Fundamentals of Machine Learning

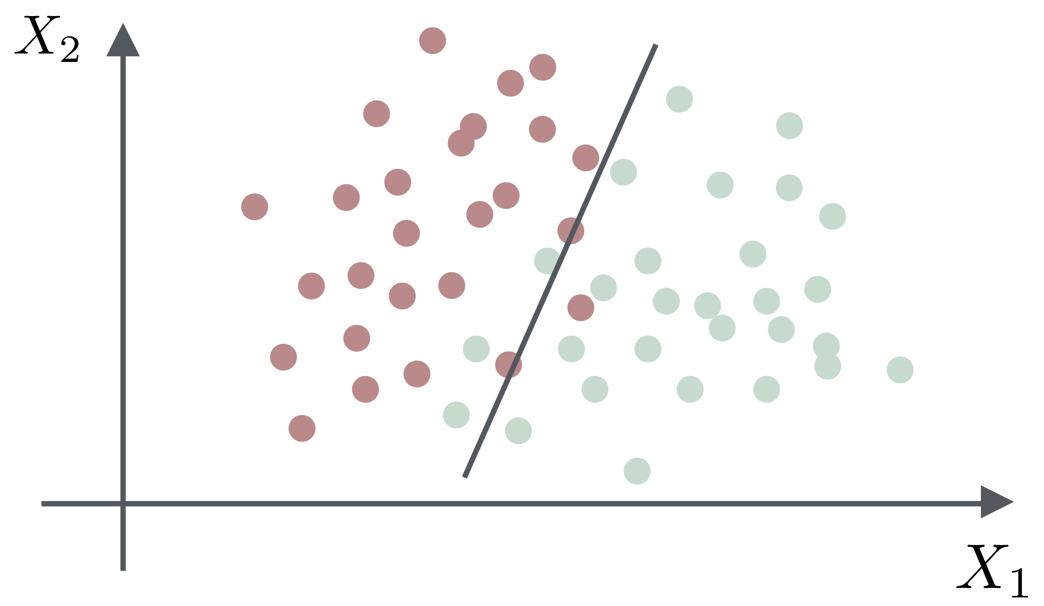
Yassine Laguel

Mail : yassine.laguel@univ-cotedazur.fr

UNIVERSITÉ CÔTE D'AZUR

Limitations of linear models

- Linear methods are great for linear tasks
  - In linear classification



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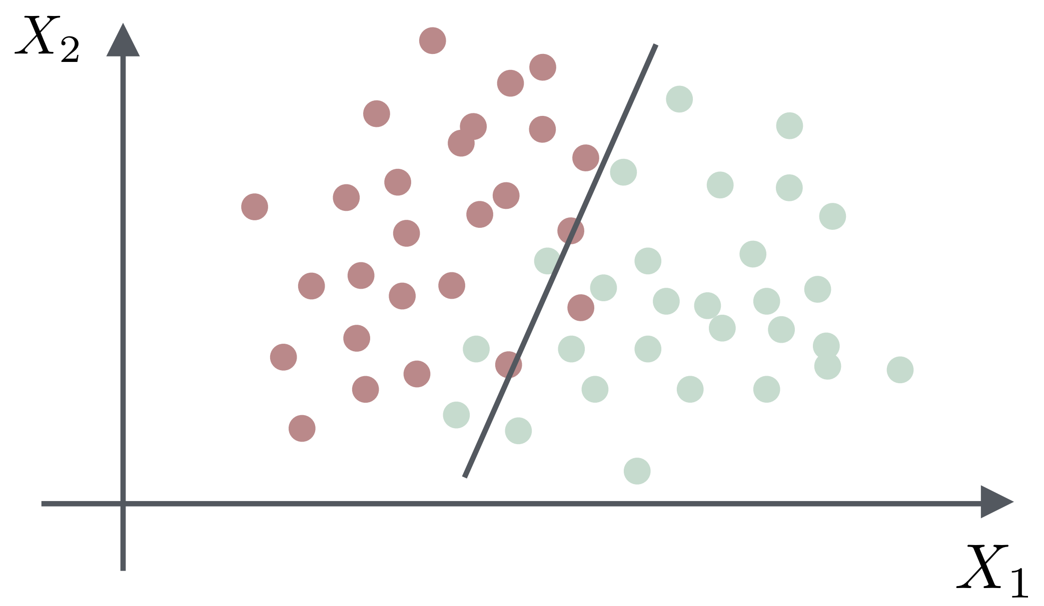

