Machine learning for graphs and with graphs

Graph kernels

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ENS DE LYON

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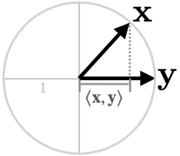
Acknowledgments

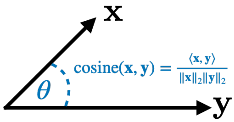
Some slides adapted from those of Jean-Philippe Vert and Rémi Flamary.

What is a kernel ?

Measuring similarities between objects

- Two "objects" $\mathbf{x}, \mathbf{y}$ in **an abstract space** $\mathcal{X}$.
- A kernel aims at measuring "how similar" is $\mathbf{x}$ from $\mathbf{y}$.
- e.g. $\mathcal{X} = \mathbb{R}^d$, $\text{kernel}(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle$ or cosine similarity.





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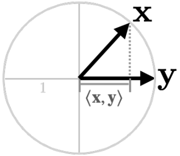
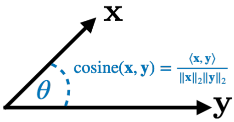
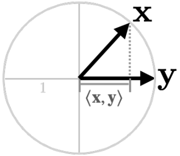




ML with kernels

- ML methods based on **pairwise comparisons**.
- By imposing constraints on the kernel (positive definite), we obtain a **general framework for learning from data** (RKHS).
- $+$ **without making any assumptions regarding the type of data** (vectors, strings, graphs, images, ...)

What is a kernel ?



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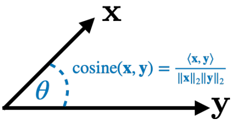

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A principle method for ERM

$\min_{f \in ?} \frac{1}{n} \sum_{i=1}^{n} \ell(\mathbf{y}_i, f(\mathbf{x}_i)) \rightarrow$ look for f in specific space (RKHS)

A feature map $\Phi : \mathcal{X} \to \mathcal{H}$

From feature map to functions: motivating example

- Feature map can be used to define functions from $\mathcal{X}$ to $\mathbb{R}$.

$$\Phi : \mathbb{R}^2 \to \mathbb{R}^3 = \mathcal{H}$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \mapsto \Phi(\mathbf{x}) = \begin{bmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{bmatrix} \text{ and } f(\mathbf{x}) = a \cdot x_1 + b \cdot x_2 + c \cdot x_1 x_2 \; (\mathbb{R}^2 \to \mathbb{R})$$

- Consider $\boldsymbol{\theta} = (a, b, c)^\top \in \mathbb{R}^3$ then $f(\mathbf{x}) = \langle \boldsymbol{\theta}, \Phi(\mathbf{x}) \rangle$.
- **Evaluation of f at $\mathbf{x}$ is an inner product in feature space.**

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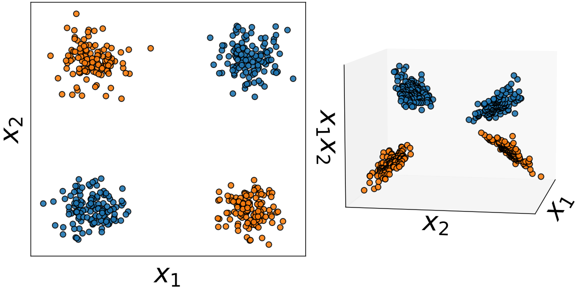
- **Evaluation of f at x is an inner product in feature space**.

Go into higher dimensions to **linearly** separate the classes !



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The definition

Positive definite (PD) kernel

Let $\mathcal{X}$ be some space. A function $\kappa : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ is a PD kernel if

- It is symmetric $\kappa(\mathbf{x}, \mathbf{y}) = \kappa(\mathbf{y}, \mathbf{x})$.
- For any $\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathcal{X}$ and $c_1, \cdots, c_n \in \mathbb{R}$

$$\sum_{i,j=1}^{n} c_i c_j \kappa(\mathbf{x}_i, \mathbf{x}_j) \geq 0 . \tag{1}$$

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$$\sum_{i,j=1}^{n} c_i c_j \kappa(\mathbf{x}_i, \mathbf{x}_j) \geq 0 \,. \qquad (1)$$

Remarks

- (1) equiv. $\mathbf{K} := (\kappa(\mathbf{x}_i, \mathbf{x}_j))_{ij} \in \mathbb{R}^{n\times n}$ is a PSD matrix $\forall \mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathcal{X}$.
- For $\kappa(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle$ if $\mathbf{X} = (\mathbf{x}_1, \cdots, \mathbf{x}_n)^\top$ then $\mathbf{c}^\top \mathbf{K} \mathbf{c} = \|\mathbf{X}^\top \mathbf{c}\|_2^2 \geq 0$.
- Works also for $\kappa(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle$ for any Φ.
- Not entirely obvious $\kappa(\mathbf{x}, \mathbf{y}) = \exp(-\|\mathbf{x} - \mathbf{y}\|_2^2 / 2\sigma^2)$. (see TD)

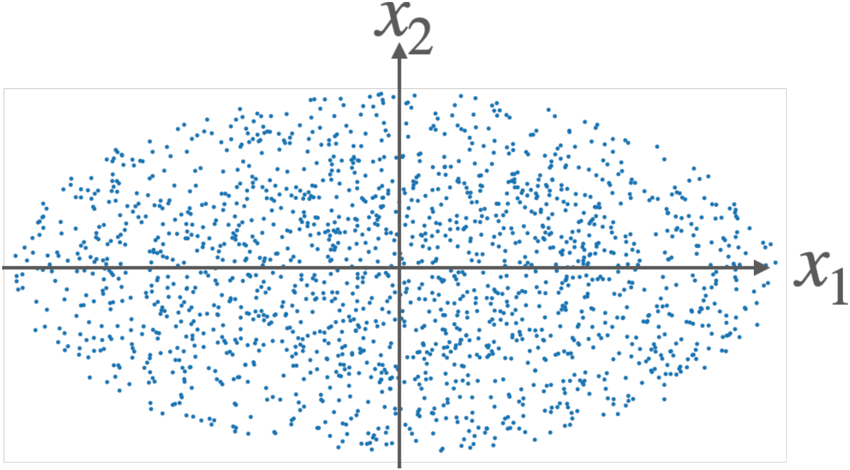
Properties of PD kernel

Basic properties (see TD)

Let $\kappa_1, \kappa_2, \cdots$ be fixed PD kernels.

