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:

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

   Answer: For each data item x_i, if its nearest centroid is closer than $\sqrt{\lambda}$, assigning x_i to the cluster will not increase the objective. On the other hand if the nearest centroid is further than $\sqrt{\lambda}$, we can create another cluster centred at x_i, and pay a penalty λ while still decreasing the overall objective.

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

   Answer: The reason is the same for K-means. The objective is non-negative, so lower bounded. Each iteration never increase the objective. There are a finite number of partitions, and the algorithm terminates if the partition does not change.

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

   Answer: Clusters are only created if an item is at least $\sqrt{\lambda}$ away from all existing clusters. So larger values of λ means that clusters are created less frequently, and each cluster will be larger (both in terms of number of items and its size in Euclidean distance). In fact a cluster cannot have a radius larger than $\sqrt{\lambda}$.

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

   Answer: The second PC maximizes the sample variance $\widehat{\text{Var}}(Z^{(2)}) = v_2^\top \widehat{\text{Cov}}(X) v_2$ of the second derived variable among the directions orthogonal to v_1, that is, it is given by the following optimisation problem:

   $$\begin{aligned} &\max_{v_2} \; v_2^\top S v_2 \\ &\text{subject to: } v_2^\top v_2 = 1, \; v_1^\top v_2 = 0. \end{aligned}$$

   Lagrangian is

   $$\mathcal{L}(v_2, \lambda_2, \gamma_2) = v_2^\top S v_2 - \lambda_2 \left(v_2^\top v_2 - 1 \right) - \gamma_2 v_1^\top v_2$$

   and setting the corresponding vector of partial derivatives to zero

   $$\frac{\partial \mathcal{L}(v_2, \lambda_2, \gamma_2)}{\partial v_2} = 2Sv_2 - 2\lambda_2 v_2 - \gamma_2 v_1 = 0.$$

   Left-multiplying the above by $v_1^\top$ gives $2v_1^\top S v_2 = \gamma_2$. However, since S is symmetric and v_1 is an eigenvector, we have

   $$\gamma_2 = 2v_1^\top S v_2 = 2v_2^\top S v_1 = 2\lambda_1 v_2^\top v_1 = 0. \tag{2}$$

   Hence $Sv_2 = \lambda_2 v_2$ and similarly as before v_2 must be the eigenvector corresponding to the second largest eigenvalue λ_2 of S.

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

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

Answer: We have

$$\begin{aligned} R(f) &= \mathbb{E}\left[(Y - f(X))^2\right] \\ &= \int \mathbb{E}\left[(Y - f(X))^2 \middle| X = x\right] g_X(x)\, dx, \end{aligned}$$

where g_X is density of X. Thus, it suffices to for every x, minimize:

$$\begin{aligned} & \mathbb{E}\left[(Y - f(X))^2 \middle| X = x\right] \\ = \;& \mathbb{E}\left[Y^2 \middle| X = x\right] - 2f(x)\,\mathbb{E}\left[Y \middle| X = x\right] + f(x)^2 \\ = \;& \text{Var}\left[Y|X = x\right] + \left(\mathbb{E}\left[Y \middle| X = x\right] - f(x)\right)^2. \end{aligned}$$

This is clearly minimized by the conditional mean:

$$f(x) = \mathbb{E}\left[Y \middle| X = x\right].$$

(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 $\tau = 1/2$?

