Kernel methods in machine learning
Homework 3

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Exercise 1 : B_n-splines

We have $k(x, y) = B_n(x - y)$. In order to show that k is a positive-definite kernel, thanks to Bochner's theorem, it is sufficient to show that $B_n \in L^1(\mathbb{R})$ and that its Fourier transform only has non-negative real values.

- I is clearly in $L^1(\mathbb{R})$, and we know that, for $f, g \in L^1(\mathbb{R})$, we have $f \star g \in L^1(\mathbb{R})$. Therefore, we can show by induction that $B_n = I \star \cdots \star I$ is in $L^1(\mathbb{R})$.
- As $B_n = I^{\star n}$, we can easily compute its Fourier transform. In fact, we have that, for $f, g \in L^1(\mathbb{R})$, $\mathcal{F}[f \star g] = \mathcal{F}[f]\mathcal{F}[g]$ where $\mathcal{F}$ is the Fourier transformation. Therefore, we have that, once again by induction,

  $$\mathcal{F}[B_n] = \mathcal{F}[I^{\star n}] = (\mathcal{F}[I])^n$$

  We need to compute $\mathcal{F}[I]$:

  $$\forall \xi \in \mathbb{R},\ \mathcal{F}[I](\xi) = \int_{\mathbb{R}} I(x) e^{-i\xi x} \mathrm{d}x = \int_{-1}^{1} e^{-i\xi x} \mathrm{d}x = -\frac{1}{i\xi}[e^{-i\xi x}]_{-1}^{1} = -\frac{e^{-i\xi} - e^{i\xi}}{i\xi} = \frac{\sin(\xi)}{\xi}$$

  So, we have that

  $$\forall \xi \in \mathbb{R},\ \mathcal{F}[B_n](\xi) = \left(\frac{\sin(\xi)}{\xi}\right)^n$$

  Therefore, $\mathcal{F}[B_n]$ has only non-negative values if, and only if n is even. Otherwise, $\mathcal{F}[B_n](-\frac{\pi}{2}) < 0$.

So, we can conclude that k is a positive-definite kernel if, and only if, n is even.

Moreover, we can describe the corresponding reproducing kernel Hilbert space thanks to a results that we saw in class. The corresponding reproducing kernel Hilbert space $\mathcal{H}$ is

$$\boxed{\mathcal{H} = \left\{ f \in L^2(\mathbb{R}) \mid \frac{1}{2\pi} \int_{\mathbb{R}} \frac{|\hat{f}(\omega)|}{B_n(\omega)} \mathrm{d}\omega > \infty \right\}}$$

endowed with the with the inner product:

$$\langle f, g \rangle_{\mathcal{H}} = \frac{1}{2\pi} \int_{\mathbb{R}} \frac{\hat{f}(\omega)\overline{\hat{g}(\omega)}}{B_n(\omega)} \mathrm{d}\omega$$

Exercise 2 : Sobolev spaces

1.

In order to show that $\mathcal{H}$ is a RHKS, we need to show several points.

Let us make a first remark : f absolutely continuous implies differentiable almost everywhere and for all $x \in [0,1]$,

$$f(x) = f(0) + \int_0^x f'(u)\mathrm{d}u \tag{1}$$

- First, let us start by showing that $\mathcal{H}$ is a Hilbert space for the given bilinear form.

  We have that $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ is symmetric bilinear form. Moreover, for $f \in \mathcal{H}$, $\langle f, f \rangle_{\mathcal{H}} = \int_0^1 (f'(x))^2 \mathrm{d}x \geq 0$. Moreover, thanks to 1 and as $f(0) = 0$ (because $f \in \mathcal{H}$), we have

  $$f(x)| = \left| \int_0^x f'(u)\mathrm{d}u \right| \leq \sqrt{x} \left(\int_0^1 (f'(u))^2 \mathrm{d}u \right)^{1/2} = \sqrt{x} \langle f, f \rangle_{\mathcal{H}} \tag{2}$$

  We used Cauchy-Schwarz's inequality in $L^2([0,1])$ between f' and $\mathbb{1}_{[0,x]}$. So $\langle f, f \rangle_{\mathcal{H}} = 0$ implies $f = 0$. So $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ is a inner product and $\mathcal{H}$ is a pre-Hilbert space.

  Let us show that $\mathcal{H}$ is complete. Let $(f_n)_{n \in \mathbb{N}}$ be a Cauchy sequence in $\mathcal{H}$. Then $(f'_n)_{n \in \mathbb{N}}$ is a Cauchy sequence in the Hilbert space $L^2([0,1])$, so $(f'_n)_{n \in \mathbb{N}}$ converges in $L^2([0,1])$ to a function $g \in L^2([0,1])$. Moreover, thanks to 2 applied to the f_n, we have that, for all $x \in [0,1]$, $(f_n(x))_{n \in \mathbb{N}}$ is a Cauchy sequence in $\mathbb{R}$, which is complete. So, for all $x \in [0,1]$, $(f_n(x))_{n \in \mathbb{N}}$ converges in $\mathbb{R}$ to a real number $f(x)$. Moreover,

  $$f(x) = \lim_n f_n(x) = \lim_n \int_0^x f'_n(u)\mathrm{d}u = \int_0^x g(u)\mathrm{d}u.$$

  So f is absolutely continuous and $f' = g$ almost everywhere, so in particular, $f' \in L^2([0,1])$. Finally, $f(0) = \lim_n f_n(0) = 0$. So we have $f \in \mathcal{H}$ and

  $$\|f_n - f\|_{\mathcal{H}} = \|f'_n - g\|_{L^2([0,1])} = 0.$$

  This shows that $\mathcal{H}$ is a Hilbert space.