- $\gamma\kappa_1$ for any $\gamma > 0$ is a PD kernel.
- $\kappa_1 + \kappa_2$ is a PD kernel.
- $\kappa(\mathbf{x}, \mathbf{y}) := \lim_{n \to +\infty} \kappa_n(\mathbf{x}, \mathbf{y})$ is a PD kernel (provided it exists).
- $\kappa(\mathbf{x}, \mathbf{y}) := \kappa_1(\mathbf{x}, \mathbf{y})\kappa_2(\mathbf{x}, \mathbf{y})$ is a PD kernel.
- If $f : \mathcal{X} \to \mathbb{R}$ then $\kappa(\mathbf{x}, \mathbf{y}) := f(\mathbf{x})\kappa_1(\mathbf{x}, \mathbf{y})f(\mathbf{y})$ is a PD kernel.

Changing the features



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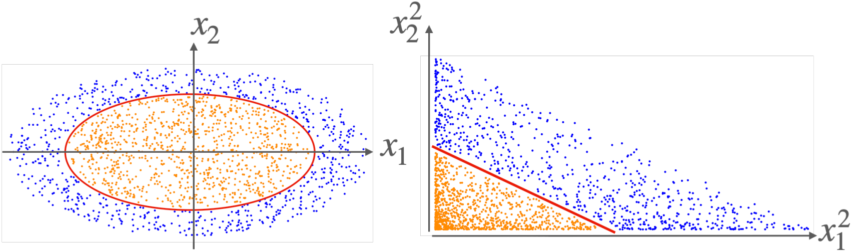


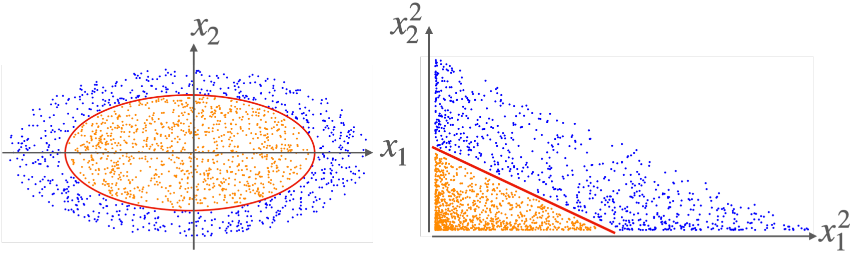
Polynomial kernel

Consider $\Phi : \mathbb{R}^2 \to \mathbb{R}^3$ defined by $\Phi(\mathbf{x} = (x_1, x_2)) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$. Then:

$$\kappa(\mathbf{x}, \mathbf{y}) := \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathbb{R}^3} = \cdots = \left(\langle \mathbf{x}, \mathbf{y} \rangle_{\mathbb{R}^2} \right)^2 .$$

Basic properties show that it defines a PD kernel.

Changing the features



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$$\kappa(\mathbf{x}, \mathbf{y}) := \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathbb{R}^3} = \cdots = (\langle \mathbf{x}, \mathbf{y} \rangle_{\mathbb{R}^2})^2 .$$

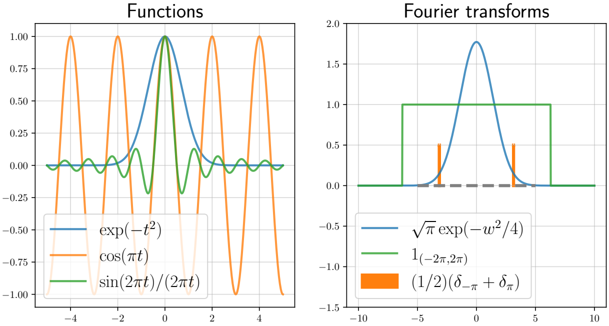
Basic properties show that it defines a PD kernel.

- More generally $\kappa(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle^m$.

Translation invariant kernels

A generic form of kernel on $\mathcal{X} = \mathbb{R}^d$

- For $\kappa_0 : \mathbb{R}^d \to \mathbb{R}$, kernel defined by
$$\kappa(\mathbf{x}, \mathbf{y}) = \kappa_0(\mathbf{x} - \mathbf{y})$$
- e.g. Gaussian kernel $\kappa(\mathbf{x}, \mathbf{y}) = \exp(-\|\mathbf{x} - \mathbf{y}\|_2^2/(2\sigma^2))$.
- Recall Fourier transform: $\widehat{f}(\boldsymbol{\omega}) = \int_{\mathbb{R}^d} f(\mathbf{x}) e^{-i\langle \boldsymbol{\omega}, \mathbf{x} \rangle} \mathrm{d}\mathbf{x}$.
- Based on Bochner's theorem (see Wendland 2004, Theorem 6.11):
$$\kappa \text{ is a PD kernel} \iff \forall \boldsymbol{\omega} \in \mathbb{R}^d, \widehat{\kappa_0}(\boldsymbol{\omega}) \geq 0$$



Main property of PD kernel

Main property: Moore–Aronszajn theorem Aronszajn 1950

A function $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a PD kernel if and only if **there exists a Hilbert space** $\mathcal{H}$ and **a mapping** $\Phi : \mathcal{X} \to \mathcal{H}$ such that

$$\forall \mathbf{x}, \mathbf{y} \in \mathcal{X}, \ \kappa(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathcal{H}} \, .$$

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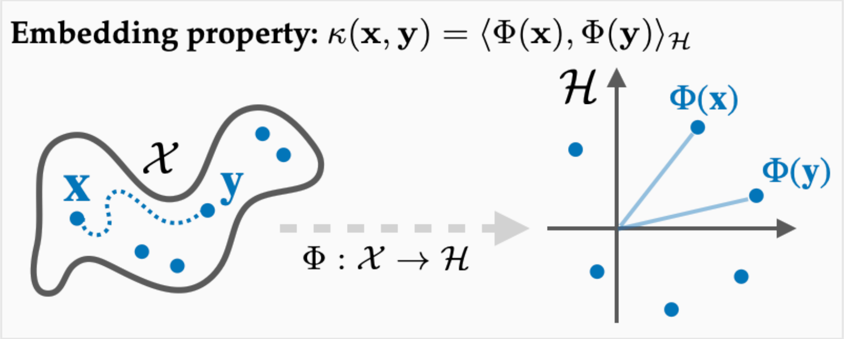


Main property of PD kernel

Some reminders

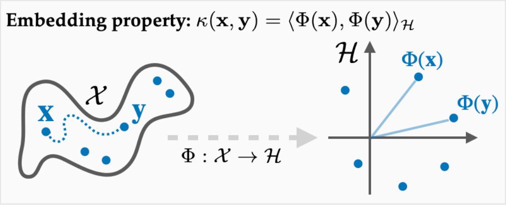
- $\langle \cdot, \cdot \rangle_{\mathcal{H}} : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ is a bilinear, symmetric and such that $\langle \mathbf{x}, \mathbf{x} \rangle_{\mathcal{H}} > 0$ for any $\mathbf{x} \neq 0$.
- A vector space endowed with an inner product is called pre-Hilbert. It is endowed with $\|\mathbf{x}\|_{\mathcal{H}} := \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle_{\mathcal{H}}}$.
- A Hilbert space is a pre-Hilbert space complete for the norm defined by the inner product.

