

**Question 1:** Let  $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  be a valid kernel function. Define

$$k_{\text{norm}}(x, z) := \frac{k(x, z)}{\sqrt{k(x, x)}\sqrt{k(z, z)}}.$$

Is  $k_{\text{norm}}$  a valid kernel? Justify your answer.

**Answer:** Yes, it is. Let  $k(x, z) = \langle \phi(x), \phi(z) \rangle$  for some mapping  $\phi : \mathcal{X} \rightarrow \mathcal{H}$ , where  $\mathcal{H}$  is a Hilbert space. Then

$$k_{\text{norm}}(x, z) = \langle \phi(x) / \|\phi(x)\|_2, \phi(z) / \|\phi(z)\|_2 \rangle$$

so that it is still a valid inner product, where the feature mapping is now  $x \mapsto \phi(x) / \|\phi(x)\|_2$  for  $\|\phi(x)\|_2^2 = \langle \phi(x), \phi(x) \rangle$ .  $\square$

**Question 2:** Consider the class of functions

$$\mathcal{H} := \{f : f(0) = 0, f' \in L^2([0, 1])\},$$

that is, functions  $f : [0, 1] \rightarrow \mathbb{R}$  with  $f(0) = 0$  that are almost everywhere differentiable, where  $\int_0^1 (f'(t))^2 dt < \infty$ . On this space of functions, we define the inner product by

$$\langle f, g \rangle = \int_0^1 f'(t)g'(t)dt.$$

Show that  $k(x, z) = \min\{x, z\}$  is the reproducing kernel for  $\mathcal{H}$ , so that it is (i) positive semidefinite and (ii) a valid kernel.

**Answer:** If we show that  $k(x, z) = \min\{x, z\}$  is indeed the reproducing kernel for  $\mathcal{H}$ , then that suffices to demonstrate that it is a positive definite function. We have for  $g(z) = k(x, z)$  that (almost everywhere)  $g'(z) = \mathbf{1}\{x \leq z\}$ , so that

$$\langle f, k(z, \cdot) \rangle = \int_0^1 f'(t)\mathbf{1}\{t \leq z\} dt = \int_0^z f'(t)dt = f(z) - f(0) = f(z).$$

Thus  $k$  is evidently a reproducing kernel, so it must be a positive definite function.

(Another way to see that, we have  $\min\{x, z\} = k(x, z) = \int_0^1 \mathbf{1}\{t \leq x\} \mathbf{1}\{t \leq z\} dt$ , so that  $\min\{x, z\}$  is evidently an inner product.)  $\square$

**Question 3:** Consider the Sobolev space  $\mathcal{F}_k$ , which is defined as the set of functions that are  $(k - 1)$ -times differentiable and have  $k$ th derivative almost everywhere on  $[0, 1]$ , where the  $k$ th derivative is square-integrable. That is, we define

$$\mathcal{F}_k := \left\{f : [0, 1] \mid f^{(k)} \in L^2([0, 1])\right\},$$

where  $f^{(k)}$  denotes the  $k$ th derivative of  $f$ . We define the inner product on  $\mathcal{F}_k$  by

$$\langle f, g \rangle = \sum_{i=0}^{k-1} f^{(i)}(0)g^{(i)}(0) + \int_0^1 f^{(k)}(t)g^{(k)}(t)dt.$$

- (a) Find the representer of evaluation for this Hilbert space, that is, find a function  $r_x : [0, 1] \rightarrow \mathbb{R}$  (defined for each  $x \in [0, 1]$ ) such that  $r_x \in \mathcal{F}_k$  and

$$\langle r_x, f \rangle = f(x)$$

for all  $x \in [0, 1]$ .

- (b) What is the reproducing kernel  $k(x, z)$  associated with this space? (Recall that  $k(x, z) = \langle r_x, r_z \rangle$  for an RKHS.)
- (c) Show that  $\mathcal{F}_k$  is a Hilbert space, meaning that  $\|f\|^2 = \langle f, f \rangle$  defines a norm and that  $\mathcal{F}_k$  is complete for the norm.