- Let us now show that the associated reproducing kernel is

  $$\forall (x,y) \in \mathbb{R}^2, \; K(x,y) = \min(x,y)$$

  First, let us show that, for $x \in \mathbb{R}$, $K_x \in \mathcal{H}$. First, we have that $K_x(0) = 0$. We can express in more details K_x :

  $$\forall y \in [0,1], \; K_x(y) = \begin{cases} y & \text{if } y \leq x \\ x & \text{if } y > x \end{cases}$$

  So, K_x is differentiable except at x and has a square integrable derivative. Therefore, $K_x \in \mathcal{H}$.

  We now need to show the reproducing property : let $f \in \mathcal{H}$ and $x \in [0,1]$, we have

  $$\langle K_x, f \rangle_{\mathcal{H}} = \int_0^1 f'(u) K'(u)\mathrm{d}u = \int_0^x f'(u)\mathrm{d}u = f(x).$$

So, we have that $\mathcal{H}$ is a RHKS and the reproducing kernel is

$$\forall (x,y) \in \mathbb{R}^2,\ K(x,y) = \min(x,y)$$

2.

Showing that $\mathcal{H}$ is a Hilbert space is the same as in question 1. In fact, the added condition on $f(1)$ does not impact the previous proof, we just need to add, when we show that $\mathcal{H}$ is complete that

$$f(1) = \lim_n f_n(1) = 0.$$

The associated reproducing kernel is

$$\forall (x,y) \in \mathbb{R}^2,\ K(x,y) = \min(x,y) - xy$$

Let us prove this statement :

- First, let $x \in [0,1]$, et let us show that $K_x \in \mathcal{H}$. First of all, we have that $K_x(0) = 0-0 = 0$ and $K_x(1) = x - x = 0$. We also have that

$$\forall y \in [0,1],\ K_x(y) = \begin{cases} y(1-x) & \text{if } y \leq x \\ x(1-y) & \text{if } y > x \end{cases}$$

  So, K_x is differentiable except at x and has a square integrable derivative. Therefore, $K_x \in \mathcal{H}$.

- Let us now show the reproducing property : let $f \in \mathcal{H}$ and $x \in [0,1]$, we have

$$\langle K_x, f\rangle_{\mathcal{H}} = \int_0^1 f'(u)K'(u)\mathrm{d}u = \int_0^x (1-x)f'(u)\mathrm{d}u - \int_x^1 xf'(u)\mathrm{d}u = \int_0^x f'(u)\mathrm{d}u - x\underbrace{\int_0^1 f'(u)\mathrm{d}u}_{[f(u)]_0^1 = 0} = f(x).$$

So, we have that $\mathcal{H}$ is a RHKS and the reproducing kernel is

$$\forall (x,y) \in \mathbb{R}^2,\ K(x,y) = \min(x,y) - xy$$

3.

- Let us start by showing that $\mathcal{H}$ is a Hilbert space when endowed with the bilinear form :

$$\forall f,g \in \mathcal{H},\ \langle f,g\rangle_{\mathcal{H}} = \int_0^1 f(u)g(u) + f'(u)g'(u)\mathrm{d}u = \langle f,g\rangle_{L^2([0,1])} + \langle f',g'\rangle_{L^2([0,1])}$$

  $\langle \cdot,\cdot\rangle_{\mathcal{H}}$ is clearly a symmetric bilinear form and we have

$$\forall f \in \mathcal{H},\ \langle f,f\rangle_{\mathcal{H}} = \|f\|^2_{L^2([0,1])} + \|f'\|^2_{L^2([0,1])} \geq 0$$

Moreover, if $\langle f, f\rangle_{\mathcal{H}} = 0$, then $\|f\|^2_{L^2([0,1])} = \|f'\|^2_{L^2([0,1])} = 0$, so $f = 0$ in $L^2([0,1])$. Therefore, $f(x) = 0$ for almost all $x \in [0,1]$. As f is continuous, we have $f = 0$.

So, $\mathcal{H}$ is a pre-Hilbert space.

