

Support Vector Machine

Lab Seminar - Senseable AI Lab

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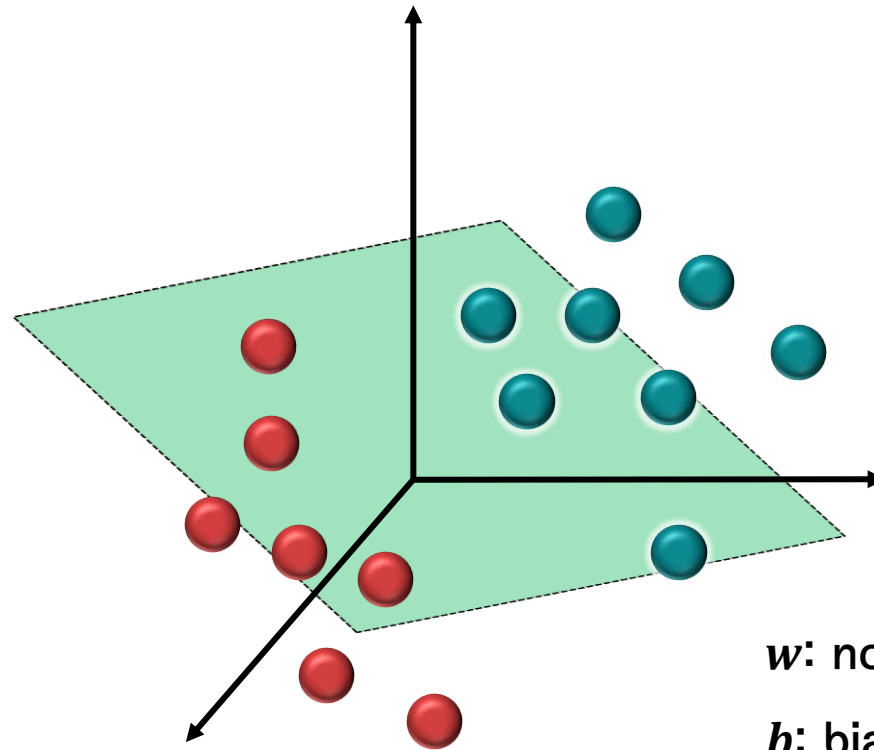
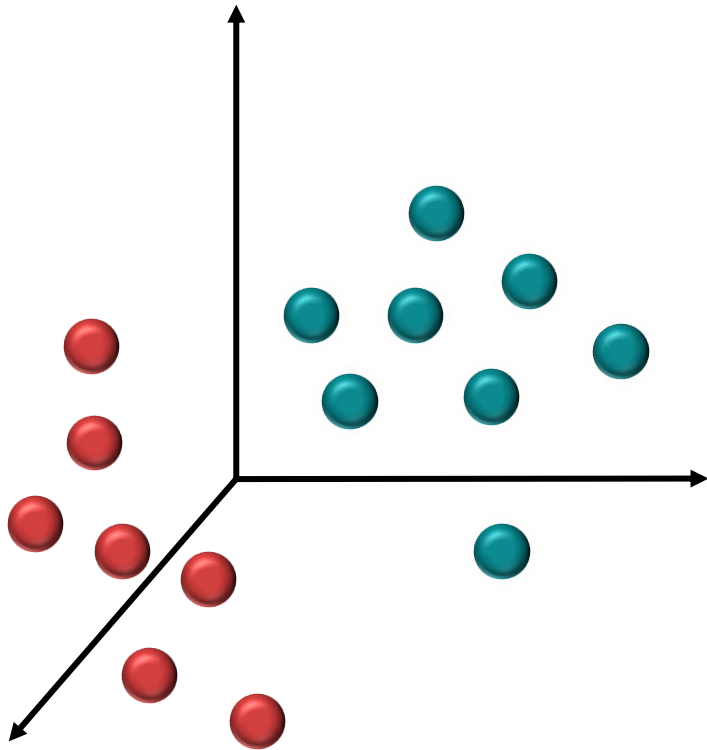
SVM

SVM has been shown to be able to achieve good generalization performance for **classification** of high-dimensional data sets and its training can be framed as solving a **quadratic programming problem**

- usually we try to maximize classification performance for the training data
- but, if the classifier is too fit for the training data, the classification ability for unknown data (i.e., the generalization ability) is degraded
- there is a trade-off between the generalization ability and fitting to the training data
- **SVM is trained so that the direct decision function maximizes the generalization ability**
- **SVM is based on statistical learning theory**