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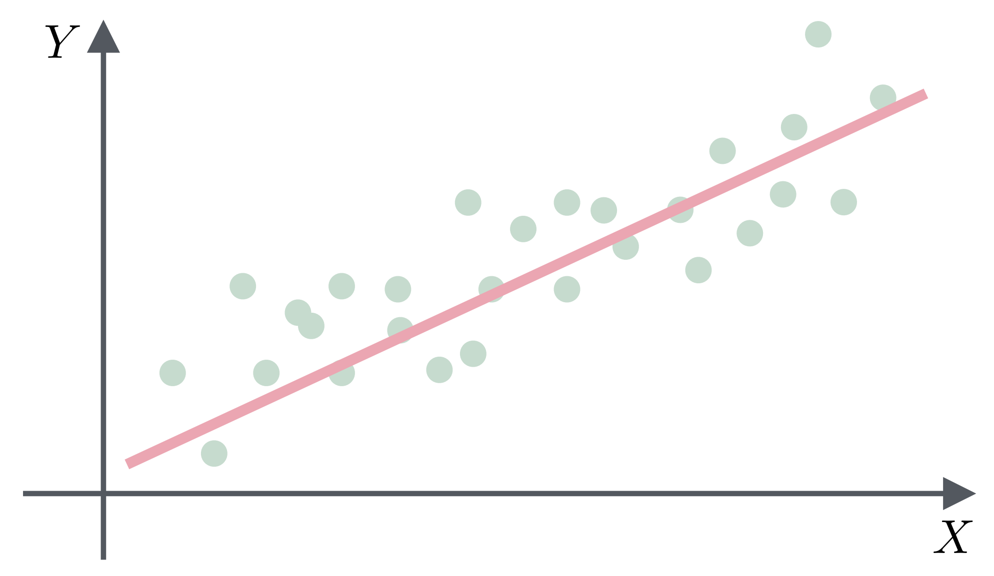

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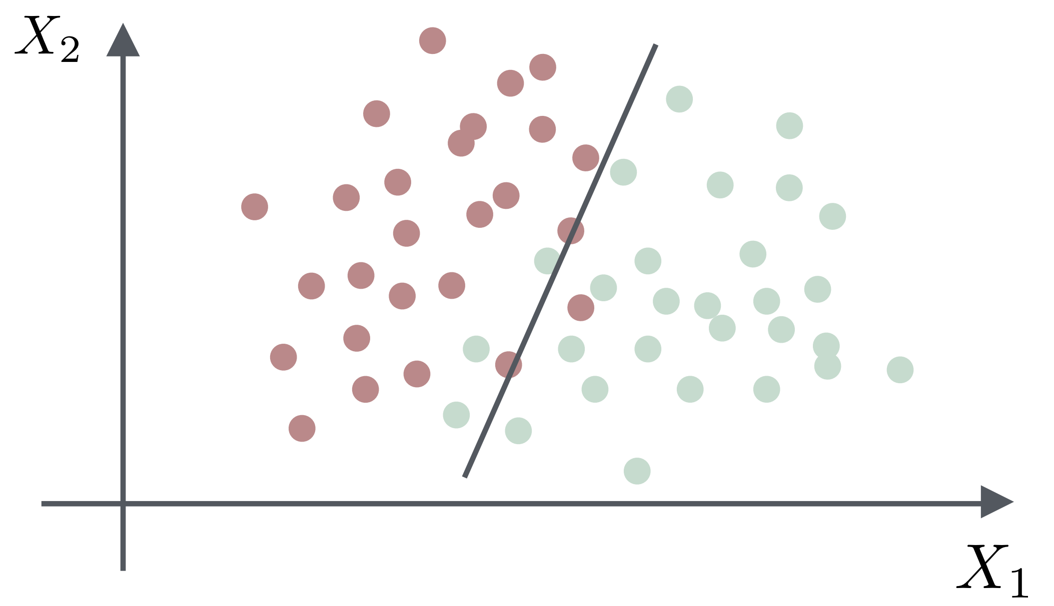

