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

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

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

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

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

$$L(w, b, \xi, \alpha, \beta) = \frac{1}{2} \|w\|_{2}^{2} + \sum_{i=1}^{m} \alpha_{i} (1 - y_{i} (\langle w, x_{i} \rangle + b) - \xi_{i}) + \sum_{i=1}^{m} \beta_{i} \xi_{i}$$
 (4)

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

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

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

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

$$0 = \nabla \frac{1}{2} \|w\|_{2}^{2} + \nabla \sum_{i=1}^{m} \alpha_{i} \left(1 - y_{i} \left(\langle w, x_{i} \rangle + b\right) - \xi_{i}\right) + \nabla \sum_{i=1}^{m} \beta_{i} \xi_{i}$$
 Stationarity
$$1 - y_{i} \left(\langle w, x_{i} \rangle + b\right) - \xi_{i} \leq 0, \quad \forall i = 1, ..., m$$
 Primal feasibility
$$\xi_{i} \geq 0$$

$$\alpha_{i} \geq 0 \quad \forall i = 1, ..., m$$
 Dual feasibility
$$\beta_{i} \geq 0 \quad \forall i = 1, ..., m$$

$$\alpha_{i} \left(1 - y_{i} \left(\langle w, x_{i} \rangle + b\right) - \xi_{i}\right) = 0, \quad \forall i = 1, ..., m$$
 Complementary slackness
$$\beta_{i} \xi_{i} = 0, \quad \forall i = 1, ..., m$$

$$(9)$$

4. It is

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

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

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 $1 = y_i (\langle w, x_i \rangle + b)$ 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 $(1 y_i (\langle w, x_i \rangle + b) \xi_i) = 0$. Let $\mathcal{S} = \{i : y_i (\langle w, x_i \rangle + b) = 1 \xi_i\}$. 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

$$h_{w,b}(x) = \operatorname{sign}(\langle w^*, x \rangle + b^*)$$

$$= \operatorname{sign}\left(\sum_{i=1}^{m} \alpha_i^* y_i \langle x_i, x \rangle + b^*\right)$$
(14)