AMATH 563 Homework 2

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1 Problem 1

Let $\Gamma : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a PDS kernel. Let $x, x' \in \mathcal{X}$. Then, the fact that Γ is PDS implies that the matrix

$$A = \begin{pmatrix} \Gamma(x,x) & \Gamma(x,x') \\ \Gamma(x,x') & \Gamma(x',x') \end{pmatrix}$$

is positive semi-definite. This implies that

$$\det(A) = \Gamma(x,x)\Gamma(x',x') - \Gamma(x,x')\Gamma(x,x') \geq 0.$$

Thus,

$$|\Gamma(x,x')|^2 \leq \Gamma(x,x)\Gamma(x',x').$$

2 Problem 2

Let K be a PDS kernel on $\mathcal{X}$ and define the normalized kernel

$$\bar{K}(x,x') = \begin{cases} 0 & \text{if } K(x,x) = 0 \text{ or } K(x',x') = 0 \\ \frac{K(x,x')}{\sqrt{K(x,x)}\sqrt{K(x',x')}} & \text{otherwise.} \end{cases}$$

We can immediately see from this definition that $\bar{K}$ is symmetric, since K is symmetric. To show that $\bar{K}$ is PDS, let $\xi \in \mathbb{R}^n$ and $x_1, \ldots, x_n \in \mathcal{X}$ and consider the sum

$$\sum_{j=1}^{n} \sum_{k=1}^{n} \xi_j \xi_k \bar{K}(x_j, x_k).$$

Now, define

$$c_j = \begin{cases} \frac{\xi_j}{\sqrt{K(x_j,x_j)}}, & K(x_j,x_j) \neq 0, \\ 0, & K(x_j,x_j) = 0, \end{cases}$$

for $j = 1, \ldots, n$. Then,

$$\sum_{j=1}^{n} \sum_{k=1}^{n} \xi_j \xi_k \bar{K}(x_j, x_k) = \sum_{j=1}^{n} \sum_{k=1}^{n} c_j c_k K(x_j, x_k) \geq 0,$$

by definition. Thus, $\bar{K}$ is also a PDS kernel.

3 Problem 3

From class, we have that the linear kernel $K(x, x') = x^T x'$ is PDS. Furthermore, the kernel $K'(x, x') = c > 0$ is also a PDS kernel. To see this, note that for any $\xi \in \mathbb{R}^n$, $x_j, x_k \in \mathcal{X}$,

$$\sum_{j=1}^{n}\sum_{k=1}^{n} \xi_j \xi_k K(x_j, x_k) = c\left(\sum_{j=1}^{n} \xi_j\right)^2 \geq 0.$$

This kernel is trivially symmetric, so it is PDS. Thus, the polynomial kernel defined by $K(x, x') = (x^T x' + c)^\alpha$ for $c > 0$ and $\alpha \in \mathbb{N}$ by the fact that PDS kernels are closed under addition and multiplication.

Again using the fact that the linear kernel, we note that the exponential function has a power series

$$\exp(x) = \sum_{j=0}^{\infty} \frac{x^j}{j!},$$

with infinite radius of convergence. Thus, the fact that PDS kernels are closed under power series implies that the exponential kernel $K(x, x') = \exp(x^T x')$ is also a PDS kernel.

In the same vein as the previous part, we have the power series

$$\exp(2\gamma^2 x) = \sum_{j=0}^{\infty} \frac{(2\gamma^2 x)^j}{j!} = \sum_{j=0}^{\infty} \frac{(2\gamma^2)^j}{j!} x^j$$

with infinite radius of convergence, so the kernel $K'(x, x') = \exp(2\gamma^2 x^T x')$ is PDS. To see that the RBF kernel $K(x, x') = \exp(-\gamma^2 \|x - x'\|_2^2)$ is also a PDS kernel, we first note that it is obviously symmetric. We then expand

$$K(x, x') = \exp(-\gamma^2 \|x\|_2^2) \exp(2\gamma^2 x^T x') \exp(-\gamma^2 \|x'\|_2^2).$$

Let $\xi_j \in \mathbb{R}^n$ and $x_1, \ldots, x_n \in \mathbb{R}^d$ and define

$$c_j = \xi_j \exp(-\gamma^2 \|x_j\|_2^2) \in \mathbb{R}.$$

Then,

$$\sum_{j=1}^{n}\sum_{k=1}^{n} \xi_j \xi_k K(x_j, x_k) = \sum_{j=1}^{n}\sum_{k=1}^{n} c_j c_k K'(x_j, x_k) \geq 0,$$

since K' is PDS. Thus, the RBF kernel is also PDS.