Proof of the theorem in the discrete case

On the board

Complete proof Steinwart and Christmann 2008, Theorem 4.16.

About the feature space



The feature map Φ and feature space $\mathcal{H}$

- The feature space may have **infinite dimension** and is **not unique**.
- Polynomial kernel in $2D$ $\kappa(\mathbf{x},\mathbf{y}) = (\langle \mathbf{x},\mathbf{y} \rangle)^2$:

$$\Phi(\mathbf{x} = (x_1, x_2)) = (x_1^2, x_2^2, x_1 x_2, x_1 x_2), \;\; \mathcal{H} = \mathbb{R}^4$$

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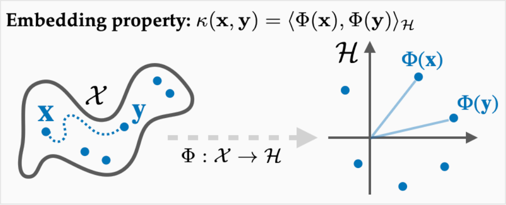

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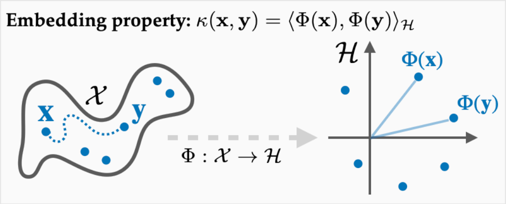
- Another possibility:

$$\Phi(\mathbf{x} = (x_1, x_2)) = (x_1^2, x_2^2, \sqrt{2} x_1 x_2), \ \mathcal{H} = \mathbb{R}^3$$

About the feature space



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$$\Phi(x) = e^{-\frac{x^2}{2\sigma^2}} \left(1, \sqrt{\frac{1}{1!\sigma^2}}x, \sqrt{\frac{1}{2!\sigma^4}}x^2, \sqrt{\frac{1}{3!\sigma^6}}x^3, \cdots\right)^\top \text{(Taylor series)}$$

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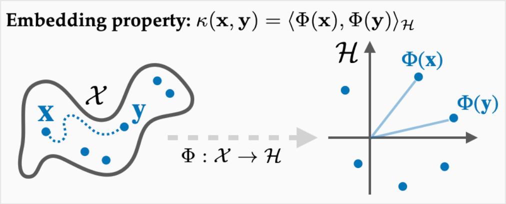

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- Or $\mathcal{H} = L_2(\mathbb{R})$ using $\kappa(x,y) = \frac{1}{\sigma}\sqrt{\frac{2}{\pi}}\int_{-\infty}^{+\infty}\exp(-\frac{(x-t)^2}{\sigma^2})\exp(-\frac{(y-t)^2}{\sigma^2})\mathrm{d}t$:

$$\Phi(x) = t \to \frac{2^{\frac{1}{4}}}{\sqrt{\sigma}\pi^{\frac{1}{4}}}\exp(-\frac{(x-t)^2}{\sigma^2})$$

Reproducing Kernel Hilbert Space (RKHS)

From kernels to functions: first idea

- **Given $\mathcal{H}$ and** $\Phi : \mathcal{X} \to \mathcal{H}_0$: defines a kernel $\kappa(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathcal{H}_0}$
- And a space of functions from $\mathcal{X}$ to $\mathbb{R}$.

$$\mathcal{H} := \{ f : \exists \boldsymbol{\theta} \in \mathcal{H}_0, \forall \mathbf{x} \in \mathcal{X}, f(\mathbf{x}) = \langle \boldsymbol{\theta}, \Phi(\mathbf{x}) \rangle_{\mathcal{H}_0} \} .$$

- Endowed with the norm

$$\|f\|_{\mathcal{H}} := \inf\{ \|\boldsymbol{\theta}\|_{\mathcal{H}_0} : \boldsymbol{\theta} \in \mathcal{H}_0 \text{ with } f = \langle \boldsymbol{\theta}, \Phi(\cdot) \rangle_{\mathcal{H}_0} \} \tag{2}$$

- It is a Hilbert space of functions called the RKHS of κ.
- We can stop here... but...

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From kernels to functions: second idea

- **Given a PSD kernel** $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.
- 1°) Find a "suitable" $(\Phi, \mathcal{H})$ such that $\kappa(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathcal{H}}$ (recall: many possible)
- 2°) Build upon it to define a suitable space of functions.

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Reproducing Kernel Hilbert Space (RKHS)

Let κ be fixed

- Among all $(\Phi, \mathcal{H})$ mentioned in Aronszjan's theorem one $\mathcal{H}$, called **RKHS**, is of interest to us.
- This is a **space of functions from $\mathcal{X}$ to** $\mathbb{R}$.
- Each data point $\mathbf{x} \in \mathcal{X}$ will be represented **by a function** given by the **canonical feature map**

$$\Phi(\mathbf{x}) = \kappa(\cdot, \mathbf{x}) : \mathcal{X} \to \mathbb{R}$$

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Example

- Consider $\mathcal{X} = \mathbb{R}$ we could decide to represent $x \in \mathbb{R}$ as a Gaussian function centered at x:

$$\Phi(x) = y \to \exp(-(x-y)^2/(2\sigma^2))$$

- What is the corresponding space $\mathcal{H}$ (if it exists)? What would be the inner-product?