Separating Hyperplane

Classification problem

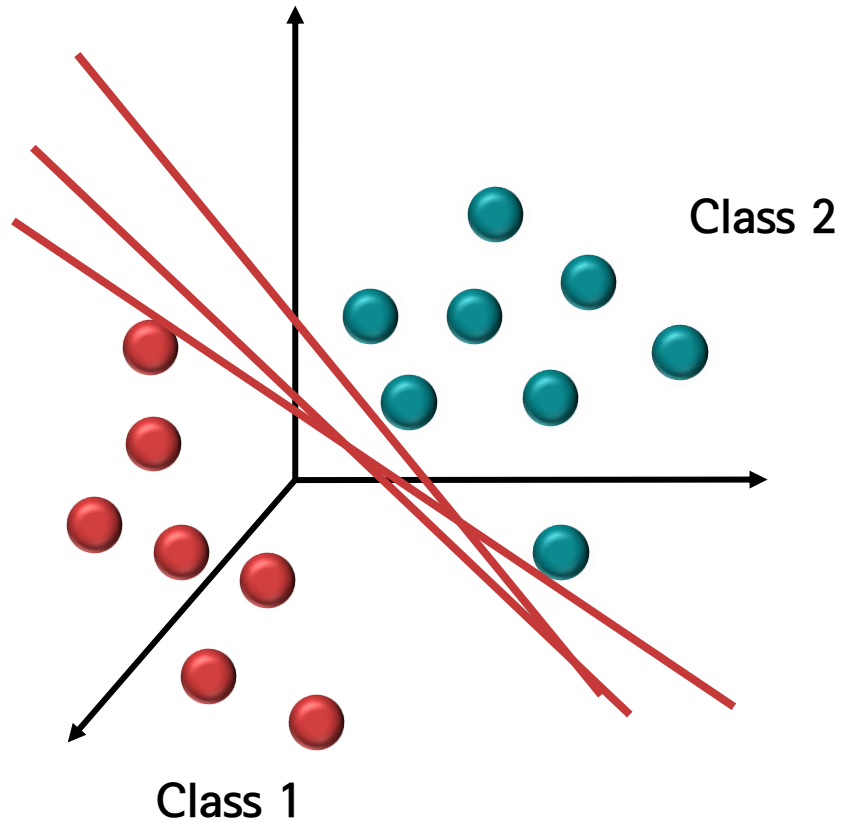


$$w^T x + b = 0$$

w : normal vector of the hyperplane

b : bias

Separating Hyperplane



- Two class classification problem
- 두 class를 나누는 hyperplane은 무한히 많음
- 어떤 hyperplane이 가장 “좋은“ hyperplane인가?
- “좋다”의 기준은?

Separating Hyperplane

Maximizing **margin** over the training set

= minimizing generalization error

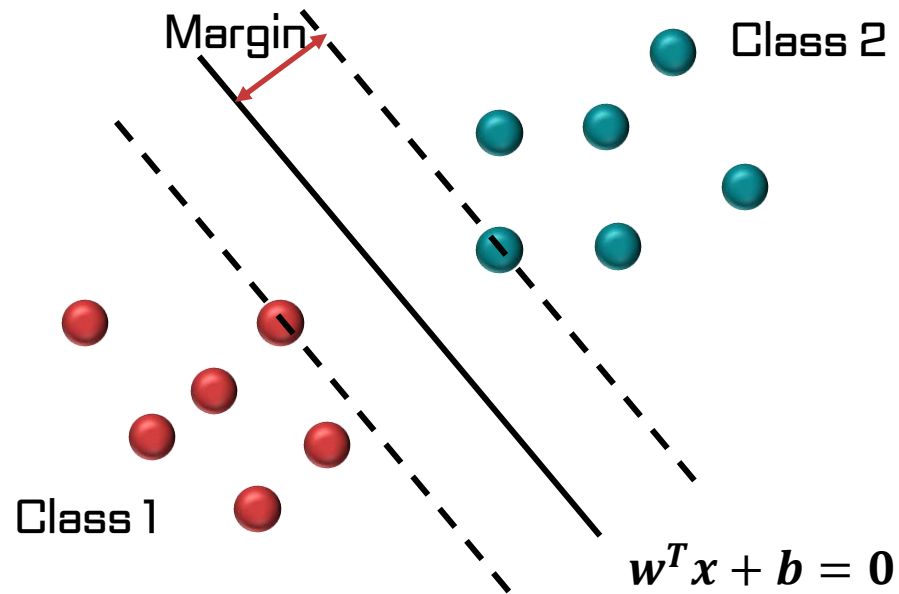
= good prediction performance

So, what is the margin?

