

Machine Learning Course 2024 Spring: Homework 2

March 31, 2024

1 Problem 1

Solution:

1. A linear SVM with $C = 0.02$.

Solution: Correspond to Figure 1.4. The decision boundary of linear SVM is linear. In comparison with Figure 1.3, the line does not separate two classes strictly, which corresponds to the case C is small and more errors are allowed.

2. A linear SVM with $C = 20$.

Solution: Correspond to Figure 1.3. The decision boundary of linear SVM is linear. In comparison with Figure 1.4, the line separates two classes strictly, which corresponds to the case C is big.

3. A hard-margin kernel SVM with $\kappa(\mathbf{u}, \mathbf{v}) = \mathbf{u}^\top \mathbf{v} + (\mathbf{u}^\top \mathbf{v})^2$.

Solution: Correspond to Figure 1.5. The decision boundary of quadratic kernel is given by $f(\mathbf{x}) = \sum_i \alpha_i (\mathbf{x}_i^\top \mathbf{x} + (\mathbf{x}_i^\top \mathbf{x})^2) + b$. Hence the decision boundary is $f(\mathbf{x}) = 0$. Since $f(\mathbf{x})$ is second order function of \mathbf{x} , the curve can be ellipse or hyperbolic curve. Figure 1.5 is hyperbolic curve.

4. A hard-margin kernel SVM with $\kappa(\mathbf{u}, \mathbf{v}) = \exp(-5\|\mathbf{u} - \mathbf{v}\|^2)$.

Solution: Correspond to Figure 1.6. We can write out the decision function as $f(\mathbf{x}) = \sum_i \alpha_i \exp(-\gamma \|\mathbf{x}_i - \mathbf{x}\|^2) + b$. If γ is large, the kernel value is quite small even if the

distance between the \mathbf{x} and \mathbf{x}_i is small. This makes the classification hard with few supporting vectors, Hence Figure 1.6 corresponds to $\gamma = 5$.

5. A hard-margin kernel SVM with $\kappa(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{1}{5}\|\mathbf{u} - \mathbf{v}\|^2\right)$.

Solution: Correspond to Figure 1.1.

□

2 Problem 2

Solution:

1. Construct the Lagrangian:

$$L(\mathbf{x}, \boldsymbol{\lambda}, \mu) = -\sum_{i=1}^n \log(\alpha_i + x_i) + \sum_{i=1}^n \lambda_i(-x_i) + \mu\left(\sum_{i=1}^n x_i - 1\right), \quad (1)$$

where $\mathbf{x} = [x_1, \dots, x_n]^\top$, $\boldsymbol{\lambda} = [\lambda_1, \dots, \lambda_n]^\top \in \mathbb{R}^n$, and $\mu \in \mathbb{R}$.

The KKT conditions are:

- (1) $-x_i^* \leq 0, i = 1, \dots, n$
- (2) $\sum_{i=1}^n x_i^* - 1 = 0$
- (3) $\lambda_i^* \geq 0, i = 1, \dots, n$
- (4) $\lambda_i^* x_i^* = 0, i = 1, \dots, n$
- (5) $\nabla_{x_i^*} L(\mathbf{x}^*, \boldsymbol{\lambda}^*, \mu^*) = -\frac{1}{\alpha_i + x_i^*} - \lambda_i^* + \mu^* = 0, i = 1, \dots, n$

2. According to the KKT conditions (3)-(5), we have

$$x_i^* \left(\mu^* - \frac{1}{\alpha_i + x_i^*} \right) = 0, i = 1, \dots, n \quad (2)$$

$$\mu^* \geq \frac{1}{\alpha_i + x_i^*}, i = 1, \dots, n \quad (3)$$

- (1) If $\mu^* < \frac{1}{\alpha_i}$, Eq.(3) is satisfied when $x_i^* > 0$. Then, according to Eq.(2), we have

$$x_i^* = \frac{1}{\mu^*} - \alpha_i;$$

- (2) If $\mu^* \geq \frac{1}{\alpha_i}$, according to Eq.(2), we have $x_i^* = 0$.