Answer: We want to find $f(x)$ to minimize

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

Note that we can write

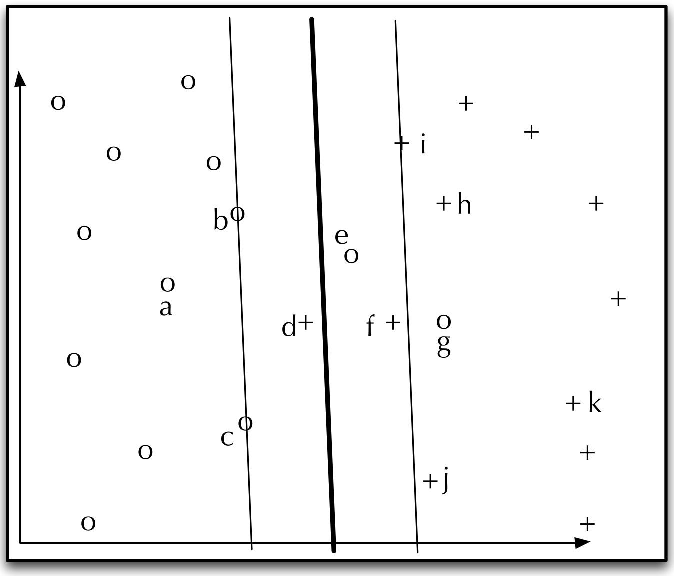
$$L(Y, f(X)) = \begin{cases} 2\tau(Y - f(X)) & \text{if } Y > f(X), \\ 2(\tau - 1)(Y - f(X)) & \text{if } Y \leq f(X). \end{cases}$$

Differentiating with respect to $f(x)$ and setting to zero, we obtain

$$2\tau\mathbb{P}(Y > f(x)|X = x) + 2(\tau - 1)\mathbb{P}(Y \leq f(x)|X = x) = 0,$$

leading to $\mathbb{P}(Y \leq f(x)|X = x) = \tau$ so the optimal $f(x)$ is the τ-quantile of the conditional distribution function $\mathbb{P}(Y \leq y|X = x)$. In the special case $\tau = 1/2$, we obtain L1 loss and the conditional median as the optimal regressor.

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 $a,\ldots,k$ are definitely support vectors? What can you say about points b, c, i? Can they be non, margin, or non-margin support vectors?

Answer: The points d, e, f, g are (non-margin) support vectors. b, c, i can in fact be non-SVs (if $\alpha = 0$), margin support vectors (if $0 < \alpha < C$) or non-margin support vectors (if $\alpha = C$).

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

Answer: Point a, the dual variable $\alpha_a = 0$ (removing a does not affect the boundary).
Point b, the dual variable $\alpha_b \in [0, C]$ (typically this is a margin support vector and typically $\alpha_b \in (0, C)$).
Point d, the dual variable $\alpha_d = C$ (margin penalty).

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).

Answer: The Lagrangian is given by

$$\frac{1}{2}\|w\|^2 - \nu\rho + \frac{1}{n}\sum_{i=1}^{n}\xi_i + \sum_{i=1}^{n}\alpha_i\left(\rho - y_i(w^\top x_i + b) - \xi_i\right) + \sum_{i=1}^{n}\beta_i\left(-\xi_i\right) + \gamma(-\rho),$$

for $\alpha_i \geq 0$, $\beta_i \geq 0$, $\gamma \geq 0$. Differentiating w.r.t. to the primal variables w, b, ξ, ρ and setting to zero gives

$$\begin{aligned} w &= \sum_{i=1}^{n}\alpha_i y_i x_i, \\ \sum_{i=1}^{n}\alpha_i y_i &= 0, \\ \alpha_i + \beta_i &= \frac{1}{n}, \\ \nu &= \sum_{i=1}^{n}\alpha_i - \gamma. \end{aligned}$$

Thus $\alpha_i \in \left[0, \frac{1}{n}\right]$, and $\nu \leq \sum_{i=1}^{n}\alpha_i$. Assume $\rho > 0$ at the global solution. This just means that the margin is non-zero. Then, by complementary slackness $\gamma = 0$, and $\sum_{i=1}^{n}\alpha_i = \nu$.