Let us now show that $\mathcal{H}$ is complete. Let $(f_n)_{n\in\mathbb{N}}$ be a Cauchy sequence in $\mathcal{H}$. As $\|f\|_{L^2([0,1])} \leq \|f\|_{\mathcal{H}}$ and $\|f'\|_{L^2([0,1])} \leq \|f\|_{\mathcal{H}}$, $(f_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in $L^2([0,1])$ and $(f_n')_{n\in\mathbb{N}}$ is also a Cauchy sequence in $L^2([0,1])$. So $(f_n)_{n\in\mathbb{N}}$ converges to $f \in L^2([0,1])$ and $(f_n')_{n\in\mathbb{N}}$ converges to $g \in L^2([0,1])$. As the convergence in L^2 implies the convergence point wise almost everywhere, like in the first question, we can show that f is is absolutely continuous and $f' = g$ almost everywhere, so in particular, $f' \in L^2([0,1])$. Finally, we have that $f(0) = \lim_n f_n(0) = 0$, so $f \in \mathcal{H}$.

Therefore, $\mathcal{H}$ is a Hilbert space.

4.

Let us start by showing the following lemma :

Lemma 1. *Let $f \in \mathcal{H}$. Then, for all $x \in [0,1]$,*

$$f(x) = \int_0^1 (x-u)_+ f''(u)\mathrm{d}u$$

In fact, we have

$$\begin{aligned}
\int_0^1 (x-u)_+ f''(u)\mathrm{d}u &= \int_0^x (x-u) f''(u)\mathrm{d}u \\
&= \left[(x-u)f'(u)\right]_0^x + \int_0^x f'(u)\mathrm{d}u \quad \text{by intergration by part} \\
&= \int_0^x f'(u)\mathrm{d}u \quad \text{as f'(0) = 0} \\
&= f(x)
\end{aligned}$$

- To show that $\mathcal{H}$ is a Hilbert space, we can do like in the first question. We just need to use a slightly different version of 2 : for all $x \in [0,1]$, using lemma 1 and Cauchy-Schwarz's inequality =

$$f(x)| = \left|\int_0^1 (x-u)_+ f''(u)\mathrm{d}u\right| \leq \left(\int_0^1 (x-u)_+\mathrm{d}u\right)^{1/2} \langle f, f\rangle_{\mathcal{H}}^{1/2} \tag{3}$$

  Therefore, we can easily show that $\mathcal{H}$ is a pre-Hilbert space.

  To show that $\mathcal{H}$ is complete, let $(f_n)_{n\in\mathbb{N}}$ be a Cauchy sequence of $\mathcal{H}$. Then, $(f_n'')_{n\in\mathbb{N}}$ is a Cauchy sequence in $L^2([0,1])$ so converges to $g \in L^2([0,1])$, and, using 3, we see that for all $x \in [0,1]$, $(f_n(x))_{n\in\mathbb{N}}$ is a Cauchy sequence in $\mathbb{R}$ so converges to $f(x) \in \mathbb{R}$. Therefore, as we did in the first question and using lemma 1, we have

$$f(x) = \lim_n f_n(x) = \lim_n \int_0^1 (x-u)_+ f_n''(u)\mathrm{d}u = \int_0^1 (x-u)_+ g(u)\mathrm{d}u$$

So $f'' = g \in L^2([0,1])$ almost everywhere, therefore f' exists and is absolutely continuous, and we easily see that $f(0) = f'(0) = 0$. So $f \in \mathcal{H}$ and therefore, $\mathcal{H}$ is complete

Thus, $\mathcal{H}$ is a Hilbert space.

- Let us now show that the associated kernel is

$$\forall (x,y) \in [0,1],\ K(x,y) = \int_0^1 (x-u)_+(y-u)_+ \mathrm{d}u$$

  - K is clearly a positive definite kernel.
  - Let us show that, for all $x \in [0,1],\ K_x \in \mathcal{H}$: to do this, we will start by computing the derivatives of K_x. As, for all $u \in [0,1]$, $y \mapsto (x-u)_+(y-u)_+$ is a $\mathcal{C}^2$ function on the compact space $[0,1]$, we can derive under the integral :

$$\forall y \in [0,1],\ K_x'(y) = \int_0^y (x-u)_+ \mathrm{d}u = \int_0^{\min(x,y)} x-u\mathrm{d}u = \left[xu - \frac{1}{2}u^2\right]_0^{\min(x,y)} = x\min(x,y) - \frac{1}{2}\min(x$$

Moreover, we also have

$$\forall y \in [0,1],\ K_x''(y) = \begin{cases} x-y \text{ if } y \leq x \\ 0 \text{ if } x \leq y \end{cases}$$

So, K_x' exists and is absolutely continuous, $K_x(0) = 0$, $K_x'(0) = 0$ and $K_x'' \in L^2([0,1])$. So $K_x \in \mathcal{H}$.

  - Finally, we need to show the reproducing property : let $f \in \mathcal{H}$ and $x \in [0,1]$:

$$\langle K_x, f\rangle_{\mathcal{H}} = \int_0^1 K_x''(u)f''(u)\mathrm{d}u = \int_0^x (x-u)f''(u)\mathrm{d}u = \int_0^1 (x-u)_+ f''(u)\mathrm{d}u = f(x)$$

thanks to lemma 1.

Therefore, we have that $\mathcal{H}$ is a RHKS and the reproducing kernel is

$$\forall (x,y) \in \mathbb{R}^2,\ K(x,y) = \int_0^1 (x-u)_+(y-u)_+ \mathrm{d}u$$