Concept of Margin

Margin: 각 클래스에서 가장 가까운 관측치 사이의 거리

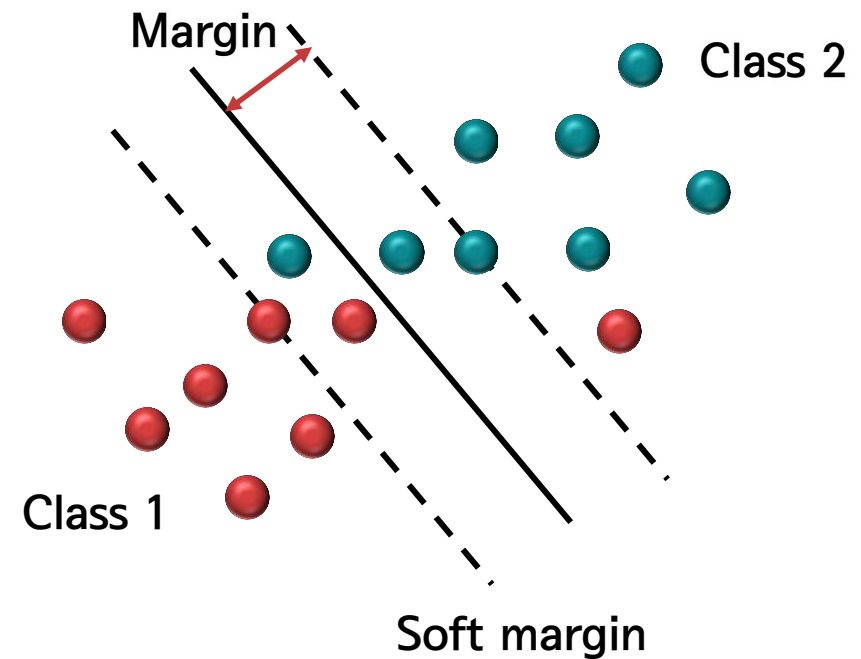
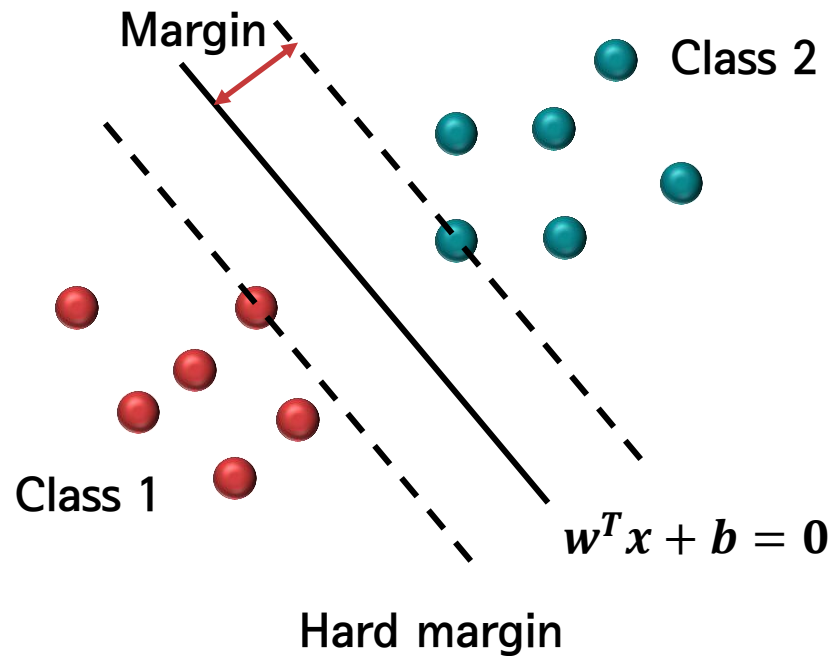
- Margin은 w (기울기)로 표현가능



