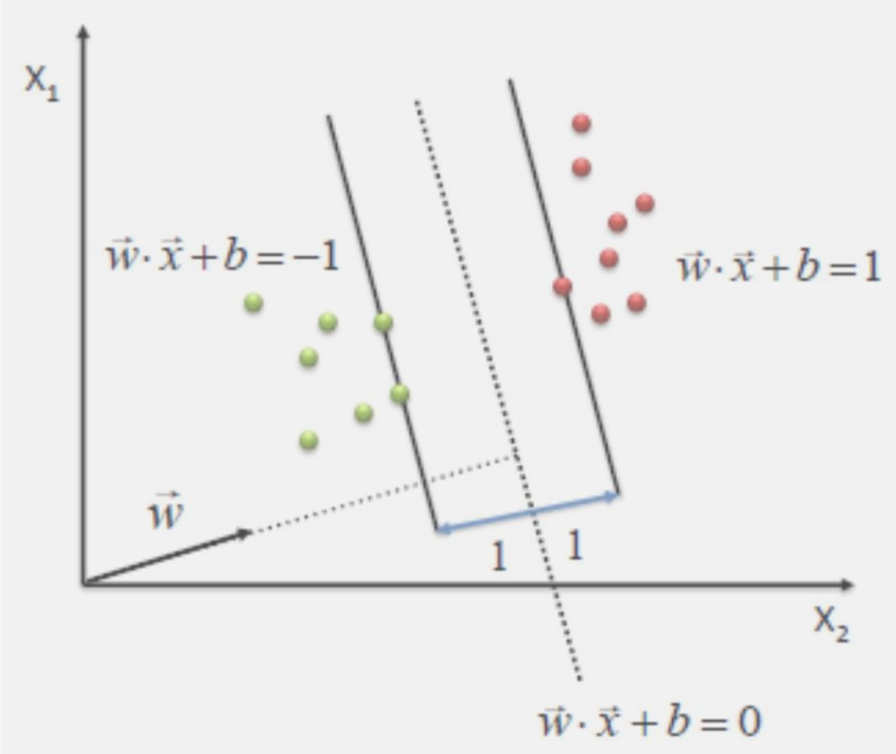
5.4 SVM 이론

Chapter 5. 서포트 벡터 머신

Contents

Margin



$w^T x^+ + b = 1$ (x^+: plusplane 상의 점)

$w^T(x^- + \lambda w) + b = 1$ ($x^+ = x^- + \lambda w$)

$w^T x^- + b + \lambda w^T w = 1$

$-1 + \lambda w^T w = 1$

$\therefore \lambda = \frac{2}{w^T w}$

Margin

$$L_2 \text{ norm} : \|W\|_2 = \left\{ \sum_{i=1}^{n} |w_i|^2 \right\}^{\frac{1}{2}}$$

$$= \sqrt{w_1^2 + w_2^2 \cdots + w_n^2} = \sqrt{W^T W}$$

$$\text{Margin} = \text{distance}(x^+, x^-)$$

$$= \|x^+ - x^-\| = \|(x^- + \lambda m) - x^-\|$$

$$= \|\lambda m\| = \lambda \sqrt{W^T \cdot W}$$

$$= \frac{2}{W^T W} \cdot \sqrt{W^T W} = \frac{2}{\sqrt{W^T W}} = \frac{2}{\|W\|_2}$$

Margin

Max margin = $\max \frac{2}{\|W\|_2} \Leftrightarrow \min \frac{1}{2}\|W\|_2$ (∵ 역수관계)

W는 제곱근을 포함하므로 계산편의를 위해 제곱

$$\min \frac{1}{2}\|W\|_2 \Leftrightarrow \min \frac{1}{2}\|w\|_2^2$$

$$= \text{minimize } \frac{1}{2}W^TW$$

minimize $\frac{1}{2}W^TW$ — 목적식 (2차식)

subject to $y_i(w^Tx_i+b) \geq 1$ — 제약식 (1차식)

→ QP문제.

