

Support Vector Machine

Primal Form

- A hyperplane that separates a n-dimensional space into two half-spaces.
- Prediction rule: $y = \text{sign}(\omega^T x + b)$
- Margin
 - Geometric margin (≥ 0): $\gamma^{(i)} = y^{(i)} \left(\left(\frac{\omega}{\|\omega\|} \right)^T x^{(i)} + \frac{b}{\|\omega\|} \right)$
 - Whole training set, the margin is $\gamma = \min_i \gamma^{(i)}$
- Goal: Learn ω and b that achieves the maximum margin $\max_{\omega, b} \min_i \gamma^{(i)}$

$$\begin{aligned} & \max_{\gamma, \omega, b} \gamma \\ & \text{s.t. } y^{(i)} (\omega^T x^{(i)} + b) \geq \gamma \|\omega\|, \quad \forall i \end{aligned}$$

- Scaling (ω, b) such that $\gamma \|\omega\| = 1$, i.e. $\omega' = \frac{\omega}{\gamma \|\omega\|}$ and $b' = \frac{b}{\gamma \|\omega\|}$.
- $\therefore \|\omega'\| = \frac{\|\omega\|}{\gamma \|\omega\|} = \frac{1}{\gamma}$, $y^{(i)} (\omega'^T x^{(i)} + b') \geq 1$
- the problem becomes

$$\begin{aligned} & \max_{\omega, b} \frac{1}{\|\omega\|} \Leftrightarrow \min_{\omega, b} \omega^T \omega \Leftrightarrow \min_{\omega, b} \frac{1}{2} \|\omega\|^2 \\ & \text{s.t. } y^{(i)} (\omega^T x^{(i)} + b) \geq 1, \quad \forall i \end{aligned}$$

- $\max_{\omega, b} \frac{1}{\|\omega\|}$ is equivalent to $\min_{\omega, b} \omega^T \omega$

Def. The primal problem

$$\begin{aligned} & \min_{\omega, b} \frac{1}{2} \|\omega\|^2 \\ & \text{s.t. } y^{(i)} (\omega^T x^{(i)} + b) \geq 1, \quad \forall i \end{aligned}$$

Duality of SVM

Preliminaries should be mastered in chapter Optimization of appendix.

- The Lagrangian problem for SVM

$$\min_{\omega, b} \max_{\alpha} \mathcal{L}(\omega, b, \alpha) = \frac{1}{2} \|\omega\|^2 + \sum_{i=1}^m \alpha_i (1 - y^{(i)} (\omega^T x^{(i)} + b))$$

- The Lagrangian dual problem for SVM is $\max_{\alpha} \mathcal{G}(\alpha) = \max_{\alpha} \inf_{\omega, b} \mathcal{L}(\omega, b, \alpha)$

$$\begin{aligned} & \max_{\alpha} \quad \mathcal{G}(\alpha) = \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i,j=1}^m y^{(i)} y^{(j)} \alpha_i \alpha_j (x^{(i)})^T x^{(j)} \\ & \text{s.t.} \quad \sum_{i=1}^m \alpha_i y^{(i)} = 0 \\ & \quad \alpha_i \geq 0 \quad \forall i \end{aligned}$$

- Proof.

$$\begin{aligned}
- \frac{\partial}{\partial \omega} \mathcal{L}(\omega, b, \alpha) &= \omega - \sum_{i=1}^m \alpha_i y^{(i)} x^{(i)} = 0 \text{ and } \frac{\partial}{\partial b} \mathcal{L}(\omega, b, \alpha) = \\
&\sum_{i=1}^m \alpha_i y^{(i)} = 0 \\
- \mathcal{L} &\text{ is a convex function.}
\end{aligned}$$

- It suffices Slater's Condition. Thus, the problem can be solved by QP solver (MATLAB, ...)
- Since we have the solution α^* for the dual problem, we can calculate the solution for the primal problem.

$$\begin{aligned}
\omega^* &= \sum_{i=1}^m \alpha_i^* y^{(i)} x^{(i)} \\
b^* &= y^{(i)} - \omega^{*T} x^{(i)} \quad \text{if } \alpha_i^* > 0
\end{aligned}$$

- For robustness, the optimal value for b is calculated by taking the averages across all b^*

$$b^* = \frac{\sum_{i: \alpha_i^* > 0} (y^{(i)} - \omega^{*T} x^{(i)})}{\sum_{i=1}^m 1(\alpha_i^* > 0)}$$