**Answer:**

- (a) By Taylor's theorem, we have

$$f(x) = f(0) + \sum_{i=1}^{k-1} f^{(i)}(0) \frac{x^i}{i!} + \frac{1}{(k-1)!} \int_0^x f^{(k)}(t) (x-t)^{k-1} dt.$$

Define the function

$$r_x(t) = \sum_{i=0}^{k-1} \frac{x^i}{i!} \frac{t^i}{i!} + \frac{(-1)^k}{(2k-1)!} \max\{x-t, 0\}^{2k-1} + \sum_{i=0}^{k-1} (-1)^{k+i+1} \frac{x^{2k-1-i}}{(2k-1-i)!} \frac{t^i}{i!}.$$

Then

$$r_x^{(i)}(0) = \frac{1}{i!} x^i + \frac{(-1)^{k+i}}{(2k-i-1)!} \max\{x, 0\}^{2k-1-i} + \frac{(-1)^{k+i+1}}{(2k-1-i)!} x^{2k-1-i} = x^i$$

for  $i < k$  and

$$r_x^{(k)}(t) = \frac{1}{(k-1)!} \max\{x-t, 0\}^{k-1}.$$

Thus we have

$$\begin{aligned} \langle f, r_x \rangle &= f(0) + f'(0)x + \frac{1}{2}f''(0)x^2 + \cdots + \frac{1}{(k-1)!}f^{(k-1)}(0)x^{k-1} + \frac{1}{(k-1)!} \int_0^1 f^{(k)}(t) [x-t]_+^{k-1} dt \\ &= \sum_{i=0}^{k-1} \frac{f^{(i)}(0)}{i!} x^i + \frac{1}{(k-1)!} \int_0^x f^{(k)}(t) (x-t)^{k-1} dt \\ &= f(x) \end{aligned}$$

where the last equality is Taylor's theorem.

- (b) For the reproducing kernel, note that

$$\begin{aligned} k(x, z) &= \langle r_x, r_z \rangle \\ &= \sum_{i=0}^{k-1} \frac{x^i}{i!} \frac{z^i}{i!} + \frac{1}{(k-1)!(k-1)!} \int_0^1 [x-t]_+^{k-1} [z-t]_+^{k-1} dt \\ &= \sum_{i=0}^{k-1} \frac{x^i}{i!} \frac{z^i}{i!} + \frac{1}{(k-1)!(k-1)!} \int_0^{\min\{x,z\}} (x-t)^{k-1} (z-t)^{k-1} dt. \end{aligned}$$

- (c) To see that  $\mathcal{F}_k$  is a Hilbert space, we must show that  $\|f\|_{\mathcal{H}}^2 = \langle f, f \rangle$  is a norm and that  $\mathcal{F}_k$  is complete for  $\|\cdot\|_{\mathcal{H}}$ . Non-negativity of  $\|\cdot\|_{\mathcal{H}}$  and the triangle inequality are trivial, as it is clear that  $\langle \cdot, \cdot \rangle$  is an inner product. Now suppose that  $\|f\|_{\mathcal{H}} = 0$ . Then  $f^{(l)}(0) = 0$  for all  $l < k$ , and  $\int_0^1 f^{(k)}(t)^2 dt = 0$ , so that  $f^{(k)} = 0$  almost everywhere. Of course, this shows that  $f^{(k-1)} \equiv 0$  by integration, and so on, so that  $f \equiv 0$ . To show completeness, let  $f_n$  be a Cauchy sequence in  $\mathcal{F}_k$ . Then since

$$\|f_n - f_m\|_{\mathcal{H}}^2 = \sum_{l=0}^{k-1} (f_n^{(l)}(0) - f_m^{(l)}(0))^2 + \int_0^1 (f_n^{(k)}(t) - f_m^{(k)}(t))^2 dt,$$

it is clear that  $f_n^{(l)}(0)$  is a Cauchy sequence in  $\mathbb{R}$  and  $f_n^{(k)}$  is a Cauchy sequence in  $L^2([0, 1])$ . Completeness of  $\mathbb{R}$  and completeness of  $L^2$  then imply the existence of  $\lim_n f_n^{(l)}(0)$  for  $l < k$  and a  $g \in L^2([0, 1])$  such that  $f_n^{(k)} \rightarrow g$  in  $L_2$ . Now define the functions  $f^{(l)}$  by

$$f^{(k)}(x) = g(x), \quad f^{(k-1)}(x) = \lim_n f_n^{(k-1)}(0) + \int_0^x g(t) dt, \quad \dots, \quad f(x) = \lim_n f_n(0) + \int_0^x f^{(1)}(t) dt.$$