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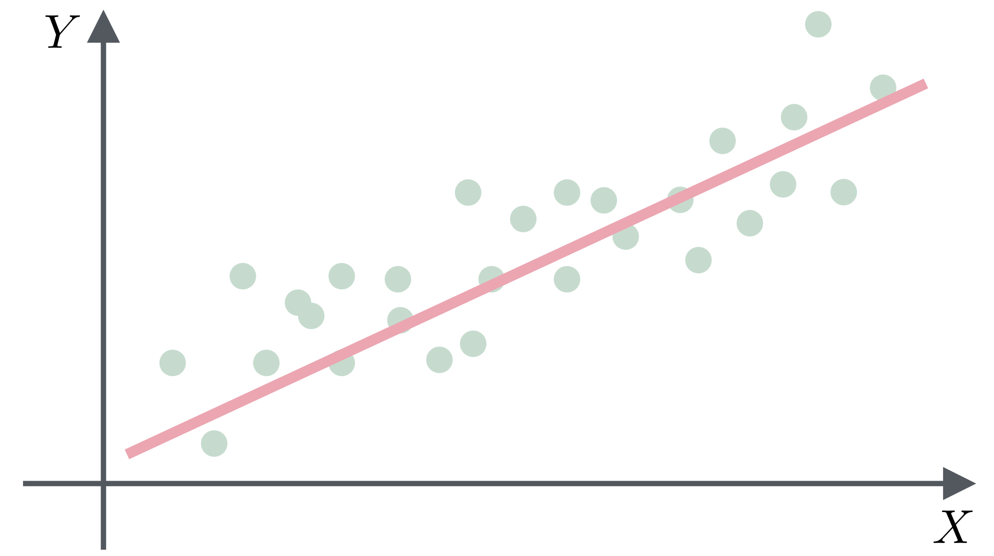

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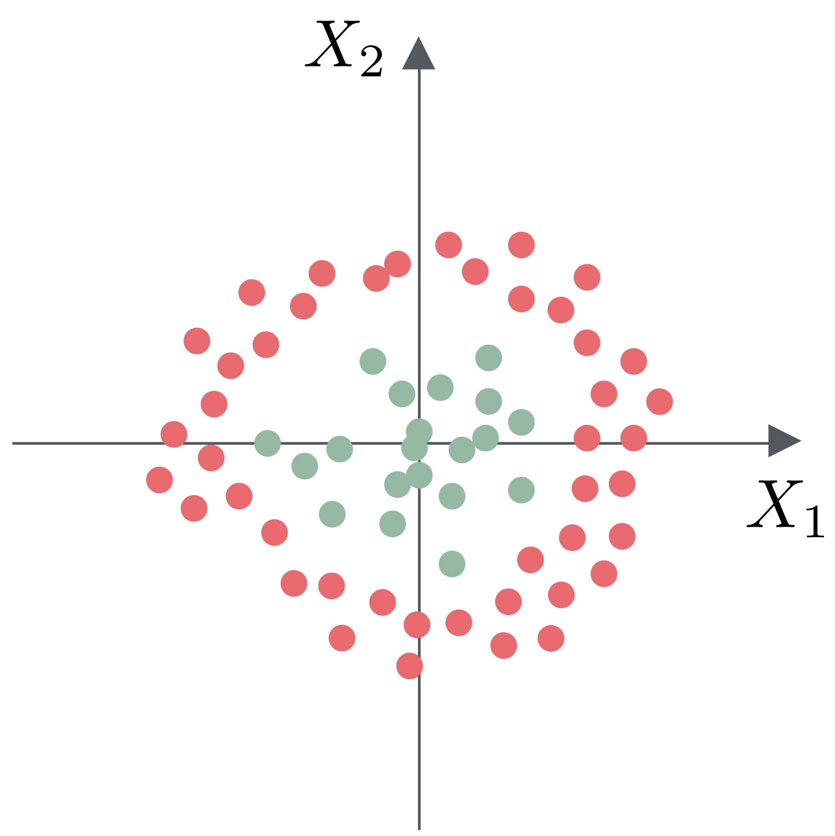
- What can we do when for non-linear tasks ?
  - In $\mathbb{R}^2$ no hyperplane separates the following two classes.



