Machine Learning

Answer Sheet for Homework 5

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December 9, 2015

Problem 1

The hard-margin support vector machine is with $d+1$ variables. For soft-margin support vector machine, there are N more variables ξ_n, $1 \leq n \leq N$.
So soft-margin support vector machine is a quadratic programming problem with $N+d+1$ variables.

$\square$

Problem 2

I wrote a `Q02.py` to help me get the answer. By using Python package `cvxopt`[2], with

$$\mathbf{z} = \begin{bmatrix} 1 & -2 \\ 4 & -5 \\ 4 & -1 \\ 5 & -2 \\ 7 & -7 \\ 7 & 1 \\ 7 & 1 \end{bmatrix}, \mathbf{y} = \begin{bmatrix} -1 \\ -1 \\ -1 \\ +1 \\ +1 \\ +1 \\ +1 \end{bmatrix} \tag{1}$$

and

$$\mathbf{Q} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \mathbf{p} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \tag{2}$$

$$\mathbf{A}^T = \begin{bmatrix} -1 & -1 & 2 \\ -1 & -4 & 5 \\ -1 & -4 & 1 \\ 1 & 5 & -2 \\ 1 & 7 & -7 \\ 1 & 7 & 1 \\ 1 & 7 & 1 \end{bmatrix}, \mathbf{c} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \tag{3}$$

To use this package, I gave `solvers.qp(`$\mathbf{Q}, \mathbf{p}, -\mathbf{A}^T, -\mathbf{c}$`)` and got

$$b = -9, \mathbf{w} = [2, 0] \tag{4}$$

So the hyperplane is

$$2z_1 - 9 = 0 \Rightarrow z_1 = 4.5 \tag{5}$$

$\square$

Problem 3

I wrote a `Q03.py` to help me get the answer. By using Python package `cvxopt`, with

$$\mathbf{Q} = \begin{bmatrix} 4 & 1 & 1 & 0 & -1 & -1 & -1 \\ 1 & 4 & 0 & -1 & -9 & -1 & -1 \\ 1 & 0 & 4 & -1 & -1 & -9 & -1 \\ 0 & -1 & -1 & 4 & 1 & 1 & 9 \\ -1 & -9 & -1 & 1 & 25 & 9 & 1 \\ -1 & -1 & -9 & 1 & 9 & 25 & 1 \\ -1 & -1 & -1 & 9 & 1 & 1 & 25 \end{bmatrix}, \mathbf{p} = \begin{bmatrix} -1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 \end{bmatrix}, \tag{6}$$

$$-\mathbf{A}^T = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}, \mathbf{c} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{7}$$

with

$$\mathbf{G} = \mathbf{y}^T = \begin{bmatrix} -1 & -1 & -1 & 1 & 1 & 1 & 1 \end{bmatrix} \text{ and } h = 0 \tag{8}$$

and To use this package, I gave `solvers.qp(`$\mathbf{Q}, \mathbf{p}, -\mathbf{A}^T, \mathbf{c}, \mathbf{G}, h$`)` and got

$$\alpha = \left[4.32 \times 10^{-9} \approx 0, 0.704, 0.704, 0.889, 0.259, 0.259, 5.27 \times 10^{-10} \approx 0\right] \tag{9}$$

where `cvxopt` needs conditions

$$-\mathbf{A}^T\boldsymbol{\alpha} \preceq \mathbf{c} \text{ and } \mathbf{G}\boldsymbol{\alpha} = h \tag{10}$$

□

Problem 4

I wrote a `Q04.py` to help me get the answer. By using python package `sympy` and

$$\mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n K\left(\mathbf{x}_n, \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) + b \tag{11}$$

$$b = y_s - \sum_{n=1}^{N} \alpha_n y_n K\left(\mathbf{x}_n, \mathbf{x}_s\right) \tag{12}$$

we have

$$\mathbf{w} = \frac{1}{9}\left(8x_1^2 - 16x_1 + 6x_2^2 - 15\right) \tag{13}$$

□

Problem 5

Since kernel function $K\left(\mathbf{x}, \mathbf{x}'\right) = \left(1 + \mathbf{x}^T\mathbf{x}'\right)^2$ is different from $\mathbf{z} = \left(\phi\left(\mathbf{x}\right), \phi\left(\mathbf{x}\right)\right)$, the curves should be different in the $\mathcal{X}$ space.

