MATH3431 Machine Learning and Neural Networks III — Epiphany term 2023

Homework 3: Support Vector Machines

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Instructions: For Formative assessment, submit the solutions to all the parts of the Exercise.

Exercise 1. ($\star\star$) Consider a training data set $\mathcal{D} = \{z_i = (x_i, y_i)\}_{i=1}^m$. Consider the Soft-SVM Algorithm that requires the solution of the following quadratic minimization problem (in a slightly modified but equivalent form to what we have discussed)

Primal problem

$$(w^*, b^*, \xi^*) = \underset{(w,b,\xi)}{\arg\min} \left(\frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^{m} \xi_i \right) \tag{1}$$

$$\text{subject to: } y_i (\langle w, x_i \rangle + b) \geq 1 - \xi_i, \ \forall i = 1, ..., m \tag{2}$$

$$\xi_i \geq 0, \ \forall i = 1, ..., m \tag{3}$$

for some user-specified fixed parameter $C > 0$. We seek to find the dual problem of 1-3.

1. Specify the Lagrangian function L associated to the above primal quadratic minimization problem, where $\{\alpha_i\}$ are the Lagrange coefficients wrt (2), and $\{\beta_i\}$ are the Lagrange coefficients wrt (3). Write down any possible restrictions on the Lagrange coefficients.

2. Compute the dual Lagrangian function denoted as $\tilde{L}$ as a function of the Lagrange coefficients and the data points $\mathcal{D}$.

3. Apply the KKT conditions to the above problem, and write them down.

4. Derive and write down the dual Lagrangian quadratic maximization problem, along with the inequality and equality constraints, where you seek to find $\{\alpha_i\}$.

5. Justify why the i-th point x_i lies on the margin boundary when $\alpha_i \in (0, C)$ (beware it is $\alpha_i \neq C$), and why the i-th point x_i lies inside the margin when $\alpha_i = C$.

6. Given optimal values $\{\alpha_i^*\}$ for Lagrangian coefficients $\{\alpha_i\}$ as they are derived by solving the dual Lagrangian maximization problem in part 4, derive the optimal values w^* and b^* for the parameters w and b as function of the support vectors. Regarding parameter b it should be in the derived in the form

$$b^* = \frac{1}{|\mathcal{M}|} \sum_{i \in \mathcal{M}} \left(y_i - \sum_{j \in \mathcal{S}} \alpha_j^* y_j \langle x_j, x_i \rangle \right)$$

where you determine the sets $\mathcal{M}$ and $\mathcal{S}$.

7. Report the halfspace predictive rule $h_{w,b}(x)$ of the above problem as a function of α^* and b^*.

Solution.

1. It is

$$L(w, b, \xi, \alpha, \beta) = \frac{1}{2} \|w\|_2^2 + \sum_{i=1}^{m} C\xi_i + \sum_{i=1}^{m} \alpha_i \left(1 - y_i \left(\langle w, x_i \rangle + b\right) - \xi_i\right) - \sum_{i=1}^{m} \beta_i \xi_i \tag{4}$$

2. Let α, β be fixed. We minimize (8) wrt w, b and we get

$$0 = \frac{\partial L}{\partial w}(w, b, \xi, \alpha, \beta) \implies w = \sum_{i=1}^{m} \alpha_i y_i x_i \tag{5}$$

$$0 = \frac{\partial L}{\partial b}(w, b, \xi, \alpha, \beta) \implies 0 = \sum_{i=1}^{m} \alpha_i y_i$$

$$0 = \frac{\partial L}{\partial \xi_i}(w, b, \xi, \alpha, \beta) \implies \alpha_i = C - \beta_i \tag{6}$$

and we substitute in (8) to get

$$\tilde{L}(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \langle x_j, x_i \rangle$$

3. They are

$$
\begin{aligned}
0 =& \nabla \frac{1}{2} \|w\|_2^2 + \nabla \sum_{i=1}^{m} C\xi_i + \nabla \sum_{i=1}^{m} \alpha_i \left(1 - y_i \left(\langle w, x_i \rangle + b\right) - \xi_i\right) - \nabla \sum_{i=1}^{m} \beta_i \xi_i && \text{Stationarity} \\
& 1 - y_i \left(\langle w, x_i \rangle + b\right) - \xi_i \leq 0, \ \ \forall i = 1, ..., m && \text{Primal feasibility} \\
& \xi_i \geq 0 \\
& \alpha_i \geq 0 \ \ \forall i = 1, ..., m && \text{Dual feasibility} \\
& && (7) \\
& \beta_i \geq 0 \ \ \forall i = 1, ..., m && (8) \\
& \alpha_i \left(1 - y_i \left(\langle w, x_i \rangle + b\right) - \xi_i\right) = 0, \ \ \forall i = 1, ..., m && \text{Complementary slackness} \\
& && (9) \\
& \beta_i \xi_i = 0, \ \ \forall i = 1, ..., m && (10)
\end{aligned}
$$

4. It is

$$
\alpha^* = \arg \max_{\alpha \in \mathbb{R}^m : \alpha \geq 0} \left(\sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \langle x_j, x_i \rangle \right) \tag{11}
$$

$$
\text{subject to } \ 0 = \sum_{i=1}^{m} \alpha_i y_i
$$

$$
\alpha_i \in [0, C] \ \ \forall i = 1, ..., m \tag{12}
$$

constrain (12) results from (6), (8), and (7).

5.

- By (5), if $\alpha_i = 0$ then x_i does not contribute to the computation of the weights.
- By (5), if $\alpha_i \neq 0$, then x_i is a support vector and contributes.
- If $\alpha_i \in (0, C)$ (where $\alpha_i \neq C$) then (6) implies that $\beta_i > 0$. By (10) if $\beta_i > 0$ then $\xi_i = 0$. Hence, given these, from (9), it is $1 = y_i \left(\langle w, x_i \rangle + b\right)$ i.e. x_i lies on the boundary.
- If $\alpha_i = C$, then x_i lies inside the boundary.

6. From (9), it is either $\alpha_i = 0$ or $\left(1 - y_i \left(\langle w, x_i \rangle + b\right) - \xi_i\right) = 0$. Let $\mathcal{S} = \{i : y_i \left(\langle w, x_i \rangle + b\right) = 1 - \xi_i\}$. From (5) , it is

$$
w^* = \sum_{i \in \mathcal{S}} \alpha_i^* y_i x_i \tag{13}
$$

Using (9) and summing up indexes in $\mathcal{M} = \{i : \alpha_i \in (0, C)\}$ for which $\xi_i = 0$ it is

$$b^* = \frac{1}{|\mathcal{M}|} \sum_{i \in \mathcal{M}} \left(y_i - \sum_{j \in \mathcal{S}} \alpha_j^* y_j \langle x_j, x_i \rangle \right)$$

7. The formula is

$$\begin{aligned} h_{w,b}(x) &= \operatorname{sign}\left(\langle w^*, x\rangle + b^*\right) \\ &= \operatorname{sign}\left(\sum_{i=1}^{m} \alpha_i^* y_i \langle x_i, x\rangle + b^*\right) \end{aligned} \tag{14}$$