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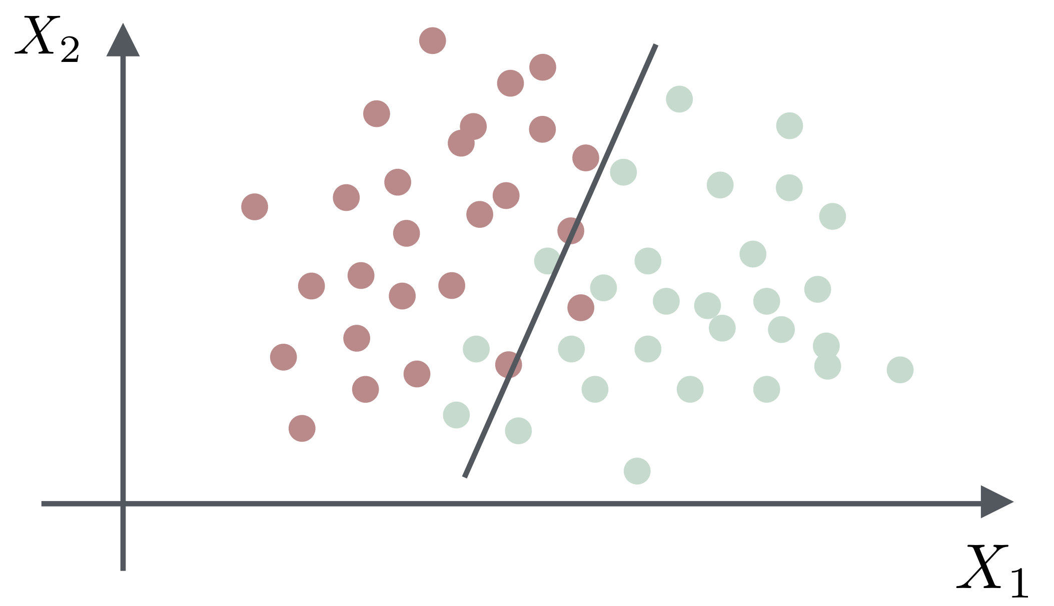

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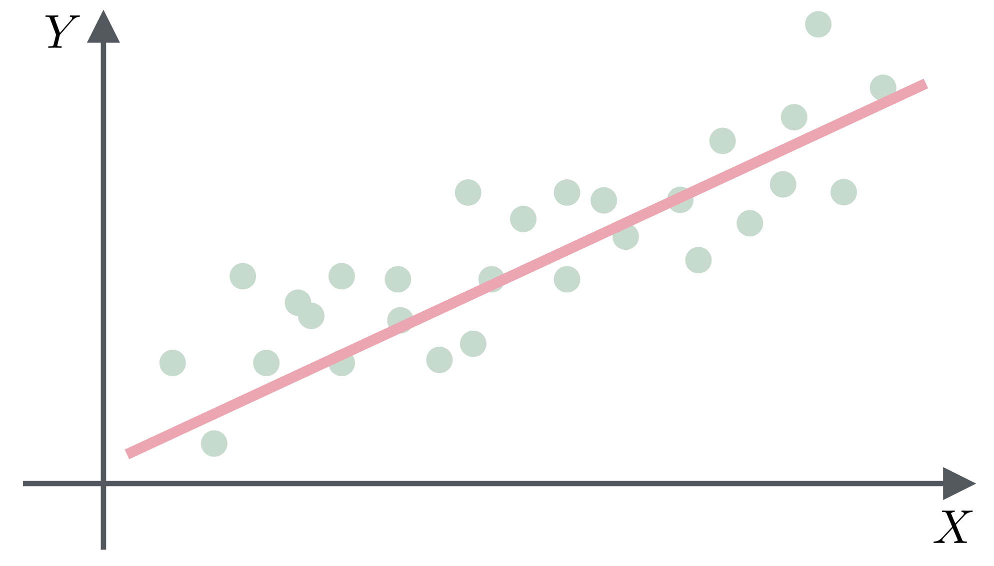