□

Problem 6

Since $\left\|\mathbf{x}_n - \mathbf{c}\right\|^2 \leq R^2$, $\forall n$, the constraint to maximize is

$$\left\|\mathbf{x}_n - \mathbf{c}\right\|^2 - R^2 \leq 0 \tag{14}$$

so $L\left(R, \mathbf{c}, \boldsymbol{\lambda}\right)$ is

$$L\left(R, \mathbf{c}, \boldsymbol{\lambda}\right) = R^2 + \sum_{n=1}^{N} \lambda_n \left(\left\|\mathbf{x}_n - \mathbf{c}\right\|^2 - R^2\right) \tag{15}$$

□

Problem 7

At the optimal $(R, \mathbf{c}, \boldsymbol{\lambda})$,

$$\frac{\partial L}{\partial R} = 2R - 2R \sum_{n=1}^{N} \lambda_n = 0 \Rightarrow \sum_{n=1}^{N} \lambda_n = 1 \text{ or } R = 0 \tag{16}$$

$$\frac{\partial L}{\partial \mathbf{c}} = 2 \sum_{n=1}^{N} \lambda_n (\mathbf{c} - \mathbf{x}_n) = \mathbf{0} \Rightarrow \mathbf{c} = \left(\sum_{n=1}^{N} \lambda_n \mathbf{x}_n \right) \Bigg/ \left(\sum_{n=1}^{N} \lambda_n \right) \text{ if } \sum_{n=1}^{N} \lambda_n \neq 0 \tag{17}$$

So the KKT conditions are

1. primal feasible: $\|\mathbf{x}_n - \mathbf{c}\|^2 \leq R^2$.
2. dual feasible: $\lambda_n \geq 0$.
3. dual-inner optimal: if $R \neq 0$, $\sum_{n=1}^{N} \lambda_n = 1$ and $\mathbf{c} = \sum_{n=1}^{N} \lambda_n \mathbf{x}_n$.
4. primal-inner optimal: $\lambda_n \left(\|\mathbf{x}_n - \mathbf{c}\|^2 - R^2 \right) = 0$.

□

Problem 8

From Problem 6, we have

$$L(R, \mathbf{c}, \boldsymbol{\lambda}) = R^2 + \sum_{n=1}^{N} \lambda_n \left(\|\mathbf{x}_n - \mathbf{c}\|^2 - R^2 \right) = R^2 + \sum_{n=1}^{N} \lambda_n \|\mathbf{x}_n - \mathbf{c}\|^2 - \sum_{n=1}^{N} \lambda_n R^2 \tag{18}$$

$$= R^2 - R^2 + \sum_{n=1}^{N} \lambda_n \|\mathbf{x}_n - \mathbf{c}\|^2 = \sum_{n=1}^{N} \lambda_n \|\mathbf{x}_n - \mathbf{c}\|^2 \tag{19}$$

where $\sum_{n=1}^{N} \lambda_n = 1$ since $R \neq 0$.
Also, from (17), we have $\mathbf{c} = \sum_{n=1}^{N} \lambda_n \mathbf{x}_n$. Hence

$$\text{Objective}(\lambda) = \sum_{n=1}^{N} \lambda_n \left\| \mathbf{x}_n - \sum_{m=1}^{N} \lambda_m \mathbf{x}_m \right\|^2 \tag{20}$$

□

Problem 9

We have

$$\sum_{n=1}^{N} \lambda_n \left\| \mathbf{x}_n - \mathbf{c} \right\|^2 = \sum_{n=1}^{N} \lambda_n \left(\mathbf{x}_n^T \mathbf{x}_n - \mathbf{x}_n^T \mathbf{c} - \mathbf{c}^T \mathbf{x}_n + \mathbf{c}^T \mathbf{c} \right) \tag{21}$$

$$= \sum_{n=1}^{N} \lambda_n \left(\mathbf{x}_n^T \mathbf{x}_n - \mathbf{x}_n^T \sum_{m=1}^{N} \lambda_m \mathbf{x}_m - \left(\sum_{m=1}^{N} \lambda_m \mathbf{x}_m \right)^T \mathbf{x}_n + \left\| \sum_{m=1}^{N} \lambda_m \mathbf{x}_m \right\|^2 \right) \tag{22}$$