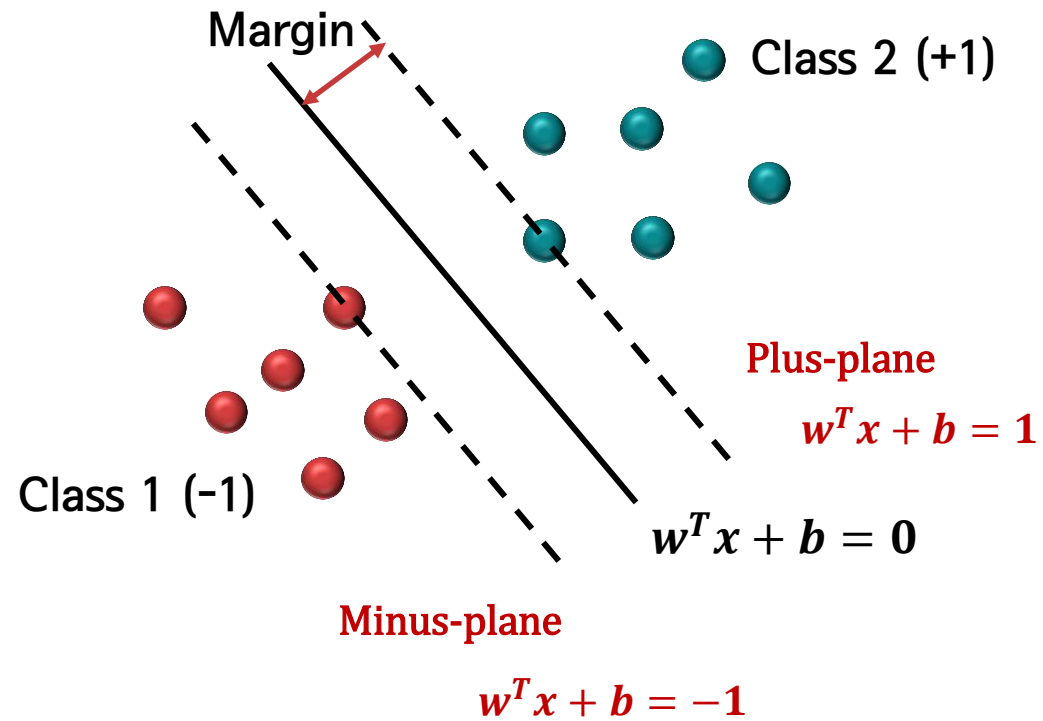
Concept of Margin

Goal of SVM model

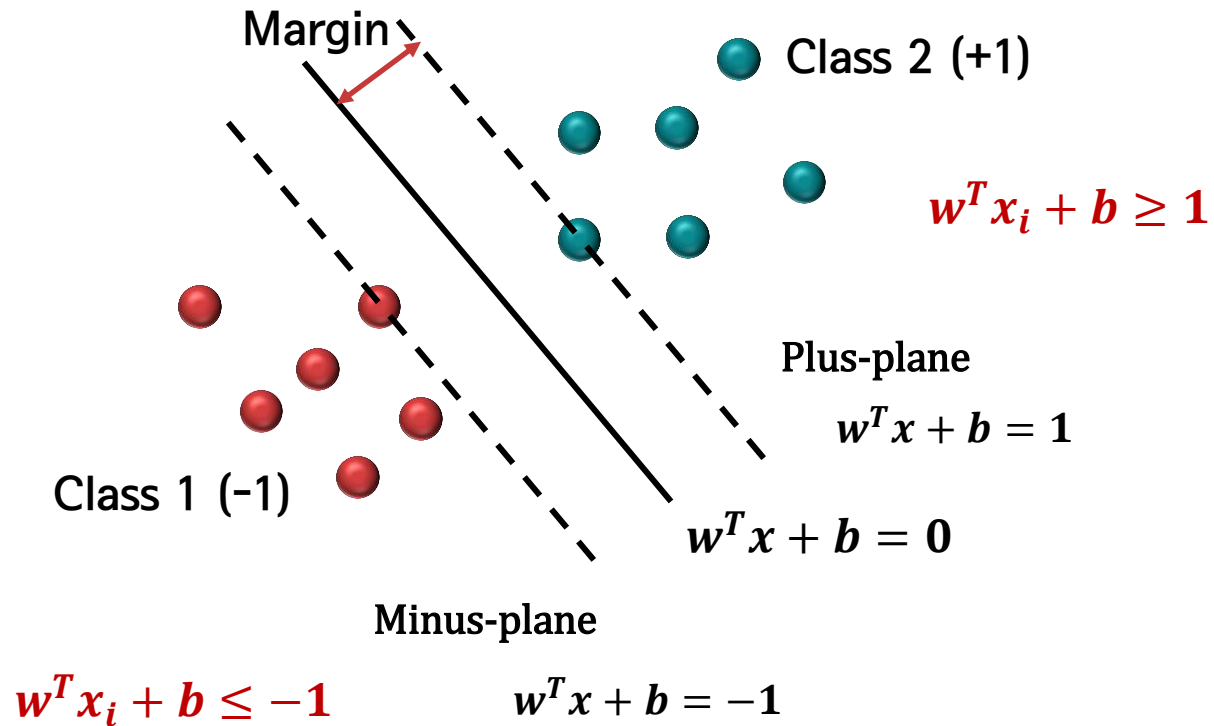
- 주어진 데이터를 통해 결정경계(decision boundary, maximum margin)를 찾는 것