Reproducing Kernel Hilbert Space (RKHS)

Reproducing kernel and RKHS

Let $\mathcal{H}$ be a **Hilbert space** of functions from $\mathcal{X}$ to $\mathbb{R}$ with inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$. $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a **reproducing kernel** of $\mathcal{H}$ if

- $\forall \mathbf{x} \in \mathcal{X}, \kappa(\cdot, \mathbf{x}) \in \mathcal{H}$
- κ satisfies the reproducing property: for any $f \in \mathcal{H}$,

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

If a reproducing kernel of $\mathcal{H}$ exists, then $\mathcal{H}$ is called a **RKHS**.

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If a reproducing kernel of $\mathcal{H}$ exists, then $\mathcal{H}$ is called a **RKHS**.

Important properties

- If $\mathcal{H}$ is a RKHS, then it has a unique reproducing kernel κ.
- (the feature map is not unique only the kernel is)
- A function κ can be the reproducing kernel of at most one RKHS.

Reproducing Kernel Hilbert Space (RKHS)

Reproducing kernel and RKHS

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If a reproducing kernel of $\mathcal{H}$ exists, then $\mathcal{H}$ is called a **RKHS**.

RKHS and feature spaces

Let $\mathcal{H}$ be a RKHS with reproducing kernel κ. Then $\mathcal{H}$ is **one** feature space associated to κ, where the feature map is $\forall \mathbf{x} \in \mathcal{X}, \Phi(\mathbf{x}) = \kappa(\cdot, \mathbf{x})$.

Examples of RKHS

So far these functions are a little bit abstract:

Two questions

- Given a PD kernel κ what is the RKHS associated to κ ?
- Given a function space, is it a RKHS and what is the reproducing kernel ?

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- Given a function space, is it a RKHS and what is the reproducing kernel ?

Battery of examples

- (on the board) The RKHS associated to $\kappa(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle$ is

$$\mathcal{H} = \{ f_{\boldsymbol{\theta}} = \mathbf{x} \to \langle \boldsymbol{\theta}, \mathbf{x} \rangle ; \boldsymbol{\theta} \in \mathbb{R}^d \}$$

  endowed with the dot product $\langle f_{\boldsymbol{\theta}_1}, f_{\boldsymbol{\theta}_2} \rangle_{\mathcal{H}} := \langle \boldsymbol{\theta}_1, \boldsymbol{\theta}_2 \rangle$.
- (homework) What is the RKHS associated to $\kappa(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle^2$?
- The space $L_2(\mathbb{R}^d)$ **is not** a RKHS.

Examples of RKHS

Battery of examples

- The Paley-Wiener space (bandwidth limited Fourier transform):

$$\mathcal{F}_\pi := \{f \in L_2(\mathbb{R}) : \operatorname{supp} \hat{f} \in [-\pi, \pi]\}$$

where $\hat{f}$ is the Fourier transform of f.

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  - Inverse Fourier transform

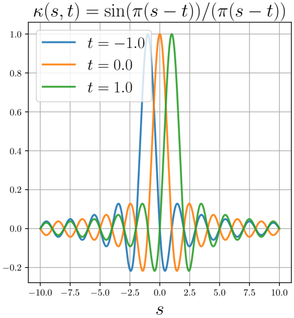
$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \hat{f}(\omega) e^{i\omega t} \mathrm{d}\omega = \langle \hat{f}, \omega \to \frac{e^{-i\omega t}}{\sqrt{2\pi}} \rangle_{L_2([-\pi,\pi])}$$

  - Plancherel-Parseval theorem

$$\forall t \in \mathbb{R},\ f(t) = \langle \hat{f}, \omega \to \frac{e^{-i\omega t}}{\sqrt{2\pi}} \rangle_{L_2([-\pi,\pi])} = \langle f, \frac{\sin(\pi(\cdot - t))}{\pi(\cdot - t)} \rangle_{L_2(\mathbb{R})}$$

  - The kernel $\kappa(s, t) = \frac{\sin(\pi(s-t))}{\pi(s-t)}$

Examples of RKHS



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- Translation invariant PD kernels on $\mathbb{R}^d$ $\kappa(\mathbf{x}, \mathbf{y}) = \kappa_0(\mathbf{x} - \mathbf{y})$ with $\kappa_0 \in L_1(\mathbb{R}^d) \cap C(\mathbb{R}^d)$ and $\forall \boldsymbol{\omega} \in \mathbb{R}^d, \widehat{\kappa_0}(\boldsymbol{\omega}) \geq 0$.

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- The corresponding RKHS is

$$\mathcal{H} = \{f \in L_2(\mathbb{R}^d) \cap C(\mathbb{R}^d) : \hat{f}/\sqrt{\widehat{\kappa_0}} \in L_2(\mathbb{R}^d)\}$$

- The inner product is given by:

$$\langle f, g \rangle_{\mathcal{H}} := (2\pi)^{-d/2} \int_{\mathbb{R}^d} \frac{\hat{f}(\boldsymbol{\omega})\overline{\widehat{g}(\boldsymbol{\omega})}}{\widehat{\kappa_0}(\boldsymbol{\omega})} \mathrm{d}\boldsymbol{\omega} \,.$$

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- Special case: Matèrn kernel $\widehat{\kappa_0}(\boldsymbol{\omega}) \propto (\alpha^2 + \|\boldsymbol{\omega}\|_2^2)^{-s}, s > d/2$
- Sobolev spaces of order s: $\|f\|_{\mathcal{H}}^2 =$ smoothness of the functions as its derivatives in $L_2(\mathbb{R}^d)$.

Reproducing Kernel Hilbert Space (RKHS)

Reproducing kernels are PD kernels

A function $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a reproducing kernel if and only if it is a PD kernel.

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Remarks

- One direction easy: a reproducing kernel is a PD kernel (on the board).
- The other more work: use Moore–Aronszajn theorem + $\mathcal{F}$ + Steinwart and Christmann 2008, Theorem 4.21.