So

$$\sum_{n=1}^{N} \lambda_n \left\| \phi(\mathbf{x}_n) - \phi(\mathbf{c}) \right\|^2 \tag{23}$$

$$= \sum_{n=1}^{N} \lambda_n K(\mathbf{x}_n, \mathbf{x}_n) - 2 \sum_{n=1}^{N} \sum_{m=1}^{N} \lambda_n \lambda_m K(\mathbf{x}_n, \mathbf{x}_m) + \sum_{n=1}^{N} \sum_{m=1}^{N} \lambda_n \lambda_m K(\mathbf{x}_n, \mathbf{x}_m) \tag{24}$$

$$= \sum_{n=1}^{N} \lambda_n K(\mathbf{x}_n, \mathbf{x}_n) - \sum_{n=1}^{N} \sum_{m=1}^{N} \lambda_n \lambda_m K(\mathbf{x}_n, \mathbf{x}_m) \tag{25}$$

□

Problem 10

From primal-inner optimal condition, pick some $\lambda_i > 0$, we have

$$\left\| \mathbf{x}_i - \mathbf{c} \right\|^2 = R^2 \tag{26}$$

so

$$R^2 = \mathbf{x}_i^T \mathbf{x}_i - \mathbf{x}_i^T \sum_{m=1}^{N} \lambda_m \mathbf{x}_m - \left(\sum_{m=1}^{N} \lambda_m \mathbf{x}_m \right)^T \mathbf{x}_i + \sum_{n=1}^{N} \sum_{m=1}^{N} \lambda_n \lambda_m \mathbf{x}_n^T \mathbf{x}_m \tag{27}$$

$$= K(\mathbf{x}_i, \mathbf{x}_i) - 2 \sum_{m=1}^{N} \lambda_m K(\mathbf{x}_i, \mathbf{x}_m) + \sum_{n=1}^{N} \sum_{m=1}^{N} \lambda_n \lambda_m K(\mathbf{x}_n, \mathbf{x}_m) \tag{28}$$

$$\Rightarrow R = \sqrt{K(\mathbf{x}_i, \mathbf{x}_i) - 2 \sum_{m=1}^{N} \lambda_m K(\mathbf{x}_i, \mathbf{x}_m) + \sum_{n=1}^{N} \sum_{m=1}^{N} \lambda_n \lambda_m K(\mathbf{x}_n, \mathbf{x}_m)} \tag{29}$$

where $R > 0$.

□

Problem 11

Claim: Let $\tilde{\mathbf{w}} = \begin{bmatrix} \mathbf{w} \\ \sqrt{2C}\cdot y_1\xi_1 \\ \sqrt{2C}\cdot y_2\xi_2 \\ \vdots \\ \sqrt{2C}\cdot y_N\xi_N \end{bmatrix}$ and $\tilde{\mathbf{x}}_n = \begin{bmatrix} \mathbf{x}_n \\ v_1 \\ v_2 \\ \vdots \\ v_N \end{bmatrix}$, where $v_i = \frac{1}{\sqrt{2C}} [\![i = n]\!]$.

Proof of Claim:

First, we have

$$\frac{1}{2}\tilde{\mathbf{w}}^T\tilde{\mathbf{w}} = \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{n=1}^{N} y_n^2\xi_n^2 = \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{n=1}^{N}\xi_n^2 \tag{30}$$

where $y_n^2 = 1$ due to $y_n \in \{+1, -1\}$.

And (P_2) can be rewritten as

$$\min_{\tilde{\mathbf{w}},b,\boldsymbol{\xi}} \left(\frac{1}{2}\tilde{\mathbf{w}}^T\tilde{\mathbf{w}}\right) \tag{31}$$

Then we have

$$\tilde{\mathbf{w}}^T\tilde{\mathbf{x}}_n = \tilde{\mathbf{w}}^T \begin{bmatrix} \mathbf{x}_n \\ v_1 \\ v_2 \\ \vdots \\ v_N \end{bmatrix} = \tilde{\mathbf{w}}^T \begin{bmatrix} \mathbf{x}_n \\ 0 \\ \vdots \\ \underbrace{\frac{1}{\sqrt{2C}}}_{i=n} \\ \vdots \\ 0 \end{bmatrix} \tag{32}$$

$$= \mathbf{w}^T\mathbf{x}_n + 0 + \cdots + y_n\xi_n + \cdots + 0 = \mathbf{w}^T\mathbf{x}_n + y_n\xi_n \tag{33}$$

