Homework 2 Solution

Problem 1. *Let $\mathcal{X}$ be a set and $\mathcal{F}$ be a Hilbert space. Let $\Psi : \mathcal{X} \to \mathcal{F}$, and $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be:*

$$\forall x, x' \in \mathcal{X}, \quad K(x, x') = \langle \Psi(x), \Psi(x') \rangle_{\mathcal{F}}$$

Show that K is a positive definite kernel on $\mathcal{X}$, and describe its RKHS $\mathcal{H}$.

Step 1 (Positive Definiteness)
for any set $X = \{x_1, \dots, x_n\}$ of points in $\mathcal{X}$, the matrix of K is the gram matrix of $\{\Psi(x_1), \dots, \Psi(x_n)\}$. Further, we know that gram matrices are positive semi-definite and symmetric (as long as the inner product is real-valued), which implies that K is a PD kernel.

Step 2 (Candidate RKHS)
Assume that we have $w = \sum_i a_i \Psi(x_i)$.

We have:

$$\begin{aligned} f_w(x) = \sum_i a_i K(x_i, x) &= \sum_i a_i \langle \Psi(x_i), \Psi(x') \rangle_{\mathcal{F}} \\ &= \langle \sum_i a_i \Psi(x_i), \Psi(x') \rangle_{\mathcal{F}} \\ &= \langle w, \Psi(x) \rangle_{\mathcal{F}} \end{aligned}$$

Let $\mathcal{H}$ be the set of all such functions endowed with the inner product:

$$\langle f_w, f_{w'} \rangle_{\mathcal{H}} = \langle w, w' \rangle_{\mathcal{F}}$$

Step 3 (Hilbert Check)
The candidate RKHS is isomorphic to $\mathcal{F}$ with the mapping $\Phi : w \to f_w$, hence it is indeed a Hilbert space.
Step 4 (RKHS properties)
First, we know that

$$K_x : y \to \langle \Psi(x), \Psi(y) \rangle_{\mathcal{F}} = f_{\Psi(x)} \in \mathcal{H}$$

Second

$$f_w(x) = \langle w, \Psi(x) \rangle_{\mathcal{F}} = \langle f_w, f_{\Psi(x)} \rangle_{\mathcal{H}}$$

on the other hand

$$f_{\Psi(x)} : y \rightarrow \langle \Psi(x), \Psi(y) \rangle_{\mathcal{F}}$$

Which is the same as K_x, hence:

$$f_w(x) = \langle f_w, K_x \rangle_{\mathcal{H}}$$

Therefore, the reproducing property holds as well, which implies that our candidate is indeed the RKHS. $\square$

Problem 2. *Prove that for any p.d. kernel K on a space $\mathcal{X}$, a function $f : \mathcal{X} \rightarrow \mathbb{R}$ belongs to the RKHS with kernel K iff there exists $\lambda > 0$ such that $K'(x, y) = K(x, y) - \lambda f(x) f(y)$ is p.d.*

$\Rightarrow$
Assume that $\mathcal{H}$ is the RKHS represented by K, and let $\langle ., . \rangle$ denote the inner product of $\mathcal{H}$, and $\|.\|$ denote the induced norm.
We can rewrite the relation as $\langle K_x, K_y \rangle - \lambda \langle f, K_x \rangle \langle f, K_y \rangle$ since $f \in \mathcal{H}$.
Note that $K_x - \frac{\alpha \langle f, K_x \rangle f}{\|f\|}$ is a member of $\mathcal{H}$ for $\alpha \in \mathbb{R}$.
We have:

$$\langle K_x - \frac{\alpha \langle f, K_x \rangle f}{\|f\|}, K_y - \frac{\alpha \langle f, K_y \rangle f}{\|f\|} \rangle$$

$$= \langle K_x, K_y \rangle + \alpha^2 \langle f, K_x \rangle \langle f, K_y \rangle - 2\alpha \frac{\langle f, K_x \rangle \langle f, K_y \rangle}{\|f\|}$$

$$= \langle K_x, K_y \rangle + (\alpha^2 - \frac{2\alpha}{\|f\|}) \langle f, K_x \rangle \langle f, K_y \rangle$$

Setting $\lambda = (\alpha^2 - \frac{2\alpha}{\|f\|})$ where $\alpha < \frac{2}{\|f\|}$, gives us a relation similar to that of K'.
Now, consider a set of points $X = \{x_1, \ldots, x_n\}$, and set
$V = \{v_1, \ldots, v_n\}$ where $v_i = K_{x_i} - \frac{\alpha \langle f, K_{x_i} \rangle f}{\|f\|}$. The matrix of K' with respect to X is positive semi-definite, since it is equal to the gram matrix of V, and gram matrices are positive semi-definite.This implies that K' is a PD kernel (Mercer's theorem).

$\Leftarrow$

Let $\mathcal{H}'$ denote the RKHS represented by K'. For any function $g \in \mathcal{H}'$ we have:

$$g(x) = \sum_i a_i K'(x_i, x) = \sum_i a_i K(x_i, x) - \lambda f(x) \sum_i a_i f(x_i)$$

or equivalently:

$$f(x) = \sum_i \frac{K(x_i, x)}{\lambda f(x_i)} - \frac{g(x)}{\lambda \sum_i a_i f(x_i)}$$

letting g be the zero function, we can see that:

$$f(x) = \sum_i c_i K(x_i, x)$$

which means that $f \in \mathcal{H}$, where $\mathcal{H}$ has the same definition as the last part of the proof. $\square$