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Important consequence

- Any PSD kernel defines a Hilbert space of functions from $\mathcal{X}$ to $\mathbb{R}$.
- These functions satisfy

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

- Abstract view of $\mathcal{H}$:

$$\mathcal{H} = \overline{\mathrm{Span}\{\kappa(\cdot, \mathbf{x}); \mathbf{x} \in \mathcal{X}\}}\ .$$

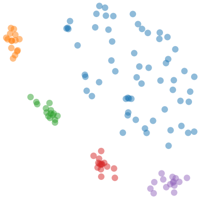
Table of contents

Recap on supervised ML

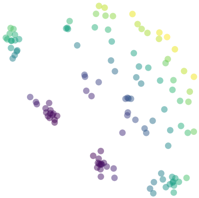
Samples + labels:

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Classification



Regression



Supervised learning

- The dataset contains the samples $(\mathbf{x}_i, y_i)_{i=1}^n$ where $\mathbf{x}_i$ is the feature sample and $y_i \in \mathcal{Y}$ its label.
- Prediction space $\mathcal{Y}$ can be:
  - $\mathcal{Y} = \{-1, 1\}$ or $\mathcal{Y} = \{1, \ldots, K\}$ for classification problems.
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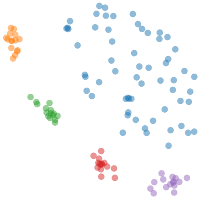

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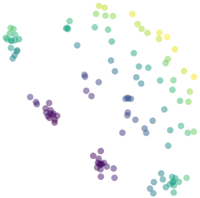

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Minimizing the averaged error on the training data

To find $f : \mathcal{X} \rightarrow \mathcal{Y}$ the idea is to minimize:

$$\min_f \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(\mathbf{x}_i)) + \lambda \operatorname{Reg}(f) \qquad \text{(ERM)}$$

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One solution

- When $\mathcal{Y} \subset \mathbb{R}$ we can consider $f \in \mathcal{H}$ where $\mathcal{H}$ is a RKHS.
- A natural candidate $\mathrm{Reg}(f) = \|f\|_{\mathcal{H}}^2$: the higher the smoother f is.
- How to ensure that this is not so difficult ?

Interpretation of minimization on a RKHS

- Suppose $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{H}$ a RKHS. Consider ERM

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(\mathbf{x}_i)) + \lambda \|f\|_{\mathcal{H}}^2$$

- Since $f \in \mathcal{H}$, then $f(\mathbf{x}) = \langle f, \kappa(\cdot, \mathbf{x}) \rangle_{\mathcal{H}} = \langle f, \Phi(\mathbf{x}) \rangle_{\mathcal{H}}$.
- Rewriting ERM in RKHS as

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Important interpretation

- $\Phi : \mathcal{X} \to \mathcal{H}$ pushes the points to a potentially very high-dimensional space (even ∞): more powerful representation.
- Then linear classification/regression is made on this high-dim space $\mathcal{H}$
- We can deduce the function in low-dim from the high-dim.

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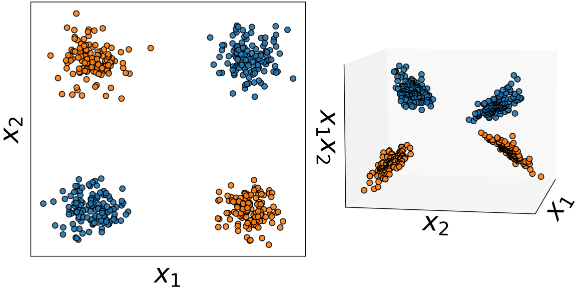
Go into higher dimensions to **linearly** separate the classes !



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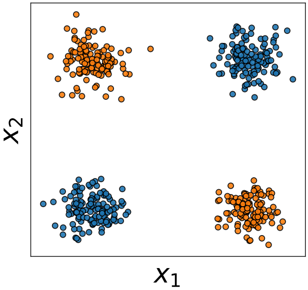
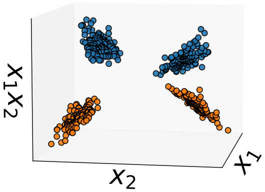
- But how to implement $\Phi(\mathbf{x}) \in \mathcal{H}$ on a computer if $\dim \mathcal{H} = \infty$?????
- How to solve ERM in $\mathcal{H}$????





The representer theorem

Main result

- Let $\mathcal{X}$ be any space, $\mathcal{D} = \{\mathbf{x}_1, \cdots, \mathbf{x}_n\} \subset \mathcal{X}$ a finite set of points.
- $\mathcal{H}$ a RKHS with reproducing kernel $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.
- Let $\Psi : \mathbb{R}^{n+1} \to \mathbb{R}$ any function that is strictly increasing with respect to the last variable.
- Then any solution $f^\star$ of the minimization problem

$$\min_{f \in \mathcal{H}} \Psi(f(\mathbf{x}_1), \cdots, f(\mathbf{x}_n), \|f\|_{\mathcal{H}}^2)$$

can be written as

$$\forall \mathbf{x} \in \mathcal{X},\ f^\star(\mathbf{x}) = \sum_{i=1}^{n} \theta_i \kappa(\mathbf{x}, \mathbf{x}_i) \text{ for some } \boldsymbol{\theta} \in \mathbb{R}^n.$$

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Important remarks

- Although the RKHS can be of infinite dimension any solution lives in $\text{Span}\{\kappa(\cdot, \mathbf{x}_1), \cdots, \kappa(\cdot, \mathbf{x}_n)\}$ which is a subspace of dimension n.
- Works for any $\mathcal{X}$ and $\Psi = \Psi_0 + g$ with $g \nearrow$!!!

Practical use of the representer theorem (1/2)

- When the representer theorem holds we can simply look for f as

$$\forall \mathbf{x} \in \mathcal{X},\ f(\mathbf{x}) = \sum_{i=1}^{n} \theta_i \kappa(\mathbf{x}, \mathbf{x}_i) \text{ for some } \boldsymbol{\theta} \in \mathbb{R}^n .$$

- Define $\mathbf{K} := (\kappa(\mathbf{x}_i, \mathbf{x}_j))_{ij}$.
- Then , for any $j \in [\![n]\!]$

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- Also

$$\begin{aligned} \|f\|_{\mathcal{H}}^2 &= \|\sum_{i=1}^{n} \theta_i \kappa(\cdot, \mathbf{x}_i)\|_{\mathcal{H}}^2 = \langle \sum_{i=1}^{n} \theta_i \kappa(\cdot, \mathbf{x}_i), \sum_{j=1}^{n} \theta_j \kappa(\cdot, \mathbf{x}_j)\rangle_{\mathcal{H}} \\ &= \sum_{ij} \theta_i \theta_j \langle \kappa(\cdot, \mathbf{x}_i), \kappa(\cdot, \mathbf{x}_j)\rangle_{\mathcal{H}} = \sum_{ij} \theta_i \theta_j \kappa(\mathbf{x}_i, \mathbf{x}_j) \\ &= \boldsymbol{\theta}^\top \mathbf{K} \boldsymbol{\theta}\,. \end{aligned}$$

