Support Vector Machine

Primal Form

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

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

- 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

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

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

  Def. The primal problem

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

Duality of SVM

Preliminaries should be mastered in chapterr Optimization of appendix.

- The Lagrangian problem for SVM

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

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

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

- Proof.

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

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

$$\omega^* = \sum_{i=1}^{m} \alpha^* y^{(i)} x^{(i)} b^* = y^{(i)} - \omega^{*T} x^{(i)}, \text{ if } \alpha^* > 0$$

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

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

- However, according to Complementary Slackness, $\alpha_i^* \left[1 - y^{(i)} \left(\omega^{*T} x^{(i)} + b^* \right) \right] = 0.$
- α_i^* is non-zero only if $x^{(i)}$ lies on the margin, i.e., $y^{(i)} \left(\omega^{*T} x^{(i)} + b^* \right) = 1.$ (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 $\phi : \mathcal{X} \to \mathcal{F}$ from input to feature space.
  - e.g., quadratic mapping $\phi : x \to \{x_1^2, x_2^2, \cdots, x_1 x_2, \cdots, x_1 x_n, \cdots, x_{n-1} x_n\}$
- Kernel $K(x, z) = \phi(x)^T \phi(z),\ K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ takes two inputs and gives their similarity in $\mathcal{F}$.

  Thereom. Mercer's Condition.

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

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

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

Applicable Algorithm

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

Kernelized SVM

- Optimization problem

$$\begin{array}{ll} \text{max}_\alpha & \sum_{i=1}^m \alpha_i - \frac{1}{2}\sum_{i,j=1}^m y^{(i)} y^{(j)} \alpha_i \alpha_j \left(x^{(i)}\right)^T x^{(j)} \\ \text{s.t.} & \sum_{i=1}^m \alpha_i y^{(i)} = 0 \\ & \alpha_i \geq 0 \quad \forall i \end{array} \Rightarrow \begin{array}{ll} \text{max}_\alpha & \sum_{i=1}^m \alpha_i - \frac{1}{2}\sum_{i,j=1}^m y^{(i)} y^{(j)} \alpha_i \alpha_j K_{i,j} \\ \text{s.t.} & \sum_{i=1}^m \alpha_i y^{(i)} = 0 \\ & \alpha_i \geq 0 \quad \forall i \end{array}$$

- Solution

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

- Prediction

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

- Kenerlized SVM needs to compute kernel when testing, whereas computed ω^* and \$b^*
\$ are enough in the unkenerlized 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

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

- 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

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

- KKT conditions (the optimal values of ω, b, ξ, α, and r should satisfy the following conditions)
  - $\nabla_\omega \mathcal{L}(\omega, b, \xi, \alpha, r) = 0 \Rightarrow \omega^* = \sum_{i=1}^m \alpha_i^* y^{(i)} x^{(i)}$
  - $\nabla_b \mathcal{L}(\omega, b, \xi, \alpha, r) = 0 \Rightarrow \sum_{i=1}^m \alpha_i^* y^{(i)} = 0$
  - $\nabla_{\xi_i} \mathcal{L}(\omega, b, \xi, \alpha, r) = 0 \Rightarrow \alpha_i^* + r_i^* = C$, for $\forall i$
  - $\alpha_i^*, r_i^*, \xi_i^* \geq 0$, for $\forall i$
  - $y^{(i)}\left(\omega^{*T} x^{(i)} + b^*\right) + \xi_i^* - 1 \geq 0$, for $\forall i$
  - $\alpha_i^*\left(y^{(i)}\left(\omega^* x^{(i)} + b^*\right) + \xi_i^* - 1\right) = 0$, for $\forall i$
  - $r_i^*\xi_i^* = 0$, for $\forall i$
- Dual problem

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

- Solution
  - $\omega^* = \sum_{i=1}^m \alpha_i^* y^{(i)} x^{(i)}$
  - $b^* = \frac{\sum_{i:0<\alpha_i^*<C}(y^{(i)} - {\omega^*}^T x^{(i)})}{\sum_{i=1}^m 1(0<\alpha_i^*<C)}$
- Proof.

$$\begin{array}{l} \because r_i^*\xi_i^* = 0 \Leftrightarrow (C - \alpha_i^*)\xi_i^* = 0 \\ \therefore \forall i, \alpha_i^* \neq C \Rightarrow \xi_i = 0 \Rightarrow \alpha_i(y^{(i)}({\omega^*}^T x^{(i)} + b^*) - 1) = 0 \\ \therefore \forall i, \alpha_i^* \in (0, C) \Rightarrow y^{(i)}({\omega^*}^T x^{(i)} + b^*) = 1 \Rightarrow {\omega^*}^T x^{(i)} + b^* = y^{(i)} \end{array}$$

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