목적식과 해

Original Prob → Lagrangian Primal (목적식과 제약식 모두 포함)

$$\max\min \mathcal{L}(w, b, \alpha) = \underbrace{\frac{1}{2}\|w\|_2^2}_{①} - \underbrace{\sum_{i=1}^{n} \alpha_i (y_i (w^T x_i + b) - 1)}_{②}$$

→ 미분을 통한 최솟값 도출

$$\Rightarrow \frac{\partial}{\partial w} : w - \sum_{i=1}^{n} \alpha_i y_i x_i = 0 \quad \rightarrow \quad w = \sum_{i=1}^{n} \alpha_i y_i x_i$$

$$\frac{\partial}{\partial b} : -\sum_{i=1}^{n} \alpha_i y_i = 0 \quad \rightarrow \quad \sum_{i=1}^{n} \alpha_i y_i = 0$$

known : x_i, y_i unknown : α_i

목적식과 해

1) $$\frac{1}{2}\|w\|_2^{\,2} = \frac{1}{2} w^T w$$

$$= \frac{1}{2} w^T \cdot \sum_{j=1}^{n} \alpha_j y_j x_j$$

$$= \frac{1}{2} \sum_{j=1}^{n} \alpha_j y_j (w^T x_j)$$

$$= \frac{1}{2} \sum_{j=1}^{n} \alpha_j y_j \left(\sum_{i=1}^{n} \alpha_i y_i x_i^T x_j \right)$$

$$= \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j x_i^T x_j$$

2) $$-\sum_{i=1}^{n} \alpha_i \left(y_i (w^T x_i + b) - 1 \right)$$

$$= -\sum_{i=1}^{n} \alpha_i y_i (w^T x_i + b) + \sum_{i=1}^{n} \alpha_i$$

$$= -\sum_{i=1}^{n} \alpha_i y_i w^T x_i \underbrace{- b \sum_{i=1}^{n} \alpha_i y_i}_{=0} + \sum_{i=1}^{n} \alpha_i$$

$$= -\sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j x_i^T x_j + \sum_{i=1}^{n} \alpha_i$$

목적식과 해

식 1)와 2)를 합치면

$$\sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j x_i^T x_j \qquad \text{where } \sum_{i=1}^{n}\alpha_i y_i = 0$$

미분을 통해 최솟값의 식을 구하였으므로 이제 maxmin → max 의 문제가 됨

위 식 또한 2차함수 (목적함수)와 1차함수 (제약함수)의 문제이므로 QP

목적식과 해

KKT에 의거하여 $\alpha_i(y_i(w^T x_i + b) - 1) = 0$

1) $\alpha_i > 0$ and $y_i(w^T x_i + b) = 1$

(= Support Vector)

$\Rightarrow$ x_i가 plus or minus plane 에 있을때 $\alpha_i > 0$

Case ①

2) $\alpha_i = 0$ and $y_i(w^T x_i + b) \neq 1$

$\Rightarrow$ x_i가 plane 위에 없으면 $\alpha_i = 0$

Case ②

$\therefore$ x_i가 SV일때만 $\alpha > 0$

목적식과 해

n개의 모든 관측치 사용X

SV에 해당하는 관측치 사용

$$w = \sum_{i=1}^{n} \alpha_i x_i y_i = \sum_{i \in SV} \alpha_i x_i y_i$$

∴ SV만 이용해서 결정 경계를 구할수 있다.

이렇게 구한 W로 b를 구한다.

SV중 임의의 점 (x_i, y_i)에서

$$w^T + b = y_{sv} \Rightarrow b = y_{sv} - \sum \alpha_i y_i x_i^T x_{sv}$$

Soft SVM

minimize $\frac{1}{2}W^TW + C\sum_{i=1}^{n}\xi_i$

subject to $y_i(w^Tx_i+b) \geq 1-\xi_i$

- C는 Margin과 training error의 trade-off 결정
- Slack variable 때문에 비선형적 데이터에도 해 존재

Original Prob → Lagrangian Primal (목적식과 제약식 모두 포함)

$$\max\min L(w,b,\alpha,\xi,r) = \underbrace{\frac{1}{2}\|w\|_2^2}_{\textcircled{1}} - \underbrace{\sum_{i=1}^{n}\alpha_i(y_i(w^Tx_i+b)-1+\xi_i)}_{\textcircled{2}} - \sum_{i=1}^{n} r_i\xi_i$$