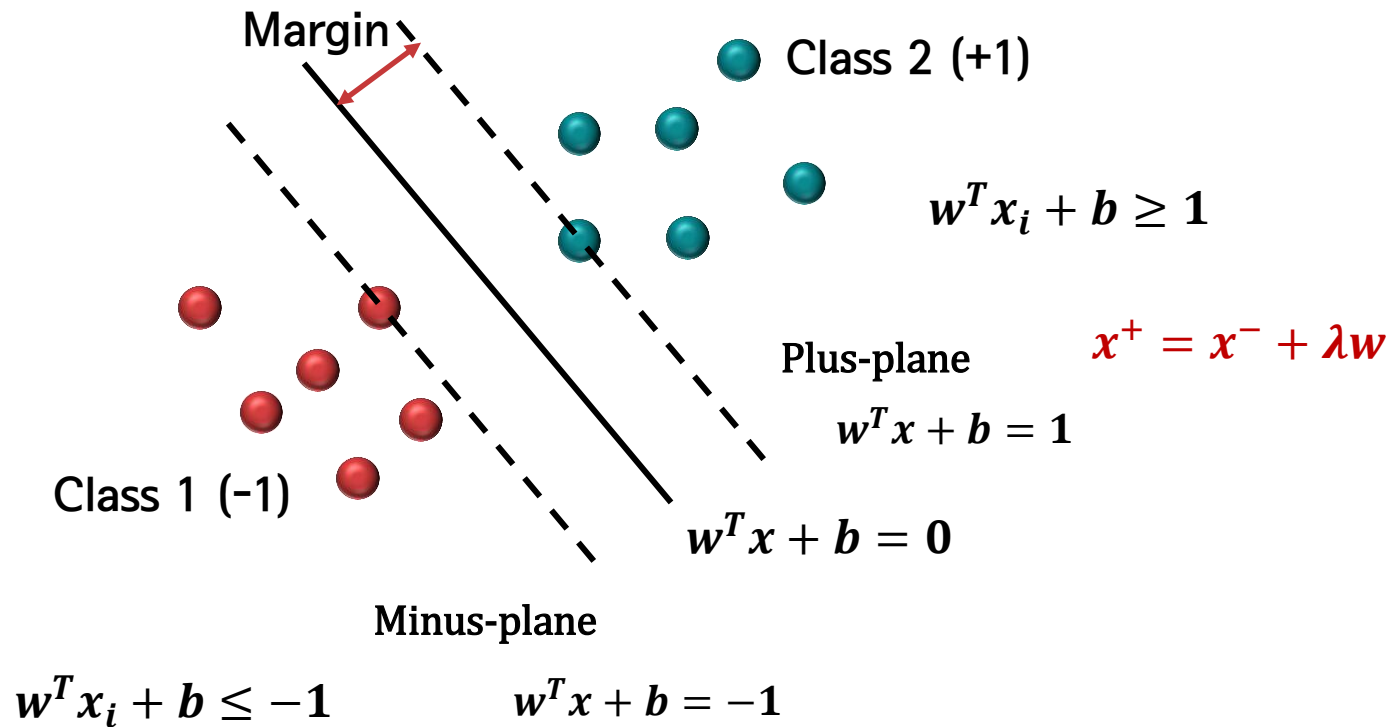
Geometric Margin



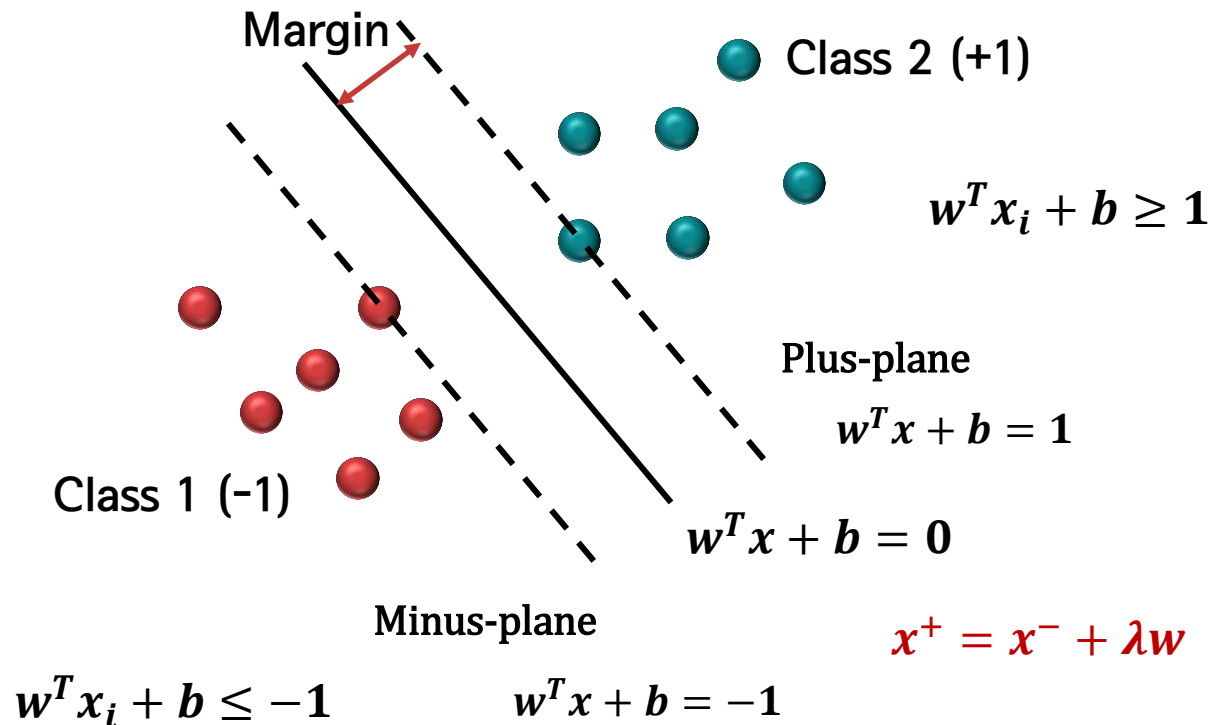
Geometric Margin



Geometric Margin



Geometric Margin



$w^T x^+ + b = 1 \rightarrow x^+$ 가 plus-plane 위의 점

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

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

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

x^- 는 minus-plane 위의 점

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

Vector norm $\|W\|_p$ ($p = 1, 2, 3, \dots$)