4 Problem 4

Let $\Omega \subseteq \mathbb{R}^d$ and let $\{\psi_j\}_{j=1}^n$ be a sequence of continuous functions on Ω and $\{\lambda_j\}_{j=1}^n$ a sequence of non-negative numbers. Consider $K(x, x') = \sum_{j=1}^{n} \lambda_j \psi_j(x) \psi_j(x')$

as a kernel on Ω. To show that it is PDS, we first observe that it is clearly symmetric. Now, let $\xi \in \mathbb{R}^m$ and $x_1, \ldots, x_m \in \Omega$. Then,

$$\sum_{i=1}^{m}\sum_{k=1}^{m} \xi_i \xi_k K(x_i, x_k) = \sum_{i=1}^{m}\sum_{k=1}^{m} \xi_i \xi_k \sum_{j=1}^{n} \lambda_j \psi_j(x_i)\psi_j(x_k)$$

$$= \sum_{j=1}^{n} \lambda_j \sum_{i=1}^{m}\sum_{k=1}^{m} \xi_i \xi_k \psi_j(x_i)\psi_j(x_k) = \sum_{j=1}^{n} \lambda_j \left(\sum_{i=1}^{m} \xi_i \psi_j(x_i)\right)^2 \geq 0.$$

Thus, K is a PDS kernel.

5 Problem 5

5.1 Part i

Let K and K' be two reproducing kernels on $\mathcal{X}$ for an RKHS $\mathcal{H}$. Then, by the reproducing property,

$$f(x) = \langle f, K(x, \cdot)\rangle = \langle f, K'(x, \cdot)\rangle$$

for all $f \in \mathcal{H}$, $x \in \mathcal{X}$. Thus,

$$0 = \langle f, K(x, \cdot) - K'(x, \cdot)\rangle$$

for all $f \in \mathcal{H}$, so

$$K(x, \cdot) - K'(x, \cdot) = 0$$

for all $x \in \mathcal{X}$. This combined with symmetry implied that $k = K'$.

5.2 Part ii

Let K be a PDS kernel, let $\mathcal{H}$ be its RHKS that we constructed in class (Lecture 7), and let $\mathcal{G}$ be another RKHS corresponding to K. Then, for any $f \in \mathcal{H}_0$[1], we have that

$$f = \sum_{j=1}^{n} c_j K(x_j, \cdot).$$

By the definition of an RKHS, we have that $K(x_j, \cdot) \in \mathcal{G}$, so $f \in \mathcal{G}$ since Hilbert spaces are closed under finite linear combinations. Thus, $\mathcal{H}_0 \subset \mathcal{G}$, but since $\mathcal{H}$ is the completion of $\mathcal{H}_0$, we must have that $\mathcal{H} \subset \mathcal{G}$. Let $g \in \mathcal{G}$. Then, we can write $g = h + h^{\perp}$ where $h \in \mathcal{H}$ and $h^{\perp} \in \mathcal{H}^{\perp}$. Then, by the reproducing property,

$$g(x) = \langle g, K(x, \cdot)\rangle = \langle h, K(x, \cdot)\rangle + \langle h^{\perp}, K(x, \cdot)\rangle = \langle h, K(x, \cdot)\rangle = h(x),$$

for any $x \in \mathcal{X}$. Thus, $g \in \mathcal{H}$, so $\mathcal{G} = \mathcal{H}$.

A detail we have glossed over here is that the $\mathcal{G}$ and $\mathcal{H}$ inner products may only be the same up to isometry, but in our case, we have chosen the identity isometry WLOG.

[1] This is the pre-Hilbert space used in the construction of $\mathcal{H}$.