# Reproducing kernels in the vectorial case

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# Some reminders on Hilbert spaces

- $H$ real **Hilbert space** : real vector space (possibly infinite dimensional) with an inner product $\langle \cdot, \cdot \rangle_H$, which is a complete metric space for the corresponding norm $\| \cdot \|_H$.
- A **linear form** on $H$ is a linear map $\mu : H \to \mathbb{R}$.
- A linear form $\mu$ on $H$ is continuous if it satifies

$$\exists C > 0, \quad \forall u \in H, \quad |\mu(u)| \leq C\|u\|_H.$$

- The space of continuous linear forms on $H$ is denoted $H^*$, the **dual space** of $H$. It is a Hilbert space with the norm

$$\|\mu\|_{H^*} := \sup\{|\mu(u)|, \ \|u\|_H \leq 1\}.$$

# Some reminders on Hilbert spaces

- **Riesz representation theorem** : every continuous linear form $\mu$ can be written as a scalar product :

$$\forall \mu \in H^*, \quad \exists!\, \tilde{\mu} \in H, \quad \forall u \in H,\ \mu(u) = \langle \tilde{\mu}, u \rangle_H.$$

- Conversely for every $v \in H$, the map $u \mapsto \langle u, v \rangle_H$ is a continuous linear form on $H$.
- The mapping $\mathcal{K}_H : \mu \mapsto \tilde{\mu}$ is an isometry between $H^*$ and $H$ : $\|\mu\|_{H^*} = \|\tilde{\mu}\|_H$.

# Reproducing kernels, the scalar case

- Let $H$ be a Hilbert space whose elements are functions $f : X \to \mathbb{R}$. $X$ can be any set.
- For $x \in X$, denote $\delta_x$ the linear form $f \mapsto f(x)$.

## Definition

- $H$ is a **Reproducing Kernel Hilbert Space (RKHS)** if all $\delta_x$ are continuous, i.e. $\forall x \in X, \quad \delta_x \in H^*$.
- The **reproducing kernel** of $H$ is the map $K_H : X \times X \to \mathbb{R}$ defined by

$$\forall x \in X, \quad K_H(\cdot, x) := \mathcal{K}_H \delta_x.$$

More concretely it satisfies :

$$\forall x \in X, \, \forall f \in H, \quad \langle K_H(\cdot, x), f \rangle_H = f(x).$$

# Reproducing kernels, the scalar case

Properties of reproducing kernels :

- **Reproducing property** :

$$\forall x, y \in X, \quad \langle K_H(\cdot, x), K_H(\cdot, y)\rangle_H = K_H(x, y).$$

- **Symetry** : $K_H(x, y) = K_H(y, x)$.
- $K_H$ is a **positive definite kernel** on $X$ : for every $n \in \mathbb{N}$, points $x_1, \dots, x_n$ in $X$, and real numbers $a_1, \dots, a_n$,

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

In other words, for every $n \in \mathbb{N}$, $x_1, \dots, x_n \in X$, the matrix $(K_H(x_i, x_j))_{1 \leq i,j \leq n}$ is a symetric positive matrix.

# Reproducing kernels, the vectorial case

- Let $H$ be a Hilbert space whose elements are functions $f : X \to E$, where $E$ is an euclidean space.
- For $x \in X$, $\alpha \in E$, denote $\delta_x^\alpha$ the linear form $f \mapsto \langle f(x), \alpha \rangle_E$.

## Definition

- $H$ is a **Reproducing Kernel Hilbert Space (RKHS)** if all $\delta_x^\alpha$ are continuous, i.e. $\forall x \in X,\ \forall \alpha \in E, \quad \delta_x^\alpha \in H^*$.
- The **reproducing kernel** of $H$ is the map $K_H : X \times X \to \mathrm{End}(E)$ defined by

$$\forall x \in X,\ \forall \alpha \in E, \quad K_H(\cdot, x)\alpha := \mathcal{K}_H \delta_x^\alpha.$$

It satisfies :

$$\forall x \in X,\ \forall \alpha \in E\ \forall f \in H, \quad \langle K_H(\cdot, x)\alpha, f \rangle_H = \langle f(x), \alpha \rangle_E.$$

# Reproducing kernels, the vectorial case

Properties of reproducing kernels :

- **Reproducing property** : $\forall x, y \in X,\ \forall \alpha, \beta \in E$,

$$\langle K_H(\cdot, x)\alpha, K_H(\cdot, y)\beta \rangle_H = \langle \alpha, K_H(x, y)\beta \rangle_E.$$

- **Symetry** : $K_H(y, x) = K_H(x, y)^*$.
- $K_H$ is a **positive definite kernel** on $X$ : for every $n \in \mathbb{N}$, points $x_1, \dots, x_n$ in $X$, and vectors $\alpha_1, \dots, \alpha_n$ in $E$,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \langle \alpha_i, K_H(x_i, x_j)\alpha_j \rangle_E \geq 0.$$

remark : more precisely, a positive definite kernel on $X$ is a function $X \times X \to \mathrm{End}(E)$ which satisfies the two last properties.

# Reproducing kernels, the vectorial case

If we are given an orthonormal basis of $E$ (e.g. the canonical basis for $E = \mathbb{R}^m$), then $K_H(x, y)$ can be considered as a $m \times m$ matrix (where $m = \dim E$). Then the two last properties can be rephrased as

- $K_H(y, x) = K_H(x, y)^T$,
- for every $n \in \mathbb{N}$ and points $x_1, \dots, x_n$ in $X$, the $nm \times nm$ matrix with $m \times m$ blocks $K_H(x_i, x_j)$ is a symetric positive matrix.

# Equivalence between reproducing kernels and positive definite kernels

**Theorem**

*Let $X$ be any set and $E$ an euclidean space. Every positive definite kernel $K : X \times X \to End(E)$ is associated to a unique RKHS $H$ of functions $f : X \to E$ such that $K_H = K$.*

For the LDDMM framework, this shows that one can start by choosing a kernel function and build all the theory from it.
Examples of commonly used kernels :

- gaussian $K_V(x, y) = \exp(-\|x - y\|^2/\sigma^2)\mathrm{Id}$ ($\sigma > 0$ is scale parameter)
- Cauchy $K_V(x, y) = 1/(1 + \|x - y\|^2/\sigma^2)\mathrm{Id}$
- Sobolev kernels, corresponding to the Sobolev spaces. They are defined using Bessel functions.

# Optimal interpolation in RKHS

Let $H$ be a RKHS of functions $f : X \to E$ with strictly positive definite repriducing kernel, $x_i \in X$ distinct points and $\gamma_i \in E$, $1 \leq i \leq n$. Consider the problem

$(P)$ Find $f \in H$ such that $f(x_i) = \gamma_i \ \forall i$ and $\|f\|_H$ is minmal.

**Proposition**

*If there exists $f \in H$ such that $f(x_i) = \gamma_i \ \forall i$, then the problem $(P)$ has a unique solution of the form*

$$f^*(x) = \sum_{i=1}^{n} K_H(x, x_i)\alpha_i$$

*for some vectors $\alpha_i \in E$ which are the solutions to*

$$\sum_{i=1}^{n} K_H(x_j, x_i)\alpha_i = \gamma_j, \ 1 \leq j \leq n.$$