* Vector norm

$$\|W\|_p = \left(\sum_i |w_i|^p \right)^{1/p}$$

L_2 norm

$$\|W\|_2 = \left(\sum_i |w_i|^2 \right)^{1/2} = \sqrt{w_1^2 + w_2^2 + \dots + w_n^2} = \sqrt{W^T W}$$

$$W^T = (w_1, w_2, \dots, w_n)$$

Geometric Margin

$$\begin{aligned}\text{Margin} &= \textit{distance}(x^+, x^-) \\ &= \|x^+ - x^-\|_2 \\ &= \|(x^- + \lambda w) - x^-\|_2 \\ &= \|\lambda w\|_2 \\ &= \lambda \sqrt{w^T w} \\ &= \frac{2}{w^T w} \sqrt{w^T w} \\ &= \frac{2}{w^T w} \\ &= \frac{2}{\|w\|_2}\end{aligned}$$

Geometric Margin

$$\max \text{Margin} = \max \frac{2}{\|w\|_2} \Leftrightarrow \min \frac{1}{2} \|w\|_2$$

$$\|w\|_2 = \sqrt{w_1^2 + w_2^2 + \dots + w_n^2}$$

- w 의 L_2 norm이 제곱근을 포함하고 있기 때문에 계산이 어려움
- → 계산상의 편의를 위해 목적함수 변형

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

Hard Margin

Convex optimization problem

- Objective function (목적식) $\text{minimize } \frac{1}{2} \|w\|_2^2$
 - objective function은 separating hyperplane으로부터 정의된 margin의 역수
- Constraint (제약식) $\text{subject to } y_i(w^T x_i + b) \geq 1, i = 1, 2, \dots, n$
 - decision variable: w, b
 - constraint는 training data를 완벽하게 separating하는 조건
- Objective function is quadratic and constraint is linear
 - quadratic programming → convex optimization
 - globally optimal solution exists (전역최적해가 존재)
 - training data가 linearly separable한 경우에만 해가 존재함

Lagrangian Formulation

Original problem

$$\text{minimize } \frac{1}{2} \|w\|_2^2$$

$$\text{subject to } y_i(w^T x_i + b) \geq 1, i = 1, 2, \dots, n$$

Lagrangian multiplier를 이용하여 문제 변환

$$\max_{\alpha} \min_{w, b} \mathcal{L}(w, b, \alpha) = \max_{\alpha} \min_{w, b} \frac{1}{2} \|w\|_2^2 - \sum_{i=1}^n \alpha_i (y_i(w^T x_i + b) - 1)$$
$$\text{subject to } \alpha_i \geq 0, i = 1, 2, \dots, n$$

Lagrangian Formulation

Original problem

$$\text{minimize } \frac{1}{2} \|w\|_2^2$$

$$\text{subject to } y_i(w^T x_i + b) \geq 1, i = 1, 2, \dots, n$$

Lagrangian multiplier를 이용하여 문제 변환

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

$\text{subject to } \alpha_i \geq 0, i = 1, 2, \dots, n$

Lagrangian Primal problem

Lagrangian Formulation

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

subject to $\alpha_i \geq 0, i = 1, 2, \dots, n$

Solving Lagrangian Primal problem

- convex, continuous 이기 때문에 미분값=0인 지점에서 최솟값

$$\frac{\partial \mathcal{L}(w, b, \alpha)}{\partial w} = 0 \quad \Rightarrow \quad w = \sum_{i=1}^n \alpha_i y_i x_i$$

$$\frac{\partial \mathcal{L}(w, b, \alpha)}{\partial b} = 0 \quad \Rightarrow \quad \sum_{i=1}^n \alpha_i y_i = 0$$

Lagrangian Formulation

Solving Lagrangian Primal problem

Recall: $\frac{\partial \mathcal{L}(w, b, \alpha)}{\partial w} = \mathbf{0} \Rightarrow w = \sum_{i=1}^n \alpha_i y_i x_i$

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

$$\frac{1}{2} \|w\|_2^2 = \frac{1}{2} w^T w = \frac{1}{2} w^T \sum_{j=1}^n \alpha_j y_j x_j$$

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

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

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

Lagrangian Formulation

Solving Lagrangian Primal problem

Recall

$$\frac{\partial \mathcal{L}(w, b, \alpha)}{\partial b} = 0 \Rightarrow \sum_{i=1}^n \alpha_i y_i = 0$$

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

- $$\begin{aligned} - \sum_{i=1}^n \alpha_i (y_i (w^T x_i + b) - 1) &= - \sum_{i=1}^n \alpha_i y_i (w^T x_i + b) + \sum_{i=1}^n \alpha_i \\ &= - \sum_{i=1}^n \alpha_i y_i w^T x_i - b \sum_{i=1}^n \alpha_i y_i + \sum_{i=1}^n \alpha_i \\ &= - \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j + \sum_{i=1}^n \alpha_i \end{aligned}$$

Lagrangian Formulation

Solving Lagrangian Primal problem

$$\begin{aligned} \min_{w,b} \frac{1}{2} \|w\|_2^2 - \sum_{i=1}^n \alpha_i (y_i (w^T x_i + b) - 1) \\ = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j \quad \text{where } \sum_{i=1}^n \alpha_i y_i = 0 \end{aligned}$$