Practical use of the representer theorem (2/2)

- Therefore the problem

$$\min_{f \in \mathcal{H}} \Psi(f(\mathbf{x}_1), \cdots, f(\mathbf{x}_n), \|f\|_{\mathcal{H}}^2)$$

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$$\min_{\boldsymbol{\theta} \in \mathbb{R}^n} \Psi([\mathbf{K}\boldsymbol{\theta}]_1, \cdots, [\mathbf{K}\boldsymbol{\theta}]_n, \boldsymbol{\theta}^\top \mathbf{K}\boldsymbol{\theta})$$

- 1°) To tackle it we only need the Gram matrix **K**: **kernel trick** !
- 2°) Can be used whatever $\mathcal{X}, \kappa$!
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Application to ERM

If we look for f in a RKHS then we need to solve

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^{n} \ell(\mathbf{y}_i, [\mathbf{K}\boldsymbol{\theta}]_i) + \lambda \boldsymbol{\theta}^\top \mathbf{K}\boldsymbol{\theta}$$

Application to regression

Setting

- $\mathbf{x}_i \in \mathcal{X}$ (not necessarily $\mathbb{R}^d$!) and $y_i \in \mathbb{R}, \mathbf{y} = (y_1, \cdots, y_n)^\top \in \mathbb{R}^n$
- We consider the square loss $\ell(y, y') = (y - y')^2$
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Kernel Ridge Regression

The ERM in the RKHS is equivalent to the minimization problem:

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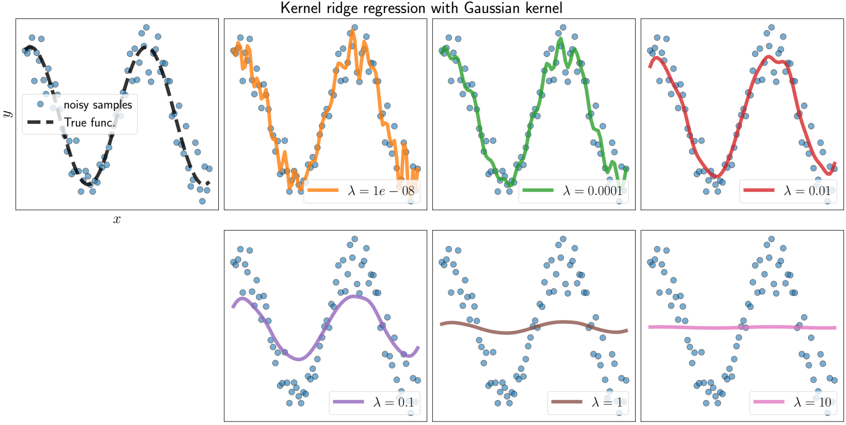
Solution

Given by $\boldsymbol{\theta}^\star = (\mathbf{K} + \lambda n \mathbf{I})^{-1}\mathbf{y}, \ \forall \mathbf{x} \in \mathcal{X}, f^\star(\mathbf{x}) = \sum_{i=1}^{n} \theta_i^\star \kappa(\mathbf{x}, \mathbf{x}_i)$.

Application to regression

- Gaussian kernel $\kappa(x, x') = \exp(-|x - x'|^2/(2\sigma^2))$
- Regularization parameter λ



Kernel ridge regression vs linear regression

- Take $\mathcal{X} = \mathbb{R}^d$ and the linear kernel $\kappa(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle$.
- Let $\mathbf{X} = (\mathbf{x}_1, \cdot, \mathbf{x}_n)^\top \in \mathbb{R}^{n \times d}$ the data. The Gram matrix is $\mathbf{K} = \mathbf{X}\mathbf{X}^\top$.
- Then corresponding function is

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- We have $\mathbf{w}^\star = \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top + \lambda n \mathbf{I}_n)^{-1} \mathbf{y}$.

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$$f^\star(\mathbf{x}) = \sum_{i=1}^{n} \theta_i^\star \kappa(\mathbf{x}, \mathbf{x}_i) = \langle \mathbf{x}, \sum_{i=1}^{n} \theta_i^\star \mathbf{x}_i \rangle = \langle \mathbf{x}, \mathbf{w}^\star \rangle.$$

- We have $\mathbf{w}^\star = \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top + \lambda n \mathbf{I}_n)^{-1} \mathbf{y}$.

ℓ_2 penalized linear regression: ridge regression

The problem

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (y_i - \mathbf{w}^\top \mathbf{x}_i)^2 + \lambda \|\mathbf{w}\|_2^2 \text{ has solution } \mathbf{w}^\star = (\mathbf{X}^\top \mathbf{X} + \lambda n \mathbf{I}_d)^{-1} \mathbf{X}^\top \mathbf{y}.$$

Kernel ridge regression vs linear regression

- Take $\mathcal{X} = \mathbb{R}^d$ and the linear kernel $\kappa(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle$.
- Let $\mathbf{X} = (\mathbf{x}_1, \cdot, \mathbf{x}_n)^\top \in \mathbb{R}^{n \times d}$ the data. The Gram matrix is $\mathbf{K} = \mathbf{X}\mathbf{X}^\top$.
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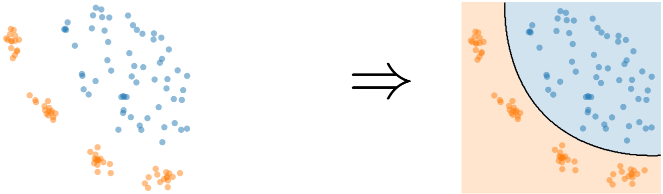
Matrix inversion lemma

$$(\mathbf{X}^\top \mathbf{X} + \lambda n \mathbf{I}_d)^{-1} \mathbf{X}^\top = \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top + \lambda n \mathbf{I}_n)^{-1}$$

- Both agree !
- Complexity roughly: KRR $O(n^3)$, RR $O(\min\{d^3, n^3\})$.

Binary classification



Objective

$$(\mathbf{x}_i, y_i)_{i=1}^n \quad \Rightarrow \quad f : \mathbb{R}^d \to \{-1, 1\}$$

- Train a function $f(\mathbf{x}) = y \in \mathcal{Y}$ predicting a binary value ($\mathcal{Y} = \{-1, 1\}$).
- $f(\mathbf{x}) = 0$ defines the boundary on the partition of the feature space.