So

$$y_n\left(\mathbf{w}^T\mathbf{x}_n + b\right) \geq 1 - \xi_n = 1 - y_n^2\xi_n \tag{34}$$

$$\Rightarrow\ y_n\left(\mathbf{w}^T\mathbf{x}_n + b\right) + y_n^2\xi_n = y_n\left(\mathbf{w}^T\mathbf{x}_n + y_n\xi_n + b\right) = y_n\left(\tilde{\mathbf{w}}^T\tilde{\mathbf{x}}_n + b\right) \geq 1 \tag{35}$$

Hence, (P_2) is equivalent to a linear hard-margin support vector machine primal problem.

□

Problem 12

Claim: $K(\mathbf{x}, \mathbf{x}') = K_1(\mathbf{x}, \mathbf{x}') + K_2(\mathbf{x}, \mathbf{x}')$ is always a valid kernel.

Proof of Calim:

Consider Mercer's conditions,

1. Symmetric

   Since K_1 and K_2 are valid kernel, both of them are symmetric. So $K_1 + K_2$ must be symmetric.

2. K is positive semi-definite

   Consider any vector $\mathbf{v}$, we have

$$\mathbf{v}^T K_1 \mathbf{v} = \begin{bmatrix} \sum_{i=1}^N v_i \phi_1(x_i)^T \phi_1(x_1') & \cdots & \sum_{i=1}^N v_i \phi_1(x_i)^T \phi_1(x_N') \end{bmatrix} \mathbf{v} \tag{36}$$

$$= \sum_{j=1}^N \sum_{i=1}^N v_i \phi_1(x_i)^T \phi_1\left(x_j'\right) v_j \geq 0 \tag{37}$$

$$\mathbf{v}^T K_2 \mathbf{v} = \begin{bmatrix} \sum_{i=1}^N v_i \phi_2(x_i)^T \phi_2(x_1') & \cdots & \sum_{i=1}^N v_i \phi_2(x_i)^T \phi_2(x_N') \end{bmatrix} \mathbf{v} \tag{38}$$

$$= \sum_{j=1}^N \sum_{i=1}^N v_i \phi_2(x_i)^T \phi_2\left(x_j'\right) v_j \geq 0 \tag{39}$$

$$\mathbf{v}^T K \mathbf{v} = \mathbf{v}^T (K_1 + K_2) \mathbf{v} = \sum_{j=1}^N \sum_{i=1}^N v_i \left(\phi_1(x_i)^T \phi_1\left(x_j'\right) + \phi_2(x_i)^T \phi_2\left(x_j'\right) \right) v_j \tag{40}$$

$$= \mathbf{v}^T K_1 \mathbf{v} + \mathbf{v}^T K_2 \mathbf{v} \geq 0 \tag{41}$$

   Hence, K is positive semi-definite.

By satisfying the Mercer's conditions, K is a valid kernel.

□

Problem 13

<u>Claim</u>: $K(\mathbf{x}, \mathbf{x}') = \exp(-K_1(\mathbf{x}, \mathbf{x}'))$ is always a valid kernel.
<u>Proof of Claim</u>:
Consider Mercer's conditions,

1. Symmetric

   Since K_1 is valid kernel, K_1 is symmetric. So K must be symmetric.

2. K is positive semi-definite

   Consider any vector $\mathbf{v}$, we have

$$\mathbf{v}^T K \mathbf{v} = \mathbf{v}^T \exp(-K_1(\mathbf{x}, \mathbf{x}')) \mathbf{v} = \mathbf{v}^T \sum_{k=1}^{\infty} \frac{1}{k!} (-K_1(\mathbf{x}, \mathbf{x}'))^k \mathbf{v} \tag{42}$$

$$= \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \left(\mathbf{v}^T (K_1(\mathbf{x}, \mathbf{x}'))^k \mathbf{v} \right) \tag{43}$$

where $\mathbf{v}^T \left(K_1\left(\mathbf{x}, \mathbf{x}'\right)\right)^k \mathbf{v} \geq 0$ for all k since K_1 is positive semi-definite. So we have

$$\sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \left(\mathbf{v}^T \left(K_1\left(\mathbf{x}, \mathbf{x}'\right)\right)^k \mathbf{v}\right) \geq 0 \Rightarrow \mathbf{v}^T K \mathbf{v} \geq 0 \tag{44}$$

Hence, K is positive semi-definite.