Lagrangian Formulation

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

subject to $\alpha_i \geq 0, i = 1, 2, \dots, n$

$$\min_{w,b} \frac{1}{2} \|w\|_2^2 - \sum_{i=1}^n \alpha_i (y_i (w^T x_i + b) - 1) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j \quad \text{where } \sum_{i=1}^n \alpha_i y_i = 0$$

Lagrangian Dual

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

subject to $\sum_{i=1}^n \alpha_i y_i = 0, \alpha_i \geq 0, i = 1, 2, \dots, n$

Lagrangian Formulation

Solving Lagrangian Dual problem

$$\begin{aligned} \max_{\alpha} \quad & \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j \\ \text{subject to} \quad & \sum_{i=1}^n \alpha_i y_i = 0, \alpha_i \geq 0, i = 1, 2, \dots, n \end{aligned}$$

- decision variable: α
- original problem formulation (primal formulation)보다 풀기 쉬운 형태
- objective function is quadratic (α_i, α_j) and constraint is linear ($\sum_{i=1}^n \alpha_i y_i = 0$)
 - \rightarrow quadratic programming \rightarrow convex optimization \rightarrow globally optimal solution exists

KKT (Karush-Kuhn-Tucker) condition

w, b, α 가 Lagrangian dual problem의 최적해가 되기 위한 조건

- 1) stationarity $\frac{\partial \mathcal{L}(w, b, \alpha)}{\partial w} = \mathbf{0} \Rightarrow w = \sum_{i=1}^n \alpha_i y_i x_i$

$$\frac{\partial \mathcal{L}(w, b, \alpha)}{\partial b} = \mathbf{0} \Rightarrow \sum_{i=1}^n \alpha_i y_i = 0$$

- 2) primal feasibility $y_i(w^T x_i + b) \geq 1, i = 1, 2, \dots, n$

- 3) dual feasibility $\alpha_i \geq 0, i = 1, 2, \dots, n$

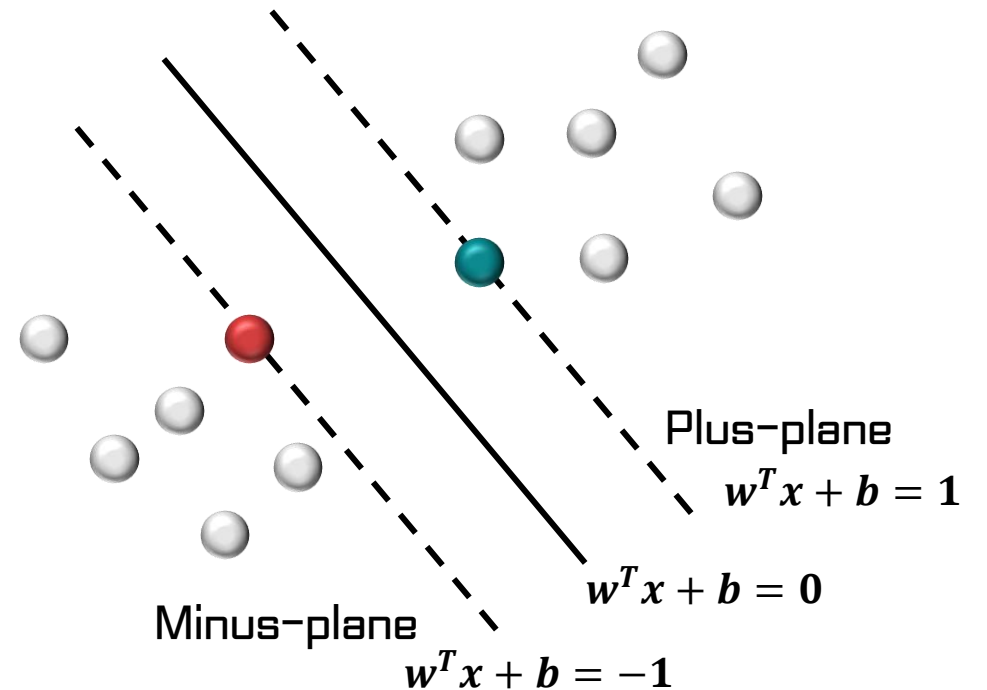
- 4) complementary slackness $\alpha_i(y_i(w^T x_i + b) - 1) = 0, i = 1, 2, \dots, n$

Characteristics of the Solutions

$$\alpha_i(y_i(w^T x_i + b) - 1) = 0, i = 1, 2, \dots, n$$

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

- x_i 가 plus-plane 또는 minus-plane (margin) 위에 있음
- margin 위에 있는 x_i 를 support vector라고 함

