SC4/SM8 Advanced Topics in Statistical Machine Learning
Problem Sheet 2

1. Let k_1 and k_2 be positive definite kernels on $\mathbb{R}^p$. Verify that the following are also valid kernels.

   [*Hint: it suffices to identify the corresponding feature.*]

   (a) $x^\top x'$,

   (b) $ck_1(x, x')$, for $c \geq 0$,

   (c) $f(x)k_1(x, x')f(x')$ for any function $f : \mathbb{R}^p \to \mathbb{R}$,

   (d) $k_1(x, x') + k_2(x, x')$,

   (e) $k_1(x, x')k_2(x, x')$,

   (f) $\exp(k_1(x, x'))$,

   (g) $\exp\left(-\frac{1}{2\gamma^2}\|x - x'\|_2^2\right)$.

2. Assume that kernel k is not strictly positive definite, but that there exist $\{a_i\}_{i=1}^n$ and $\{x_i\}_{i=1}^n$, such that

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

   Show that then

$$f(x) = \sum_{i=1}^n a_i k(x_i, x) = 0 \quad \forall x \in \mathcal{X}.$$

   Hence conclude that the RKHS functions of the form $f(x) = \sum_{i=1}^n a_i k(x_i, x)$ have zero norm if and only if they are identically equal to zero. [*Hint: assume contrary for some $x = x_{n+1}$ and consider $\sum_{i=1}^{n+1} \sum_{j=1}^{n+1} a_i a_j k(x_i, x_j)$*]

3. (**One-Class SVM**) A Gaussian RBF kernel on $\mathcal{X} = \mathbb{R}^p$ is given by

$$k(x, x') = \exp\left(-\frac{1}{2\sigma^2}\left\|x - x'\right\|^2\right). \tag{1}$$

   (i) What is $k(x, x)$ for this kernel? What can you conclude about the norm of the features $\varphi(x)$ of x? What values can the angles between $\varphi(x)$ and $\varphi(x')$ take? Sketch the set $\{\varphi(x) : x \in \mathcal{X}\}$ as if the features lived in a 2D space.

   (ii) Let $\{x_i\}_{i=1}^n$ be a set of points in $\mathcal{X} = \mathbb{R}^p$ (no labels are given). The one-class Support Vector Machine (SVM) is a method for outlier detection which in its primal form is defined as

$$\min_{w,\xi,\rho} \frac{1}{2}\|w\|^2 + \frac{1}{\nu n}\sum_{i=1}^n \xi_i - \rho, \quad \text{subject to } \langle w, \varphi(x_i)\rangle \geq \rho - \xi_i,\ \xi_i \geq 0,$$

   where ν is a given SVM parameter, features $\varphi(x)$ correspond to the RBF kernel in (1), and ξ_i's are the non-negative slack variables. The fitted hyperplane $\langle w, \varphi(x)\rangle - \rho$ in the feature space separates the majority of points from the origin (while pushing away from the origin as much as possible) and is used to determine "atypical" x-instances.

   Using the 2D intuition from (i), sketch the corresponding hyperplane in the feature space and annotate with ρ, w and a non-zero slack ξ_j for an "outlier" x_j. Would it make sense to use the one-class SVM with a linear kernel?

(iii) Write the dual form of the one-class SVM, using Lagrangian duality.
[*Hint: setting to zero the derivative of the Lagrangian with respect to* w *should give* $w = \sum_{i=1}^{n} \alpha_i \varphi(x_i)$, *where* $\alpha_i \geq 0$ *are the Lagrange multipliers of the constraints* $\langle w, \varphi(x_i) \rangle \geq \rho - \xi_i$]

4. Derive the Gram matrix $\tilde{\mathbf{K}}$ of centred features $\tilde{\varphi}(x_i) = \varphi(x_i) - \frac{1}{n}\sum_{r=1}^{n} \varphi(x_r)$ as a function of kernel values $\mathbf{K}_{i,j} = k(x_i, x_j) = \varphi(x_i)^\top \varphi(x_j)$. Show that it takes the form $\mathbf{HKH}$, where $\mathbf{H}$ is a matrix you should specify. Verify that $\mathbf{H}$ is symmetric and idempotent, i.e., $\mathbf{H}^2 = \mathbf{H}$.

5. Show that

$$\mathrm{MMD}_k\left(P, Q\right) = \sup_{f \in \mathcal{H}_k \colon \|f\|_{\mathcal{H}_k} \leq 1} \left| \mathbb{E}_{X \sim P} f(X) - \mathbb{E}_{Y \sim Q} f(Y) \right|.$$

6. Let $\mathbf{L}$ be an unnormalized Laplacian matrix of a graph with C connected components. Verify that

   (a) Column vector $\mathbf{1}$ is the eigenvector of $\mathbf{L}$ with eigenvalue 0.

   (b) $\mathbf{L}$ is positive semi-definite.

   (c) v is an eigenvector of $\mathbf{L}$ corresponding to 0-eigenvalue if and only if $v \in \mathrm{span}\{e_1, \ldots, e_C\}$, where
   $$e_{ci} = \begin{cases} 1, & \text{vertex } i \text{ belongs to the connected component } c, \\ 0, & \text{otherwise.} \end{cases}$$

7. Verify that for a given partition $C_1, C_2, \ldots, C_K$ and column vectors $h_k \in \mathbb{R}^n$ defined as $h_{k,i} = \frac{1}{\sqrt{|C_k|}} \mathbf{1}_{\{i \in C_k\}}$, we have

$$\text{ratio-cut}\left(C_1, \ldots, C_K\right) = \sum_{k=1}^{K} h_k^\top \mathbf{L} h_k.$$