Since  $f^{(k)} \in L^2([0, 1])$ , it is clear that each of the  $f^{(l)}$  are absolutely continuous, and the derivative of  $f^{(l)}$  is  $f^{(l+1)}$ . So  $f_n$  indeed has a limit  $f$ . □

**Question 4:** The variation distance between probability distributions  $P$  and  $Q$  on a space  $\mathcal{X}$  is defined by  $\|P - Q\|_{\text{TV}} = \sup_{A \subset \mathcal{X}} |P(A) - Q(A)|$ .

- (a) Show that

$$2\|P - Q\|_{\text{TV}} = \sup_{f: \|f\|_{\infty} \leq 1} \{\mathbb{E}_P[f(X)] - \mathbb{E}_Q[f(X)]\}$$

where the supremum is taken over all functions with  $f(x) \in [-1, 1]$ , and the first expectation is taken with respect to  $P$  and the second with respect to  $Q$ . You may assume that  $P$  and  $Q$  have densities.

**Answer:** Using the assumption that we have a density and that  $P(A) - Q(A) = 1 - P(A^c) - (1 - Q(A^c)) = Q(A^c) - P(A^c)$ , we have

$$\begin{aligned} \|P - Q\|_{\text{TV}} &= \sup_{A \subset \mathcal{X}} \{P(A) - Q(A)\} = \sup_A \int \mathbf{1}\{x \in A\} (p(x) - q(x)) dx \\ &= \int \mathbf{1}\{p(x) \geq q(x)\} (p(x) - q(x)) dx. \end{aligned}$$

Similarly, we have  $\|P - Q\|_{\text{TV}} = \sup_A \{Q(A) - P(A)\}$ , and combining these yields

$$2\|P - Q\|_{\text{TV}} = \int (\mathbf{1}\{p(x) \geq q(x)\} - \mathbf{1}\{p(x) \leq q(x)\}) (p(x) - q(x)) dx.$$

But of course,  $\sup_{a \in [-1, 1]} a(p - q) = (p - q)(\mathbf{1}\{p \geq q\} - \mathbf{1}\{p \leq q\})$ , which proves the result. □

**Question 5:** In a number of experimental situations, it is valuable to determine if two distributions  $P$  and  $Q$  are the same or different. For example,  $P$  may be the distribution of widgets produced by one machine,  $Q$  the distributions of widgets by a second machine, and we wish to test if the two distributions are the same (to within allowable tolerances). Let  $\mathcal{H}$  be an RKHS of functions with domain  $\mathcal{X}$  and reproducing kernel  $k$ , and let  $P$  and  $Q$  be distributions on  $\mathcal{X}$ .

(a) Let  $\|\cdot\|_{\mathcal{H}}$  denote the norm on the Hilbert space  $\mathcal{H}$ . Show that

$$D_k(P, Q)^2 := \sup_{f: \|f\|_{\mathcal{H}} \leq 1} \left\{ |\mathbb{E}_P[f(X)] - \mathbb{E}_Q[f(Z)]|^2 \right\} = \mathbb{E}[k(X, X')] + \mathbb{E}[k(Z, Z')] - 2\mathbb{E}[k(X, Z)]$$

where  $X, X' \stackrel{\text{iid}}{\sim} P$  and  $Z, Z' \stackrel{\text{iid}}{\sim} Q$ .

(b) A kernel  $k: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  is called *universal* if the induced RKHS  $\mathcal{H}$  of functions  $f: \mathcal{X} \rightarrow \mathbb{R}$  can arbitrarily approximate continuous functions. That is, for any  $\phi: \mathcal{X} \rightarrow \mathbb{R}$  continuous and  $\epsilon > 0$ , there is some  $f \in \mathcal{H}$  such that

$$\sup_{x \in \mathcal{X}} |f(x) - \phi(x)| \leq \epsilon.$$

Show that if  $k$  is universal, then

$$D_k(P, Q) = 0 \text{ if and only if } P = Q.$$

You may assume  $\mathcal{X}$  is a metric space and that  $P = Q$  iff  $P(A) = Q(A)$  for all compact  $A \subset \mathcal{X}$ .