subject to $\alpha_i \cdot r_i \geq 0,\ i=1,2,\cdots n.$

→ 미분을 통한 최솟값 도출

Soft SVM

$$\Rightarrow \frac{\partial}{\partial w} : w - \sum_{i=1}^{n} \alpha_i y_i x_i = 0 \quad \rightarrow \quad w = \sum_{i=1}^{n} \alpha_i y_i x_i$$

$$\frac{\partial}{\partial b} : -\sum_{i=1}^{n} \alpha_i y_i = 0 \quad \rightarrow \quad \sum_{i=1}^{n} \alpha_i y_i = 0$$

$$\frac{\partial}{\partial \xi_i} : C - \alpha_i - r_i = 0 \quad \rightarrow \quad C = \alpha_i + r_i$$

known : x_i. y_i ξ_i unknown : α_i

$$\min \frac{1}{2}\|w\|_2^2 + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n}\alpha_i\left(y_i(w^T x_i + b) - 1 + \xi_i\right) - \sum_{i=1}^{n} r_i \xi_i$$

$$= \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j x_i^T x_j \quad \text{where } \sum_{i=1}^{n}\alpha_i y_i = 0 \text{ and } C - \alpha_i - r_i = 0$$

한편 $\alpha_i \geq 0,\ r_i \geq 0$ and $C - \alpha_i - r_i = 0$ $\Rightarrow 0 \leq \alpha_i \leq C$

Soft SVM

Lagrangian dual로 Hard / Soft Margin SVM 표현 시

Soft) $\max \frac{1}{2}\|w\|_2^2 - \sum_{i=1}^{n} \alpha_i \alpha_j y_i y_j x_i^T x_j$ subject to $\sum_{i=1}^{n} \alpha_i y_i = 0$, $0 \le \alpha_i \le C$

Hard) $\max \frac{1}{2}\|w\|_2^2 - \sum_{i=1}^{n} \alpha_i \alpha_j y_i y_j x_i^T x_j$ subject to $\sum_{i=1}^{n} \alpha_i y_i = 0$, $0 \le \alpha_i$

→ 둘의 차이 : α의 범위 뿐.

KKT에 의거하여 $\alpha_i(y_i(w^T x_i + b) - 1 + \xi) = 0$, $\alpha_i = C - r_i$, $r_i \xi_i = 0$

1) $\alpha_i = 0 \Rightarrow r_i = C$

$\Rightarrow \xi_i = 0 \; (\because r_i \neq 0)$

$\Rightarrow \{y_i(w^T x_i + b) - 1\} \neq 0$ $\Rightarrow$ x가 plane 위에 없음

2) $0 < \alpha_i < C \Rightarrow r_i > 0$

$\Rightarrow \xi_i = 0$

$\Rightarrow \{y_i(w^T x_i + b) - 1\} = 0$ $\Rightarrow$ x가 plane 위에 있음

3) $\alpha_i = C \Rightarrow r_i = 0$

$\Rightarrow \xi_i > 0$

$\Rightarrow \alpha_i(y_i(w^T x_i + b) - 1) = -\alpha_i \xi_i \neq 0$ $\Rightarrow$ x가 두 plane의 사이에 있음

비선형적 Decision Boundary

$x = (x_1, x_2 \cdots x_n) \Rightarrow \varphi(x) = z = (z_1, z_2, \cdots z_n)$

Inout Space R^p $(p < q)$ Feature Space R^q

선형으로 구분할 수 있는 q차원으로 transform 후 학습

그 후 boundary를 p차원으로 가져오면 비선형적 경계 생김

비선형적 Decision Boundary

$$\sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j x_i^T x_j \qquad \text{where } \sum_{i=1}^{n}\alpha_i y_i = 0$$

고차원 변형식

$$\Big\downarrow \; x_i \rightarrow \varphi(x_i)$$

$$\sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \varphi(x_i^T)\varphi(x_j) \qquad \text{where } \sum_{i=1}^{n}\alpha_i y_i = 0$$

$\Big\downarrow$ K라는 φ의 형태를 몰라도 구현가능한 커널 함수를 적용해도 동일한 효과를 얻을 수 있음

$$\sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j K(x_i^T x_j) \qquad \text{where } \sum_{i=1}^{n}\alpha_i y_i = 0$$