SC4/SM8 Advanced Topics in Statistical Machine Learning
Problem Sheet 1

1. This question pertains to the DP-means algorithm.

   (a) Show that each iteration of Step 2 locally minimises the following objective:

   $$W_\lambda(\{C_k\}, \{\mu_k\}, K) = \sum_{k=1}^{K} \sum_{i \in C_k} \|x_i - \mu_k\|_2^2 + \lambda K. \tag{1}$$

   (b) Conclude that the DP-means algorithm will terminate after a finite number of iterations.

   (c) Describe how the tuning parameter λ controls the number of clusters returned by the algorithm.

2. Show that the second PC is the eigenvector corresponding to the second largest eigenvalue.

3. For a given loss function L, the risk R of real-valued $f : \mathcal{X} \to \mathbb{R}$ is given by the expected loss

   $$R(f) = \mathbb{E}\left[L(Y, f(X))\right].$$

   Derive the optimal regression functions (which minimize the true risk) for the following losses:

   (a) The squared error loss

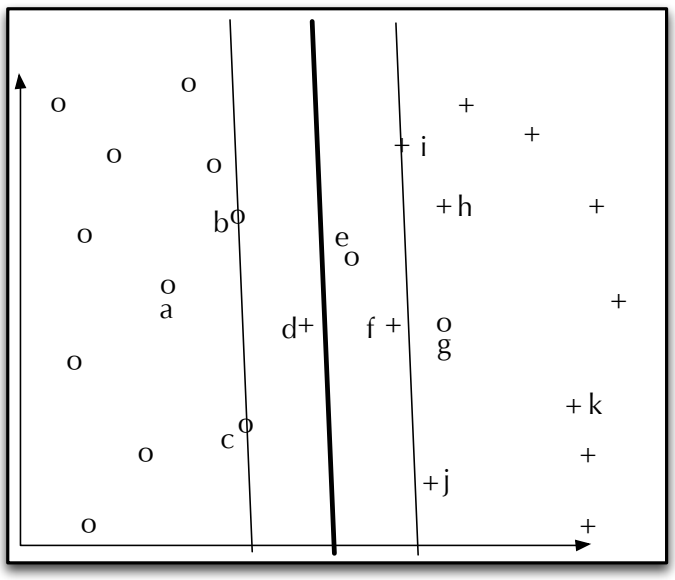
   $$L(Y, f(X)) = (Y - f(X))^2$$

   (b) The τ-pinball loss, for general $\tau \in (0, 1)$, given by

   $$L(Y, f(X)) = 2 \max\left\{\tau(Y - f(X)), (\tau - 1)(Y - f(X))\right\}.$$

   What happens in the case $\tau = 1/2$?

4. The figure below shows a binary classification dataset and the optimal the decision boundary and margins of a soft-margin C-SVM for some value C.



(a) Which of the points a,...,k are definitely support vectors? What can you say about points b, c, i? Can they be non, margin, or non-margin support vectors?

(b) For points a, b and d what are the range of possible values for the corresponding dual variables?

5. Parameter C in C-SVM can sometimes be hard to interpret. An alternative parametrization is given by ν-SVM:

$$\min_{w,b,\rho,\xi} \left(\frac{1}{2}\|w\|^2 - \nu\rho + \frac{1}{n}\sum_{i=1}^{n} \xi_i \right)$$

subject to

$$\begin{aligned} \rho &\geq 0, \\ \xi_i &\geq 0, \\ y_i \left(w^\top x_i + b \right) &\geq \rho - \xi_i. \end{aligned}$$

(note that we now directly adjust the constraint threshold ρ).

Using complementary slackness, show that ν is an upper bound on the proportion of non-margin support vectors (margin errors) and a lower bound on the proportion of all support vectors with non-zero weight (both those on the margin and margin errors). You can assume that $\rho > 0$ at the optimum (non-zero margin).

6. Consider the regression problem to the real-valued output $y \in \mathbb{R}$. Let $\epsilon > 0$ and define the ϵ-insensitive loss function L_ϵ as

$$L_\epsilon(y, f(x)) = \begin{cases} 0 & \text{if } |y - f(x)| < \epsilon, \\ |y - f(x)| - \epsilon & \text{otherwise,} \end{cases}$$

and the regularized empirical risk objective defined as

$$J(w, b) = C \sum_{i=1}^{n} L_\epsilon(y_i, f(x_i)) + \frac{1}{2}\|w\|_2^2,$$

where we used a linear model $f(x) = w^\top x + b$ for regression functions.

(a) Introduce the slack variables $\xi_i^+ = \max\{y_i - f(x_i) - \epsilon, 0\}$ and $\xi_i^- = \max\{f(x_i) - y_i - \epsilon, 0\}$. Verify that $L_\epsilon(y_i, f(x_i)) = \xi_i^+ + \xi_i^-$.