(c) You wish to estimate  $D_k(P, Q)$  given samples from each of the distributions. Assume that  $k(x, z) \in [-B, B]$  for all  $x, z \in \mathcal{X}$ . Let  $X_i \stackrel{\text{iid}}{\sim} P$ ,  $i = 1, \dots, n_1$  and  $Z_i \stackrel{\text{iid}}{\sim} Q$ ,  $i = 1, \dots, n_2$ . Define

$$\hat{K}(X_{1:n_1}) := \binom{n_1}{2}^{-1} \sum_{1 \leq i < j \leq n_1} k(X_i, X_j), \quad \hat{K}(Z_{1:n_2}) := \binom{n_2}{2}^{-1} \sum_{1 \leq i < j \leq n_2} k(Z_i, Z_j),$$

and

$$\hat{K}(X_{1:n_1}, Z_{1:n_2}) := \frac{1}{n_1 n_2} \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} k(X_i, Z_j).$$

Show that  $\mathbb{E}[\hat{K}(X_{1:n})] = \mathbb{E}[k(X, X')]$  and  $\mathbb{E}[\hat{K}(X_{1:n_1}, Z_{1:n_2})] = \mathbb{E}[k(X, Z)]$  for  $X, X' \stackrel{\text{iid}}{\sim} P$  and  $Z, Z' \stackrel{\text{iid}}{\sim} Q$ . Show for some numerical constant  $c > 0$  that for all  $t \geq 0$ ,

$$\mathbb{P} \left( \left| \hat{K}(X_{1:n}) - \mathbb{E}[k(X, X')] \right| \geq t \right) \leq 2 \exp \left( -c \frac{nt^2}{B^2} \right)$$

and

$$\mathbb{P} \left( \left| \hat{K}(X_{1:n_1}, Z_{1:n_2}) - \mathbb{E}[k(X, Z)] \right| \geq t \right) \leq 2 \exp \left( -c \frac{n_1 t^2}{B^2} \right) + 2 \exp \left( -c \frac{n_2 t^2}{B^2} \right).$$

(d) Define the empirical Hilbert distances

$$\hat{D}_k^2(P, Q) := \binom{n_1}{2}^{-1} \sum_{1 \leq i < j \leq n_1} k(X_i, X_j) + \binom{n_2}{2}^{-1} \sum_{1 \leq i < j \leq n_2} k(Z_i, Z_j) - \frac{2}{n_1 n_2} \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} k(X_i, Z_j).$$

Show that for all  $t \geq 0$ ,

$$\mathbb{P} \left( \left| \hat{D}_k^2(P, Q) - D_k^2(P, Q) \right| \geq t \right) \leq C \exp \left( -c \frac{\min\{n_1, n_2\} t^2}{B^2} \right)$$

where  $0 < c, C < \infty$  are numerical constants.

**Answer:**

- (a) As  $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  is the reproducing kernel for  $\mathcal{H}$ , we have for any  $f \in \mathcal{H}$  such that  $\|f\|_{\mathcal{H}} \leq 1$

$$\begin{aligned} \mathbb{E}[f(X)] - \mathbb{E}[f(Z)] &= \mathbb{E}[\langle f, k(X, \cdot) \rangle] - \mathbb{E}[\langle f, k(Z, \cdot) \rangle] \\ &\stackrel{(i)}{=} \langle f, \mathbb{E}[k(X, \cdot) - k(Z, \cdot)] \rangle \\ &\stackrel{(ii)}{\leq} \|f\|_{\mathcal{H}} \|\mathbb{E}[k(X, \cdot) - k(Z, \cdot)]\|_{\mathcal{H}} \leq \|\mathbb{E}[k(X, \cdot) - k(Z, \cdot)]\|_{\mathcal{H}}, \end{aligned}$$