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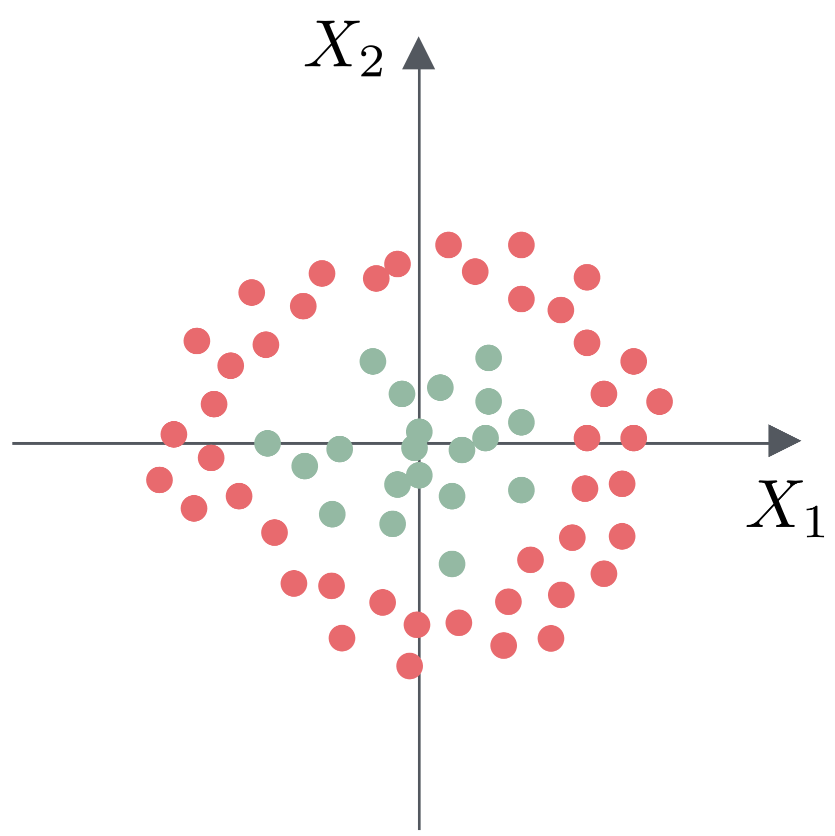
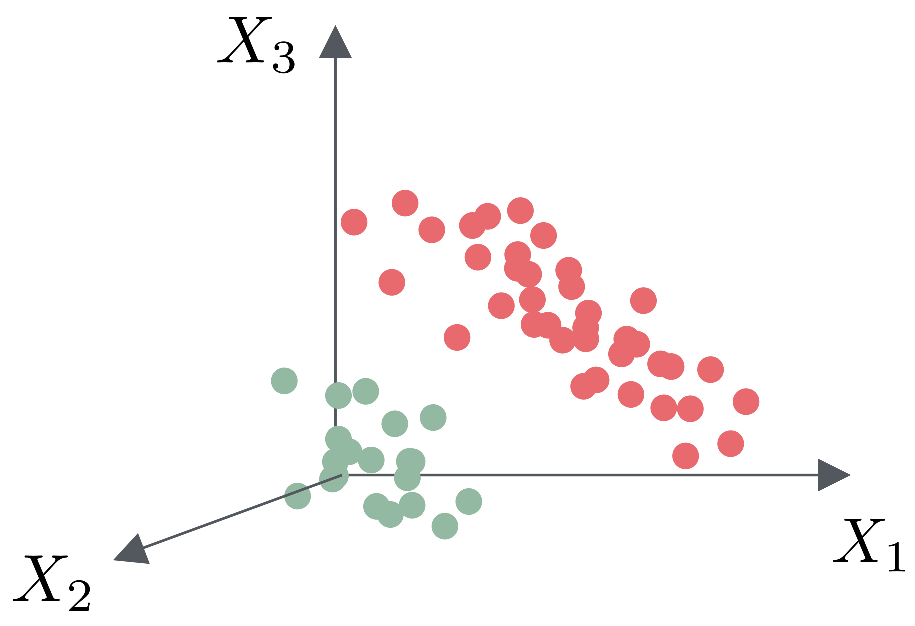


  - Yet, if we apply the transformation $x \mapsto \varphi(x) = \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right)^\top$.

    We obtain linearly separable data points in $\mathbb{R}^3$.



Positive Definite Kernels

A First definition

Definition : Positive definite Kernel

A positive definite kernel on a set $\mathcal{X}$ is a function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ which satisfies

$$\text{(symmetry) (i)} \quad K(x, x') = K(x', x), \quad \forall x, x' \in \mathcal{X}^2$$

$$\text{(positive-definiteness) (ii)} \quad \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j K(\mathbf{x}_i, \mathbf{x}_j) \geq 0 \qquad \forall (x_1, \ldots, x_n) \in \mathcal{X}^n$$

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Remarks :

- In other words, K is a p.d. kernel if and only if, for any $N \in \mathbb{N}$, and any set of points $(x_1, \ldots, x_n) \in \mathcal{X}^N$, the similarity matrix $\boldsymbol{K}_{i,j} = K(x_i, x_j)$ is positive definite.

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Stability properties

Proposition : Stability through elementary operations

Let K_1, K_2 be two positive definite kernels. Let $c > 0$.

Then

(i) $K_1 + K_2$ is a positive definite kernel.

(ii) $c \cdot K_1$ is a positive definite kernel.

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Proof : on the blackboard.

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Proposition : Pointwise limit of p.d. kernels

Let $(K_i)_{i \geq 0}$ be a sequence of p.d. kernels that converges pointwise to a function K. Then K is also a p.d. kernel.

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  - e^K is a p.d. kernel.