- Non-margin support vectors are those with $\alpha_i = \frac{1}{n}$, for which by complementary slackness $y_i\left(w^\top x_i + b\right) = \rho - \xi_i$, and from $\alpha_i + \beta_i = \frac{1}{n}$, $\beta_i = 0$, so potentially $\xi_i > 0$ (margin error). Denote this set by $N(\alpha)$. Then

$$\frac{|N(\alpha)|}{n} = \sum_{i\in N(\alpha)}\frac{1}{n} = \sum_{i\in N(\alpha)}\alpha_i \leq \sum_{i=1}^{n}\alpha_i = \nu.$$

- Denote margin support vectors, i.e. those with $\alpha_i \in (0, \frac{1}{n})$, with $M(\alpha)$. For these $\beta_i > 0$ and thus $\xi_i = 0$, so $y_i\left(w^\top x_i + b\right) = \rho$. Furthermore,

$$\nu = \sum_{i=1}^{n}\alpha_i = \sum_{i\in N(\alpha)}\frac{1}{n} + \sum_{i\in M(\alpha)}\alpha_i \leq \sum_{i\in M(\alpha)\cup N(\alpha)}\frac{1}{n} = \frac{|N(\alpha) + M(\alpha)|}{n}.$$

Thus ν is an upper bound on the number of margin errors and a lower bound on the number of support vectors.

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 $L_\epsilon(y_i, f(x_i)) = \xi_i^+ + \xi_i^-$.

Answer: $L_\epsilon(y_i, f(x_i))$ is non-zero only if either $y_i - f(x_i) > \epsilon$, in which case it is equal to ξ_i^+, or if $f(x_i) - y_i > \epsilon$, in which case it is equal to ξ_i^-. Furthermore, if $\xi_i^+ > 0$, then $f(x_i) - y_i - \epsilon < -2\epsilon$, so $\xi_i^- = 0$.

(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

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

Answer: The primal problem is given by

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

subject to

$$\begin{array}{ll} \xi_i^+ \geq 0 & \xi_i^+ \geq y_i - f(x_i) - \epsilon, i = 1, \ldots, n, \\ \xi_i^- \geq 0 & \xi_i^- \geq f(x_i) - y_i - \epsilon, i = 1, \ldots, n. \end{array}$$

Lagrangian is given by

$$\begin{aligned} \mathcal{L} &= \frac{1}{2}\|w\|^2 + C \sum_{i=1}^n \left(\xi_i^+ + \xi_i^-\right) - \sum_{i=1}^n (\nu_i^+ \xi_i^+ + \nu_i^- \xi_i^-) \\ &\quad + \sum_{i=1}^n \alpha_i^+ (y_i - f(x_i) - \epsilon - \xi_i^+) + \sum_{i=1}^n \alpha_i^- (f(x_i) - y_i - \epsilon - \xi_i^-), \end{aligned}$$

where the Lagrange multipliers $\alpha_i^+, \alpha_i^-, \nu_i^+, \nu_i^-$ are all ≥ 0. By differentiating with respect to primal variables and setting to zero,

$$\begin{aligned} \partial_b \mathcal{L} &= \sum_{i=1}^n (\alpha_i^+ - \alpha_i^-) = 0, \\ \partial_w \mathcal{L} &= w - \sum_{i=1}^n (\alpha_i^+ - \alpha_i^-) x_i = 0, \\ \partial_{\xi_i^\pm} \mathcal{L} &= C - \alpha_i^\pm - \nu_i^\pm = 0, \end{aligned}$$

and substituting back in, we obtain the desired dual problem.

(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?

Answer: The partial derivatives of the Lagrangian with respect to primal variables have to vanish for optimality. From $\partial_w \mathcal{L}$, it follows that $w = \sum_{i=1}^n (\alpha_i^+ - \alpha_i^-) x_i$. Also, from $\partial_{\xi_i^\pm} \mathcal{L}$, it follows that $\nu_i^\pm = C - \alpha_i^\pm$. Now, by complementary slackness, also $\nu_i^\pm \xi^\pm = 0$ for all i. Hence, if an error larger than ϵ is committed ($\xi_i^\pm > 0$), it must be that $\nu_i^\pm = 0$ and hence $\alpha_i^\pm = C$. On the other hand, with $|f(x_i) - y_i| < \epsilon$, we have $\xi_i^+ = \xi_i^- = 0$ and $f(x_i) - y_i - \epsilon$ and $y_i - f(x_i) - \epsilon$ are both nonzero, so $\alpha_i^+ = \alpha_i^- = 0$ by complementary slackness. Therefore, we have a sparse expansion of w in terms of x_i. To compute b, take any $\alpha_i^\pm \in (0, C)$ – it must be $|y_i - f(x_i)| = \epsilon$, so we can compute $b = y_i - w^\top x_i \pm \epsilon$.