where we have used linearity in (i) and Cauchy-Schwarz in (ii), and that  $\|f\|_{\mathcal{H}} \leq 1$  in the final line. Equality holds in step (ii) if

$$f(\cdot) = \frac{\mathbb{E}[k(X, \cdot) - k(Z, \cdot)]}{\|\mathbb{E}[k(X, \cdot) - k(Z, \cdot)]\|_{\mathcal{H}}},$$

and we have

$$\begin{aligned} \|\mathbb{E}[k(X, \cdot) - k(Z, \cdot)]\|_{\mathcal{H}}^2 &= \langle \mathbb{E}[k(X, \cdot) - k(Z, \cdot)], \mathbb{E}[k(X', \cdot) - k(Z', \cdot)] \rangle \\ &= \langle \mathbb{E}[k(X, \cdot)], \mathbb{E}[k(X', \cdot)] \rangle + \langle \mathbb{E}[k(Z, \cdot)], \mathbb{E}[k(Z', \cdot)] \rangle - 2 \langle \mathbb{E}[k(X, \cdot)], \mathbb{E}[k(Z, \cdot)] \rangle \\ &= \mathbb{E}[k(X, X')] + \mathbb{E}[k(Z, Z')] - 2\mathbb{E}[k(X, Z)], \end{aligned}$$

where the final equality uses the linearity of the inner product and independence of  $X, X', Z, Z'$ .

- (b) Suppose that  $P = Q$ . Then certainly  $\mathbb{E}_P[f(X)] - \mathbb{E}_Q[f(Z)] = \mathbb{E}_P[f(X)] - \mathbb{E}_P[f(X)] = 0$  for all  $f \in \mathcal{H}$ . Now suppose  $P \neq Q$ . Then there exists a compact set  $A$  such that  $P(A) \neq Q(A)$ . For  $n \in \mathbb{N}$ , define the function

$$\phi_n(x) = \max\{1 - n \cdot \text{dist}(x, A), 0\} = [1 - n \text{dist}(x, A)]_+,$$

which satisfies  $\phi_n(x) = 1$  for  $x \in A$ ,  $\phi_n(x) = 0$  for  $x$  such that  $\text{dist}(x, A) \geq 1/n$ , and is Lipschitz continuous. Moreover, we have  $\phi_n(x) \downarrow \mathbf{1}_{\{x \in A\}}$  for all  $x \in A$  as  $n \rightarrow \infty$ . Thus the monotone convergence theorem gives that

$$\lim_n \mathbb{E}_P[\phi_n(X)] = P(A) \quad \text{and} \quad \lim_n \mathbb{E}_Q[\phi_n(Z)] = Q(A).$$

Let  $\epsilon > 0$  be such that  $|P(A) - Q(A)| \geq 4\epsilon$ . Choose  $N$  such that  $n \geq N$  implies  $|\mathbb{E}_P[\phi_n] - P(A)| < \epsilon$  and  $|\mathbb{E}_Q[\phi_n] - Q(A)| < \epsilon$ , and let  $n \geq N$ . Choose  $f \in \mathcal{H}$  such that  $\sup_x |f(x) - \phi_n(x)| \leq \epsilon$ . Then

$$|\mathbb{E}_P[f(X)] - \mathbb{E}_Q[f(Z)]| \geq |\mathbb{E}_P[\phi_n(X)] - \mathbb{E}_Q[\phi_n(Z)]| - 2\epsilon > |P(A) - Q(A)| - 4\epsilon \geq 4\epsilon - 4\epsilon = 0.$$

Dividing by  $\|f\|_{\mathcal{H}}$  we have

$$D_k(P, Q) = \sup_{g: \|g\|_{\mathcal{H}} \leq 1} |\mathbb{E}_P[g] - \mathbb{E}_Q[g]| \geq \frac{|\mathbb{E}_P[f(X)] - \mathbb{E}_Q[f(Z)]|}{\|f\|_{\mathcal{H}}} > 0.$$

- (c) The expectation equalities are immediate.