- However, according to Complementary Slackness, $\alpha_i^* [1 - y^{(i)} (\omega^{*T} x^{(i)} + b^*)] = 0$.
- α_i^* is non-zero only if $x^{(i)}$ lies on the margin, i.e., $y^{(i)} (\omega^{*T} x^{(i)} + b^*) = 1$. (Support Vector, \mathcal{S}).

$$\therefore \omega = \sum_{s \in \mathcal{S}} \alpha_s y^{(s)} x^{(s)}$$

Kernel

- Basic idea: mapping data to higher dimensions where it exhibits linear patterns.
- Each kernel K has an associated feature mapping $\phi : \mathcal{X} \rightarrow \mathcal{F}$ from input to feature space.
 - e.g., quadratic mapping $\phi : x \rightarrow \{x_1^2, x_2^2, \dots, x_1 x_2, \dots, x_1 x_n, \dots, x_{n-1} x_n\}$
- Kernel $K(x, z) = \phi(x)^T \phi(z)$, $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ takes two inputs and gives their similarity in \mathcal{F} .

Theorem. Mercer's Condition.

For K to be a kernel function if K is a positive definite function.

$$\int \int f(x) K(x, z) f(z) dx dz > 0 \forall f, \text{ s.t. } \int_{-\infty}^{\infty} f^2(x) dx < \infty$$

- Composing rules
 - Direct sum $K(x, z) = K_1(x, z) + K_2(x, z)$
 - Scalar product $K(x, z) = \alpha K_1(x, z)$
 - Direct product $K(x, z) = K_1(x, z) K_2(x, z)$

Def. Kernel Matrix.

$$K_{i,j} = K(x^{(i)}, x^{(j)}) = \phi(x^{(i)})^T \phi(x^{(j)})$$

Example Kernel

- Linear (trivial) Kernel $K(x, z) = x^T z$
- Quadratic Kernel $K(x, z) = (x^T z)^2$ or $(1 + x^T z)^2$
- Polynomial Kernel (of degree d) $K(x, z) = (x^T z)^d$ or $(1 + x^T z)^d$
- Gaussian Kernel $K(x, z) = \exp\left(-\frac{\|x-z\|^2}{2\sigma^2}\right)$
- Sigmoid Kernel $K(x, z) = \tanh(\alpha x^T z + c)$

Applicable Algorithm

- SVM, linear regression, etc.
- K-means, PCA, etc.

Kernelized SVM

- Optimization problem

$$\begin{aligned} \max_{\alpha} \quad & \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i,j=1}^m y^{(i)} y^{(j)} \alpha_i \alpha_j (x^{(i)})^T x^{(j)} \\ \text{s.t.} \quad & \sum_{i=1}^m \alpha_i y^{(i)} = 0 \\ & \alpha_i \geq 0 \quad \forall i \end{aligned}$$

\Downarrow

$$\begin{aligned} \max_{\alpha} \quad & \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i,j=1}^m y^{(i)} y^{(j)} \alpha_i \alpha_j K_{i,j} \\ \text{s.t.} \quad & \sum_{i=1}^m \alpha_i y^{(i)} = 0 \\ & \alpha_i \geq 0 \quad \forall i \end{aligned}$$

- Solution

$$\begin{aligned} \omega^* &= \sum_{i: \alpha_i^* > 0} \alpha_i^* y^{(i)} \phi(x^{(i)}) \\ b^* &= y^{(i)} - \omega^{*T} \phi(x^{(i)}) \\ &= y^{(i)} - \sum_{j: \alpha_j^* > 0} \alpha_j^* y^{(j)} \phi^T(x^{(j)}) \phi(x^{(i)}) \\ &= y^{(i)} - \sum_{j: \alpha_j^* > 0} \alpha_j^* y^{(j)} K_{ij} \end{aligned}$$

- Prediction

$$\begin{aligned} y &= \text{sign} \left(\sum_{i: \alpha_i^* > 0} \alpha_i^* y^{(i)} \phi(x^{(i)})^T \phi(x) + b^* \right) \\ &= \text{sign} \left(\sum_{i: \alpha_i^* > 0} \alpha_i^* y^{(i)} K(x^{(i)}, x) + b^* \right) \end{aligned}$$

- Kernelized SVM needs to compute kernel when testing, whereas computed ω^* and b^* are enough in the unkernelized version.