By satisfying the Mercer's conditions, K is a valid kernel.

Note: Prove A^k is positive semi-definite if A is positive semi-definite $k \in \mathbb{N}$.
Since A is positive semi-definite, all eigenvalues λ_i of A is non-negative. Hence for any vector $\mathbf{v}$

$$\mathbf{v}^T A^k \mathbf{v} = \mathbf{v}^T A^{k-1} \left(A\mathbf{v}\right) = \mathbf{v}^T A^{k-1} \left(\sum_{i=1}^{N} \lambda_i v_i\right) = \mathbf{v}^T A^{k-2} \left(\sum_{i=1}^{N} \lambda_i^2 v_i\right) \tag{45}$$

$$= \cdots = \sum_{i=1}^{N} \lambda_i^k v_i^2 \geq 0 \text{ since } \lambda_i \geq 0, \forall i \tag{46}$$

$\square$

Problem 14

Claim: $\tilde{C} = \dfrac{C}{p}$, $\tilde{\beta}_n = \dfrac{\beta_n}{p} = \dfrac{C}{p} - \dfrac{\alpha_n}{p} = \tilde{C} - \tilde{\alpha}_n$, $\forall n$ for optimal solution.
Proof of Claim:

$$\tilde{g}_{\text{SVM}}(\mathbf{x}) = \text{sign}\left(\sum_{n=1}^{N} \tilde{\alpha}_n y_n \tilde{K}\left(\mathbf{x}_n, \mathbf{x}\right) + b\right) \tag{47}$$

$$= \text{sign}\left(\sum_{n=1}^{N} \tilde{\alpha}_n y_n \left(pK\left(\mathbf{x}_n, \mathbf{x}\right) + q\right) + b\right) \tag{48}$$

$$= \text{sign}\left(p\sum_{n=1}^{N} \tilde{\alpha}_n y_n K\left(\mathbf{x}_n, \mathbf{x}\right) + q\sum_{n=1}^{N} \tilde{\alpha}_n y_n + b\right) \tag{49}$$

$$= \text{sign}\left(p\sum_{n=1}^{N} \left(\tilde{C} - \tilde{\beta}_n\right) y_n K\left(\mathbf{x}_n, \mathbf{x}\right) + q \cdot 0 + b\right) \tag{50}$$

$$= \text{sign}\left(\sum_{n=1}^{N} \left(p \cdot \frac{C}{p} - p\tilde{\beta}_n\right) y_n K\left(\mathbf{x}_n, \mathbf{x}\right) + b\right) \tag{51}$$

$$= \text{sign}\left(\sum_{n=1}^{N} \left(C - p\tilde{\beta}_n\right) y_n K\left(\mathbf{x}_n, \mathbf{x}\right) + b\right) \tag{52}$$

where $\sum_{n=1}^{N} \tilde{\alpha}_n y_n = 0$ due to optimal constraint.

Since $\tilde{\beta}_n = \frac{\beta_n}{p}$, then we have

$$\tilde{g}_{\text{SVM}}(\mathbf{x}) = \operatorname{sign}\left(\sum_{n=1}^{N} (C - \beta_n) y_n K(\mathbf{x}_n, \mathbf{x}) + b\right) \tag{53}$$

$$= \operatorname{sign}\left(\sum_{n=1}^{N} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b\right) \tag{54}$$

$$= g_{\text{SVM}}(\mathbf{x}) \tag{55}$$

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Problem 15

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Problem 16

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Problem 17

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Problem 18

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Problem 19

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Problem 20

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Reference

[1] Lecture Notes by Hsuan-Tien LIN, Department of Computer Science and Information Engineering, National Taiwan University, Taipei 106, Taiwan.

[2] Quadratic Programming with Python and CVXOPT

https://courses.csail.mit.edu/6.867/wiki/images/a/a7/Qp-cvxopt.pdf