We apply bounded differences for the first statement. We first look at  $f(x_{1:n}) = \widehat{K}(x_{1:n})$ . As the function is symmetric, we fix index  $i = 1$ . Then for  $x, x' \in \mathcal{X}$ , we have

$$f(x, x_{2:n}) - f(x', x_{2:n}) = \binom{n}{2}^{-1} \sum_{j=2}^n (k(x, X_j) - k(x', X_j))$$

and using that  $k(x, x') \in [-B, B]$ , the summands are each bounded by  $2B$  in magnitude. Thus

$$|f(x, x_{2:n}) - f(x', x_{2:n})| \leq \frac{2}{n(n-1)} \cdot 2B(n-1) = \frac{4B}{n}.$$

Bounded differences (McDiarmid's inequality) implies

$$\mathbb{P}\left(\left|\widehat{K}(X_{1:n}) - \mathbb{E}[\widehat{K}(X_{1:n})]\right| \geq t\right) \leq 2 \exp\left(-\frac{nt^2}{8B^2}\right).$$

The argument about  $\widehat{K}(X_{1:n_1}, Z_{1:n_2})$  is a bit more complex. Define

$$\widehat{K}(X_{1:n_1}, Q) = \frac{1}{n_1} \sum_{i=1}^{n_1} \mathbb{E}_Q[k(X_i, Z) \mid X_i].$$

Then we have

$$\mathbb{E}[\widehat{K}(X_{1:n_1}, Z_{1:n_2}) \mid X_{1:n_1}] = \widehat{K}(X_{1:n_1}, Q)$$

by the independence of  $Z_i, X_j$ . Fixing  $X_{1:n_1}$ , define the function  $g(z_{1:n_2} \mid X_{1:n_1})$  by

$$g(z_{1:n_2} \mid X_{1:n_1}) = \widehat{K}(X_{1:n_1}, z_{1:n_2}).$$

Then  $g$  satisfies bounded differences with parameter  $4B/n_2$ , as above, and so *conditional on*  $X_{1:n_1}$ , we have

$$\mathbb{P}\left(\left|g(Z_{1:n_2} \mid X_{1:n_1}) - \widehat{K}(X_{1:n_1}, Q)\right| \geq t \mid X_{1:n_1}\right) \leq 2 \exp\left(-\frac{n_2 t^2}{8B^2}\right). \quad (1)$$

Now we argue that

$$x_{1:n_1} \mapsto \widehat{K}(x_{1:n_1}, Q)$$

satisfies bounded differences as well. Note that  $\mathbb{E}[\widehat{K}(X_{1:n_1}, Q)] = \mathbb{E}[k(X, Z)]$  by construction. Without loss of generality let us fix  $x_{2:n_1}$  and modify  $x_1 \in \{x, x'\}$ . Then

$$\widehat{K}(x, x_{2:n_1}, Q) - \widehat{K}(x', x_{2:n_1}, Q) = \frac{1}{n_1} \mathbb{E}_Q[k(x, Z) - k(x', Z)] \in \left[-\frac{2B}{n_1}, \frac{2B}{n_1}\right],$$

satisfying bounded differences with parameter  $2B/n_1$ . Thus we have

$$\mathbb{P}\left(\left|\widehat{K}(X_{1:n_1}, Q) - \mathbb{E}[k(X, Z)]\right| \geq t\right) \leq 2 \exp\left(-\frac{n_1 t^2}{2B^2}\right). \quad (2)$$

Combining the bounds (1) and (2) and applying the tower property of expectation and the triangle inequality, we have

$$\begin{aligned} & \mathbb{P}\left(\left|\widehat{K}(X_{1:n_1}, Z_{1:n_2}) - \mathbb{E}[k(X, Z)]\right| \geq t\right) \\ & \leq \mathbb{E}\left[\mathbb{P}\left(\left|g(Z_{1:n_2} \mid X_{1:n_1}) - \widehat{K}(X_{1:n_1}, Q)\right| \geq t/2 \mid X_{1:n_1}\right)\right] + \mathbb{P}\left(\left|\widehat{K}(X_{1:n_1}, Q) - \mathbb{E}[k(X, Z)]\right| \geq t/2\right) \\ & \leq 2 \exp\left(-\frac{n_2 t^2}{32B^2}\right) + 2 \exp\left(-\frac{n_1 t^2}{8B^2}\right). \end{aligned}$$

□