ERM in RKHS

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \ell(y_i, f(\mathbf{x}_i)) + \lambda \|f\|_{\mathcal{H}}^2 \,.$$

Loss functions

A focus on classification problems $\mathcal{Y} = \{-1, 1\}$

$$\ell(y_i, f(\mathbf{x}_i)) = \Phi(y_i f(\mathbf{x}_i)) \text{ with } \Phi \text{ non-increasing.}$$

Loss functions

A focus on classification problems $\mathcal{Y} = \{-1, 1\}$

$$\ell(y_i, f(\mathbf{x}_i)) = \Phi(y_i f(\mathbf{x}_i)) \text{ with } \Phi \text{ non-increasing.}$$

- $y_i f(\mathbf{x}_i)$ is **the margin**.
- $\ell(y_i, f(\mathbf{x}_i)) = \mathbf{1}_{y_i f(\mathbf{x}_i) \leq 0}$ (0/1 loss)
- $\ell(y_i, f(\mathbf{x}_i)) = \max\{0, 1 - y_i f(\mathbf{x}_i)\}$ (hinge loss: **SVM**)
- $\ell(y_i, f(\mathbf{x}_i)) = \log(1 + e^{-y_i f(\mathbf{x}_i)})$ (logistic loss)

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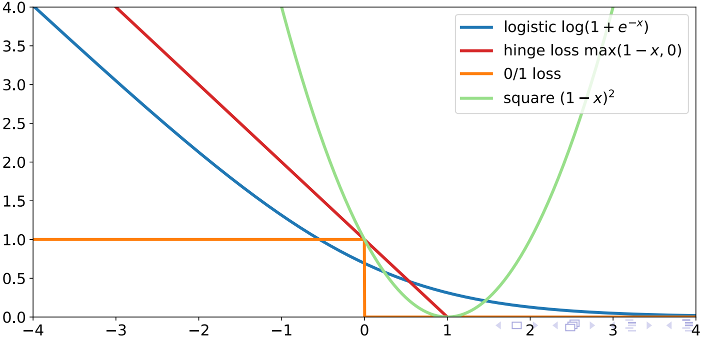
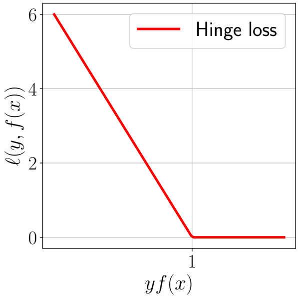


Support Vector Machines (SVM)

Definition

- The hinge-loss is the function $\mathbb{R} \to \mathbb{R}_+$:

$$\Phi_{\text{hinge}}(x) = \max(1 - x, 0)$$
$$= \begin{cases} 0 & \text{if } x \geq 1 \\ 1 - x & \text{otherwise} \end{cases}$$



Interpretation of the loss $\ell(y, f(x)) = \Phi_{\text{hinge}}(yf(x))$

- When $yf(x) \geq 0$: $\text{sign}(y) = \text{sign}(f(x))$ thus good prediction $\to$ the loss should be "small".
- When $yf(x) \geq 1$: if $y = +1 \implies f(x) \geq 1$, if $y = -1 \implies f(x) \leq -1 \to$ zero loss is a good idea.
- When $yf(x) \leq 1$ we can do better.

Support Vector Machines (SVM)

Definition

- SVM is the corresponding large-margin classifier, which solves:

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \Phi_{\text{hinge}}(y_i f(\mathbf{x}_i)) + \lambda \|f\|_{\mathcal{H}}^2 .$$

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- SVM is the corresponding large-margin classifier, which solves:

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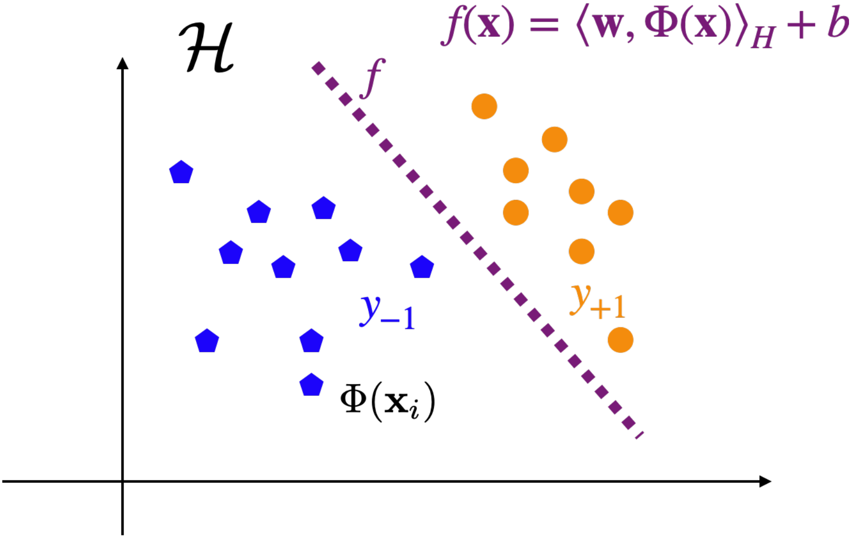
Solving for the SVM (details in Steinwart and Christmann 2008)

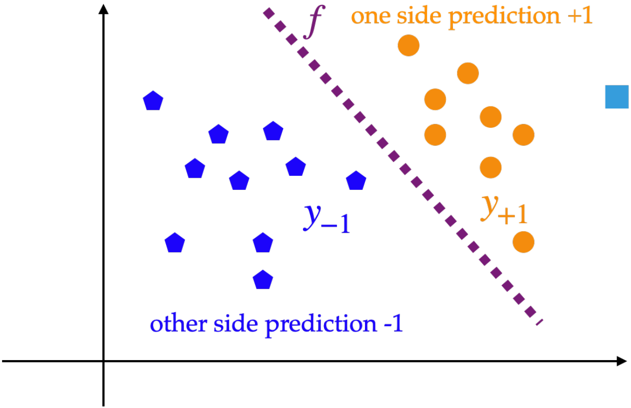
- Representer theorem: sol. of the form $f^\star(\mathbf{x}) = \sum_{i=1}^{n} \theta_i^\star \kappa(\mathbf{x}, \mathbf{x}_i)$.
- $\boldsymbol{\theta}^\star$ can be found by solving a quadratic program (QP).
- Again: we only need to know the Gram matrix $\mathbf{K} = (\kappa(\mathbf{x}_i, \mathbf{x}_j))_{ij}$.

What is SVM doing ?