Soft Margin

- Relax the constraints from $y^{(i)}(\omega^T x^{(i)} + b) \geq 1$ to $y^{(i)}(\omega^T x^{(i)} + b) \geq 1 - \xi_i$
- $\xi_i \geq 0$ is called slack variable

Def. Soft Margin SVM

$$\begin{aligned} \min_{\omega, b, \xi} \quad & \frac{1}{2} \|\omega\|^2 + C \sum_{i=1}^m \xi_i \\ \text{s.t.} \quad & y^{(i)}(\omega^T x^{(i)} + b) \geq 1 - \xi_i, \quad \forall i = 1, \dots, m \\ & \xi_i \geq 0, \quad \forall i = 1, \dots, m \end{aligned}$$

- C is a hyper-parameter that controls the relative weighting between $\frac{1}{2} \|\omega\|^2$ for larger margins and $\sum_{i=1}^m \xi_i$ for fewer misclassified examples.
- Lagrangian function

$$\mathcal{L}(\omega, b, \xi, \alpha, r) = \frac{1}{2} \omega^T \omega + C \sum_{i=1}^m \xi_i - \sum_{i=1}^m \alpha_i [y^{(i)} (\omega^T x^{(i)} + b) - 1 + \xi_i] - \sum_{i=1}^m r_i \xi_i$$

- KKT conditions (the optimal values of ω, b, ξ, α , and r should satisfy the following conditions)

$$\begin{aligned} - \nabla_{\omega} \mathcal{L}(\omega, b, \xi, \alpha, r) = 0 & \Rightarrow \omega^* = \sum_{i=1}^m \alpha_i^* y^{(i)} x^{(i)} \\ - \nabla_b \mathcal{L}(\omega, b, \xi, \alpha, r) = 0 & \Rightarrow \sum_{i=1}^m \alpha_i^* y^{(i)} = 0 \\ - \nabla_{\xi_i} \mathcal{L}(\omega, b, \xi, \alpha, r) = 0 & \Rightarrow \alpha_i^* + r_i^* = C, \text{ for } \forall i \\ - \alpha_i^*, r_i^*, \xi_i^* & \geq 0, \text{ for } \forall i \\ - y^{(i)} (\omega^{*T} x^{(i)} + b^*) + \xi_i^* - 1 & \geq 0, \text{ for } \forall i \\ - \alpha_i^* (y^{(i)} (\omega^{*T} x^{(i)} + b^*) + \xi_i^* - 1) & = 0, \text{ for } \forall i \\ - r_i^* \xi_i^* & = 0, \text{ for } \forall i \end{aligned}$$

- Dual problem

$$\begin{aligned} \max_{\alpha} \quad & \mathcal{J}(\alpha) = \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i,j=1}^m y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \quad \forall i = 1, \dots, m \\ & \sum_{i=1}^m \alpha_i y^{(i)} = 0 \end{aligned}$$

- Solution

$$\begin{aligned} - \omega^* &= \sum_{i=1}^m \alpha_i^* y^{(i)} x^{(i)} \\ - b^* &= \frac{\sum_{i: 0 < \alpha_i^* < C} (y^{(i)} - \omega^{*T} x^{(i)})}{\sum_{i=1}^m 1(0 < \alpha_i^* < C)} \end{aligned}$$

- Proof.

$$\because r_i^* \xi_i^* = 0 \Leftrightarrow (C - \alpha_i^*) \xi_i^* = 0$$

$$\therefore \forall i, \alpha_i^* \neq C \Rightarrow \xi_i = 0 \Rightarrow \alpha_i (y^{(i)} (\omega^{*T} x^{(i)} + b^*) - 1) = 0$$

$$\therefore \forall i, \alpha_i^* \in (0, C) \Rightarrow y^{(i)} (\omega^{*T} x^{(i)} + b^*) = 1 \Rightarrow \omega^{*T} x^{(i)} + b^* = y^{(i)}$$

- Corollaries of KKT conditions for soft-margin SVM
 - When $\alpha_i^* = 0$, $y^{(i)} (\omega^{*T} x^{(i)} + b^*) \geq 1$, correctly classified.
 - When $\alpha_i^* = C$, $y^{(i)} (\omega^{*T} x^{(i)} + b^*) \leq 1$, misclassified.
 - When $0 < \alpha_i^* < C$, $y^{(i)} (\omega^{*T} x^{(i)} + b^*) = 1$, support vector.