Thus we have,

$$x_i^* = \max\{0, \frac{1}{\mu^*} - \alpha_i\}. \quad (4)$$

Substituting Eq.(4) into the condition (2), we can obtain

$$\sum_{i=1}^n \max\{0, \frac{1}{\mu^*} - \alpha_i\} = 1. \quad (5)$$

Therefore, the optimal solution of the problem is $x_i^* = \max\{0, \frac{1}{\mu^*} - \alpha_i\}, i = 1, \dots, n$, where μ^* satisfies Eq.(5)

□

3 Problem 3

1. Solution:

$$\begin{aligned} & \|\phi(\mathbf{x}_i) - \phi(\mathbf{x}_j)\|^2 \\ &= \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_i) + \phi(\mathbf{x}_j)^\top \phi(\mathbf{x}_j) - 2\phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j) \\ &= \kappa(\mathbf{x}_i, \mathbf{x}_i) + \kappa(\mathbf{x}_j, \mathbf{x}_j) - 2\kappa(\mathbf{x}_i, \mathbf{x}_j) \\ &= 1 + 1 - 2 \exp(-\frac{1}{2}\|\mathbf{x}_i - \mathbf{x}_j\|^2) \\ &< 2 \end{aligned}$$

□

2. Proof:

Consider a simpler kernel function $\kappa'(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^\top \mathbf{x}_j + c$ first. For any dataset $D = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m\}$, the kernel matrix \mathbf{K}' is:

$$\mathbf{K}' = \begin{pmatrix} \kappa'(\mathbf{x}_1, \mathbf{x}_1) & \cdots & \kappa'(\mathbf{x}_1, \mathbf{x}_m) \\ \vdots & \ddots & \vdots \\ \kappa'(\mathbf{x}_m, \mathbf{x}_1) & \cdots & \kappa'(\mathbf{x}_m, \mathbf{x}_m) \end{pmatrix} = \begin{pmatrix} \mathbf{x}_1^\top \mathbf{x}_1 + c & \cdots & \mathbf{x}_1^\top \mathbf{x}_m + c \\ \vdots & \ddots & \vdots \\ \mathbf{x}_m^\top \mathbf{x}_1 + c & \cdots & \mathbf{x}_m^\top \mathbf{x}_m + c \end{pmatrix}. \quad (6)$$

The kernel matrix can be further rewritten as

$$\begin{aligned}
\mathbf{K}' &= \begin{pmatrix} \mathbf{x}_1^\top \mathbf{x}_1 & \cdots & \mathbf{x}_1^\top \mathbf{x}_m \\ \vdots & \ddots & \vdots \\ \mathbf{x}_m^\top \mathbf{x}_1 & \cdots & \mathbf{x}_m^\top \mathbf{x}_m \end{pmatrix} + \begin{pmatrix} c & \cdots & c \\ \vdots & \ddots & \vdots \\ c & \cdots & c \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_m^\top \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 & \cdots & \mathbf{x}_m \end{pmatrix} + c \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \begin{pmatrix} 1 & \cdots & 1 \end{pmatrix} \\
&= \mathbf{X}\mathbf{X}^\top + c\mathbf{1}\mathbf{1}^\top,
\end{aligned} \tag{7}$$

where $\mathbf{X} \in \mathbb{R}^{m \times d}$ is the data matrix. Considering the positive definiteness of matrix \mathbf{K}' , for any non-zero vector $\mathbf{w} \in \mathbb{R}^m$, we have

$$\begin{aligned}
\mathbf{w}^\top \mathbf{K}' \mathbf{w} &= \mathbf{w}^\top (\mathbf{X}\mathbf{X}^\top + c\mathbf{1}\mathbf{1}^\top) \mathbf{w} \\
&= \mathbf{w}^\top \mathbf{X}\mathbf{X}^\top \mathbf{w} + c\mathbf{w}^\top \mathbf{1}\mathbf{1}^\top \mathbf{w} \\
&= (\mathbf{X}^\top \mathbf{w})^\top (\mathbf{X}^\top \mathbf{w}) + c(\mathbf{1}^\top \mathbf{w})^\top (\mathbf{1}^\top \mathbf{w}) \\
&= \|\mathbf{X}^\top \mathbf{w}\|^2 + c(\mathbf{1}^\top \mathbf{w})^2.
\end{aligned} \tag{8}$$

- (a) When $c \geq 0$, we have $\mathbf{w}^\top \mathbf{K}' \mathbf{w} \geq 0$, thus, \mathbf{K}' is semi-positive definite. According to Mercer's Theorem (refer to page 55 of Lecture 6 slides), $\kappa'(\mathbf{x}_i, \mathbf{x}_j)$ is a kernel function. According to the kernels' composition rule (refer to page 57 of Lecture 6 slides), $\kappa(\mathbf{x}_i, \mathbf{x}_j) = (\kappa'(\mathbf{x}_i, \mathbf{x}_j))^N$ is also a kernel function as a multiplication of N kernel functions.
- (b) When $c < 0$, it cannot be guaranteed that $\mathbf{w}^\top \mathbf{K}' \mathbf{w} \geq 0$, thus, \mathbf{K}' is not semi-positive definite. Consequently, $\kappa(\mathbf{x}_i, \mathbf{x}_j)$ is not a kernel function.

□