Find a separating hyperplane in the RKHS



What is SVM doing ?



- Classification:

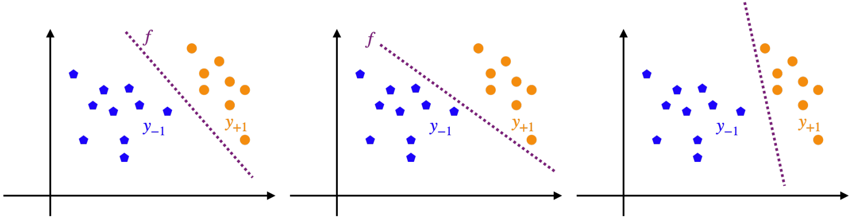
$$\text{sign}(f)$$

$$\textit{if } f(\mathbf{x}) > 0 \rightarrow +1$$

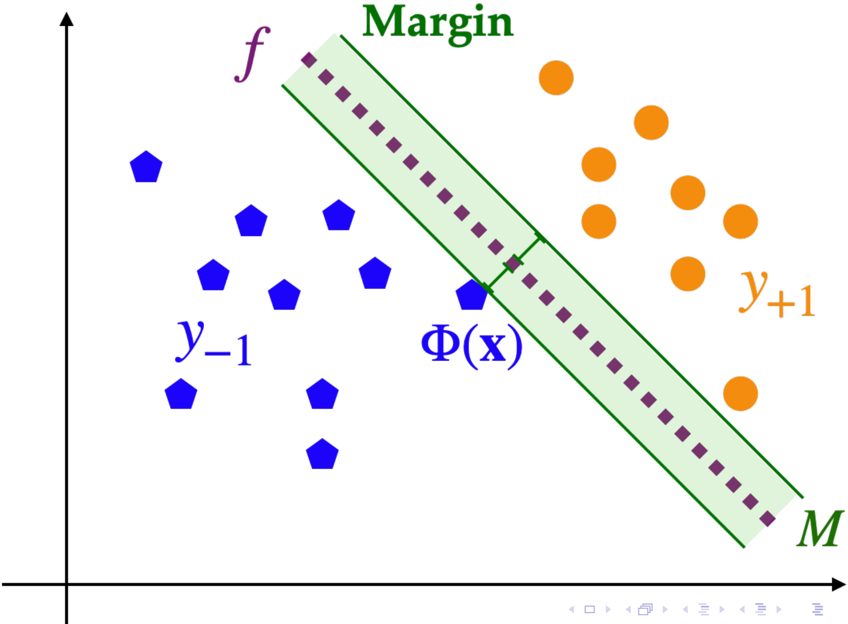
$$\textit{if } f(\mathbf{x}) < 0 \rightarrow -1$$

What is SVM doing ?

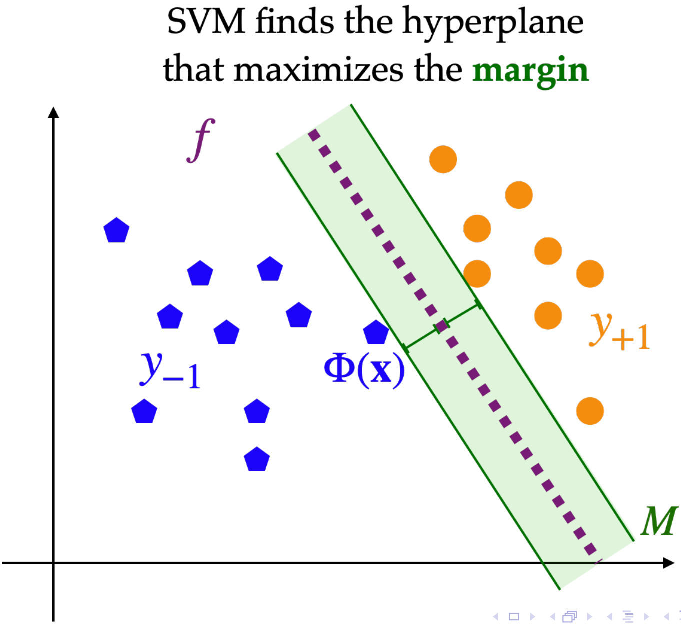
But there could be an infinity of separating hyperplanes or zero !



What is SVM doing ?

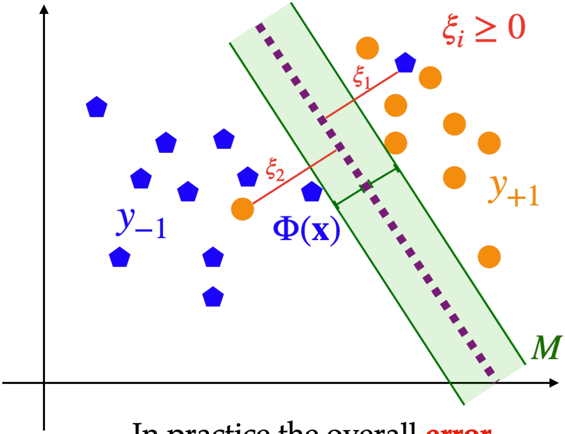


What is SVM doing ?



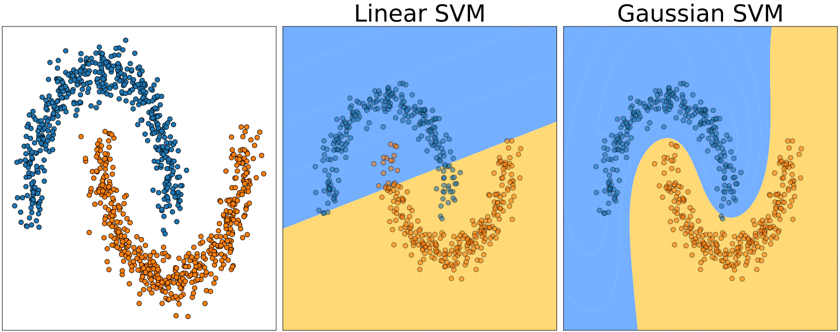
What is SVM doing ?

+ We allow **some errors** to be made



In practice the overall **error**
is controlled by a regularization param. C

Example



Conclusion

- Kernel theory is very rich, kernels are quite simple but also versatile.
- Defines a very general way of learning classifiers/regressors on any kind of space.
- Based on the representer theorem: we only need the Gram matrix !
- Difficulties: the choice of the kernel (see TD), also can be expensive.

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