Implementation

Reproducing Kernel Hilbert space

- Kernels as inner products

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Let $\mathcal{X}$ be a set and $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ be a class of functions forming a (real) Hilbert space with inner product $\langle ., . \rangle_{\mathcal{H}}$.

The function $K : \mathcal{X}^2 \mapsto \mathbb{R}$ is called a **reproducing kernel** of $\mathcal{H}$ if

(i) $\mathcal{H}$ contains all functions of the form $K_x : u \mapsto K(x, u),$ for $x \in \mathcal{X}$.

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Unicity results for the kernel and the RKHS

Proposition : Continuity. of the evaluation map

A Hilbert space of functions $H \subset \mathbb{R}^{\mathcal{X}}$ is a RKHS if and only if for any $x \in \mathcal{X}, f \mapsto f(x)$ from $\mathcal{H}$ to $\mathbb{R}$ is continuous.

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If two RKHS have the same reproducing kernel, then they are equal.

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Kernels as inner products

Definition : Reproducing Kernel Hilbert space

Let $\mathcal{X}$ be a set and $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ be a class of functions forming a (real) Hilbert space with inner product $\langle ., . \rangle_{\mathcal{H}}$.

The function $K : \mathcal{X}^2 \mapsto \mathbb{R}$ is called a **reproducing kernel** of $\mathcal{H}$ if

(i) $\mathcal{H}$ contains all functions of the form $K_x : u \mapsto K(x,u)$, for $x \in \mathcal{X}$.

(ii) For every $\mathbf{x} \in \mathcal{X}$ and $f \in \mathcal{H}$, we have $f(x) = \langle f, K_x \rangle_{\mathcal{H}}$.

Remarks :

- As a recall, a Hilbert space is a complete vector space endowed with an inner product.
- Property (ii) is often called the reproducing property.
- For $\mathcal{H}$ given, if a reproducing kernel exists, then $\mathcal{H}$ is called a **reproducing kernel Hilbert space**.

Proposition : Reproducing kernels are p.d. kernels

Reproducing kernels are positive definite kernels.

Proof : On the black board

Unicity results for the kernel and the RKHS

Proposition : Continuity. of the evaluation map

A Hilbert space of functions $H \subset \mathbb{R}^{\mathcal{X}}$ is a RKHS if and only if for any $x \in \mathcal{X}, f \mapsto f(x)$ from $\mathcal{H}$ to $\mathbb{R}$ is continuous.

Proof : On the blackboard.

Proposition : Unicity of the reproducing kernel

If two reproducing kernel exist for a Hilbert space, then they are equal.

Proof : On the blackboard.

Proposition : Unicity of the. RKHS

If two RKHS have the same reproducing kernel, then they are equal.

Proof : On the blackboard.

Correspondence property and representation theorem

- Aronszajn theorem

Proposition : Aronszajn theorem

$K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a p.d. kernel on $\mathcal{X}$ if and only if there exists a Hilbert space $\mathcal{H}$ and a mapping $\varphi : \mathcal{X} \to \mathcal{H}$ such that

$$K\left(\mathbf{x}, \mathbf{x}'\right) = \left\langle \Phi(\mathbf{x}), \Phi\left(\mathbf{x}'\right) \right\rangle_{\mathcal{H}}, \quad \forall x, x' \in \mathcal{X}.$$

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- In other words, the kernel operates a measure of similarity on data, made explicit as an inner product after application of φ.

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- Any algorithm that solely involves dot products on $\mathcal{X} \times \mathcal{X}$ may be generalized at a cheap cost by replacing the dot product with a p.d. kernel: this procedure is often called the **kernel trick**.

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Representation theorem

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Let $\mathcal{X}$ be a set with a p.d. kernel K, $\mathcal{H}$ be the corresponding RKHS, and $S = \{x_1, \ldots, x_n\} \subset \mathcal{X}$ a finite set of points in $\mathcal{X}$.

Let $\psi : \mathbb{R}^{n+1} \to \mathbb{R}$ be a function of $n+1$ variables strictly increasing w.r.t. the last variable. Then any solution of

$$\min_{f \in \mathcal{H}} \psi\left(f(\mathbf{x}_1), \cdots, f(\mathbf{x}_n), \|f\|_{\mathcal{H}}\right)$$

admits a representation of the form :

$$f(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i K(\mathbf{x}_i, \mathbf{x}) = \sum_{i=1}^{n} \alpha_i K_{\mathbf{x}_i}(\mathbf{x}), \quad \forall \mathbf{x} \in \mathcal{X}.$$

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Implementation