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.

Answer: We can write the empirical risk as

$$\frac{1}{n} \|\mathbf{y} - \mathbf{X}w\|_2^2$$

Differentiating wrt w and setting to 0,

$$\begin{aligned}
(\mathbf{X}w - \mathbf{y})^\top \mathbf{X} &= 0 \\
w^\top (\mathbf{X}^\top \mathbf{X}) - \mathbf{y}^\top \mathbf{X} &= 0 \\
\hat{w} &= (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}
\end{aligned}$$

(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

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

Answer: The objective becomes:

$$\frac{1}{n}\|\mathbf{y}-\mathbf{X}w\|_2^2+\frac{\lambda}{n}\|w\|_2^2$$

Again differentiating and setting derivative to 0,

$$\begin{aligned}(\mathbf{X}w-\mathbf{y})^\top\mathbf{X}+\lambda w^\top &= 0\\ w^\top(\lambda I+\mathbf{X}^\top\mathbf{X})-\mathbf{y}^\top\mathbf{X} &= 0\\ \hat{w} &= (\lambda I+\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}\end{aligned}$$

(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:

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

Answer: To prove the identity in the hint, we have

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

Now, using $\mathbf{\Phi}$ instead of $\mathbf{X}$, we would get

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

instead. Multiply by $\mathbf{\Phi}$,

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

Finally, for a test vector $x_\star$, let $\varphi_\star = \varphi(x)$. Then the prediction is $\varphi_\star^\top \hat{w}$, which gives

$$\begin{aligned}
&\varphi_\star^\top(\mathbf{\Phi}^\top\mathbf{\Phi} + \lambda I)^{-1}\mathbf{\Phi}^\top\mathbf{y} \\
=&\varphi_\star^\top\mathbf{\Phi}^\top(\mathbf{\Phi}\mathbf{\Phi}^\top + \lambda I)^{-1}\mathbf{y} \\
=&\varphi_\star^\top\mathbf{\Phi}^\top(\mathbf{K} + \lambda I)^{-1}\mathbf{y}
\end{aligned}$$

where we note that $\varphi_\star^\top\mathbf{\Phi}^\top$ is a row vector with ith entry $k(x_\star, x_i)$.

In particular, the nonlinear model can be "kernelized" and all computations can be carried out without explicit computation of $\varphi(x)$ nor of the "primal" weight vector $\hat{w}$.

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

$$\min_w \sum_{i=1}^n -\log\sigma(y_i w^\top\varphi(x_i)) + \lambda\|w\|_2^2 \tag{3}$$

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:* $\sigma'(t) = \sigma(t)\sigma(-t)$]

Answer:

The first step, albeit without regularisation, was derived in the lecture notes - it just suffices to check that the logistic function $\rho(t) = \log(1+e^{-t}) = -\log\sigma(t)$ is convex, which is true since $\rho''(t) = e^t/(1+e^t)^2 \geq 0$. Regularisation just adds λI to the Hessian.

For the second part, we write $w^\top\varphi(x_i) = \alpha^\top\mathbf{k}_i$ where $\mathbf{k}_i = [k(x_i, x_1), \ldots, k(x_i, x_n)]^\top$ to get the problem expressed in terms of α:

$$\min_\alpha \sum_{i=1}^n -\log\sigma(y_i\alpha^\top\mathbf{k}_i) + \lambda\alpha^\top\mathbf{K}\alpha, \tag{4}$$

with Hessian

$$\frac{\partial^2 J}{\partial\alpha\partial\alpha^\top} = \sum_{i=1}^n \sigma(y_i\alpha^\top\mathbf{k}_i)\sigma(-y_i\alpha^\top\mathbf{k}_i)\mathbf{k}_i\mathbf{k}_i^\top + 2\lambda\mathbf{K},$$

which is positive semidefinite. There is actually nothing special here about the logistic loss - the same argument works for any differentiable loss convex in $yf(x)$.