(b) Re-express the regularized empirical risk objective $J(w, b)$ as a constrained optimization problem over w, b, ξ^+ and ξ^-. Write down Lagrangian and show that the dual problem can be written as

$$\max_{\alpha^+,\alpha^-} \left\{ -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}(\alpha_i^+ - \alpha_i^-)(\alpha_j^+ - \alpha_j^-)x_i^\top x_j + \sum_{i=1}^{n}(\alpha_i^+ - \alpha_i^-)y_i - \epsilon\sum_{i=1}^{n}(\alpha_i^+ + \alpha_i^-) \right\},$$

subject to

$$\sum_{i=1}^{n}(\alpha_i^+ - \alpha_i^-) = 0, \quad \alpha_i^+ \in [0, C], \quad \alpha_i^- \in [0, C], \quad i = 1, \ldots, n.$$

(c) Considering derivatives of the Lagrangian and complementary slackness, express the weight vector w using dual coefficients α_i^+ and α_i^-. Show that those examples (x_i, y_i) which lie outside of the ϵ-insensitive tube around f, must have corresponding $\alpha_i^+ = C$ or $\alpha_i^- = C$ and that those examples (x_i, y_i) for which $|f(x_i) - y_i)| < \epsilon$ (they lie strictly inside the ϵ-tube), must have $\alpha_i^+ = \alpha_i^- = 0$. How can you compute b using the dual solution?

7. **(Kernel Ridge Regression)** Let $(x_i, y_i)_{i=1}^n$ be our dataset, with $x_i \in \mathbb{R}^p$ and $y_i \in \mathbb{R}$. Classical linear regression can be formulated as empirical risk minimization, where the model is to predict y using a class of functions $f(x) = w^\top x$, parametrized by vector $w \in \mathbb{R}^p$ using the squared loss, i.e. we minimize

$$\hat{R}(w) = \frac{1}{n}\sum_{i=1}^{n}(y_i - w^\top x_i)^2.$$

(a) Show that the optimal parameter vector is

$$\hat{w} = (\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{y}$$

where $\mathbf{X}$ is a $n \times p$ matrix with ith row given by $x_i^\top$, and $\mathbf{y}$ is a $n \times 1$ column vector with i-th entry y_i.

(b) Consider regularizing our empirical risk by incorporating an L_2 regularizer. That is, find w minimizing

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - w^\top x_i)^2 + \frac{\lambda}{n}\|w\|_2^2$$

Show that the optimal parameter is given by the ridge regression estimator

$$\hat{w} = (\mathbf{X}^\top \mathbf{X} + \lambda I)^{-1}\mathbf{X}^\top \mathbf{y}$$

(c) Suppose that we now wish to introduce nonlinearities into the model, by transforming $x \mapsto \varphi(x)$. Let $\mathbf{\Phi}$ be a matrix with ith row given by $\varphi(x_i)^\top$. The optimal parameters $\hat{w}$ would then be given by (previous part):

$$\hat{w} = (\mathbf{\Phi}^\top \mathbf{\Phi} + \lambda I)^{-1}\mathbf{\Phi}^\top \mathbf{y}.$$

Can we make predictions without computing $\hat{w}$?

First, express the predicted y values on the training set, $\mathbf{\Phi}\hat{w}$, only in terms of $\mathbf{y}$ and the Gram matrix $\mathbf{K} = \mathbf{\Phi}\mathbf{\Phi}^\top$, with $\mathbf{K}_{ij} = \varphi(x_i)^\top\varphi(x_j) = k(x_i, x_j)$ where k is some kernel function. Then, compute an expression for the value of $y_\star$ predicted by the model at an unseen test vector $x_\star$.

Hint: You may find it useful to first prove that:

$$(\mathbf{\Phi}^\top \mathbf{\Phi} \ + \lambda I)^{-1}\mathbf{\Phi}^\top = \mathbf{\Phi}^\top(\mathbf{\Phi}\ \mathbf{\Phi}^\top \ + \lambda I)^{-1}.$$

8. Denote $\sigma(t) = 1/(1 + e^{-t})$. Verify that the ERM corresponding to the logistic loss over the functions of the form $f(x) = w^\top\varphi(x)$ can be written as

$$\min_w \sum_{i=1}^{n} -\log\sigma(y_i w^\top \varphi(x_i)) + \lambda\|w\|_2^2 \tag{2}$$

and is a convex optimisation problem in w. Assume that you can write $w = \sum_{i=1}^{n} \alpha_i \varphi(x_i)$. Show that the criterion in (3) is also convex in the so called dual coefficients $\alpha \in \mathbb{R}^n$. [*Hint:* $\sigma'(t) = \sigma(t)\sigma(-t)$]