universal Kernel/RKHS

- ▶ **Universal kernel** (Steinwart, JMLR 2001): A kernel k on a compact metric space, \mathcal{X} is said to be universal if the RKHS, \mathcal{H} is dense (w.r.t. uniform norm) in the space of continuous functions on \mathcal{X} .

Any continuous function on \mathcal{X} can be approximated arbitrarily by a function in \mathcal{H} .

- ▶ (Steinwart and Christmann, 2008) For certain conditions on L , if k is universal, then

$$\inf_{f \in \mathcal{H}} \mathcal{R}_{L, \mathbf{P}}(f) = \mathcal{R}_{L, \mathbf{P}}(f^*),$$

i.e., approximation error is zero.

- ▶ Squared loss, Hinge loss,...

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When is k Universal?

k is **universal** if and only if

$$\int_{\mathcal{X}} \int_{\mathcal{X}} k(x, y) d\mu(x) d\mu(y) > 0$$

for all non-zero finite signed measures, μ on \mathcal{X} .

(Carmeli et al., 2010; S et al., 2011)

Generalization of strictly positive definite kernels

- ▶ In Lecture 2, we will explore more by relating it to the **Hilbert space embedding of measures**.
- ▶ **Examples:** Gaussian, Laplacian, etc. (No finite dimensional RKHS is universal!!)

Advanced Topics

- ▶ Consistency and convergence rates of KRR (Caponnetto and De Vito, 2007; Steinwart et al., 2009)
- ▶ Consistency and convergence rates of KPCA (Blanchard et al., 2007; Rudi et al., 2013)
- ▶ Spectral regularization
- ▶ Stochastic gradient descent methods for KRR

Questions

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Suggested Readings

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