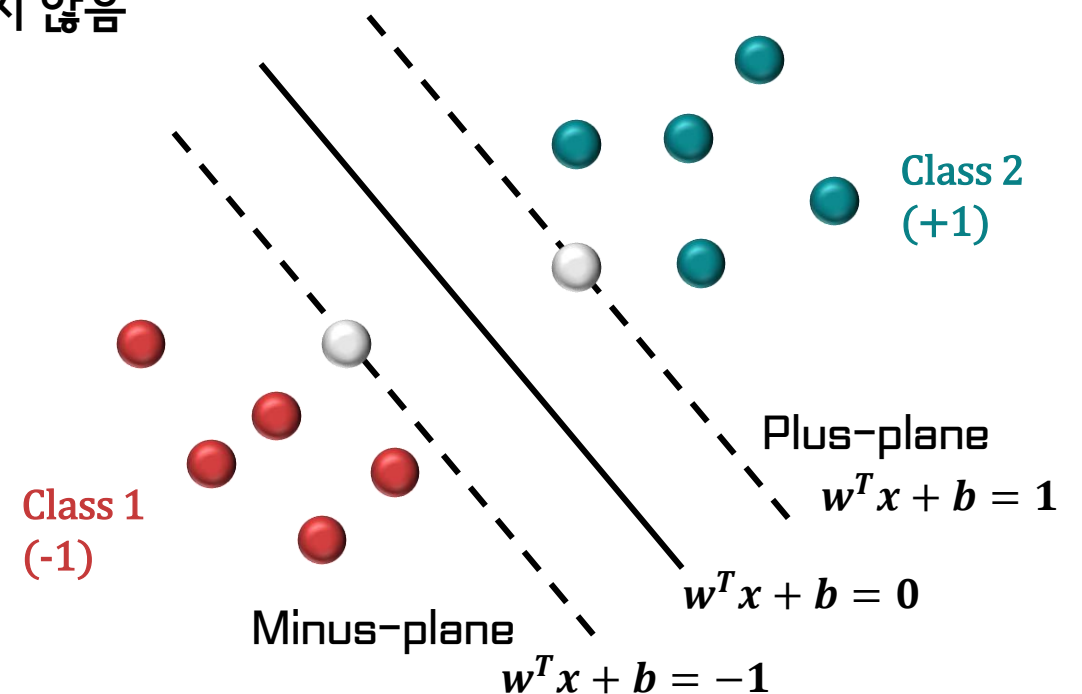


Characteristics of the Solutions

$$\alpha_i(y_i(w^T x_i + b) - 1) = 0, i = 1, 2, \dots, n$$

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

- x_i 가 plus-plane 또는 minus-plane (margin) 위에 있지 않음
- Hyperplane을 구축하는데 영향을 미치지 않음



Characteristics of the Solutions

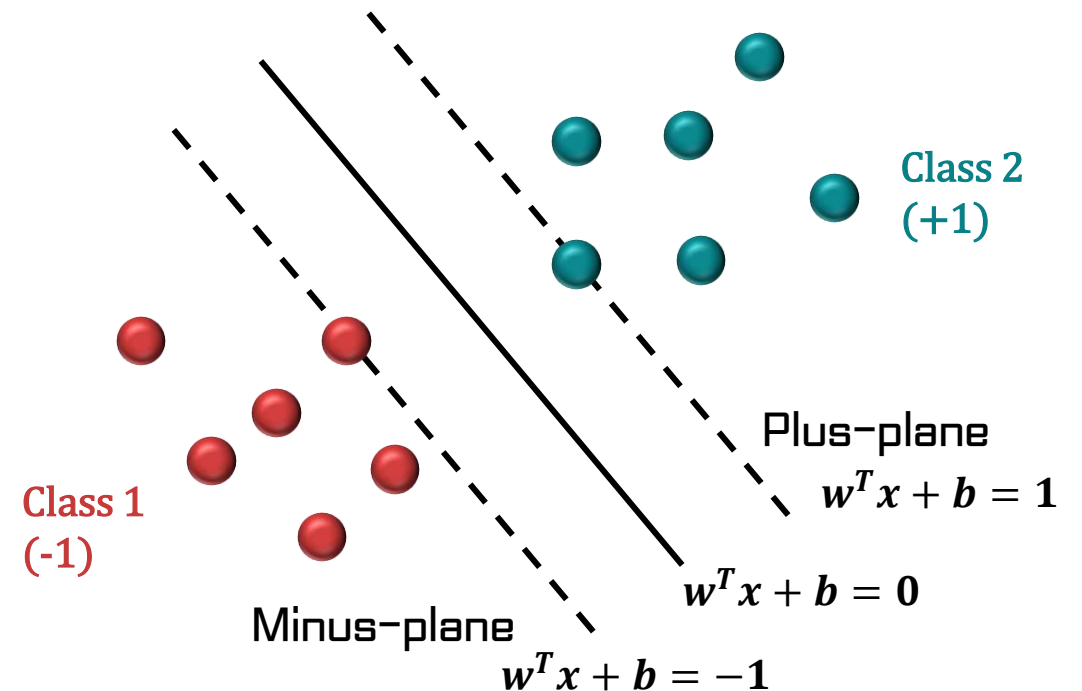
즉, x_i 가 support vector인 경우에만 $\alpha_i^* > 0$ 이므로

- $w^* = \sum_{i=1}^n \alpha_i^* y_i x_i = \sum_{i \in SV} \alpha_i^* y_i x_i$
- x_i 만을 사용하여 decision boundary를 구할 수 있음
 - 임의의 support vector 하나를 이용하여 b^*

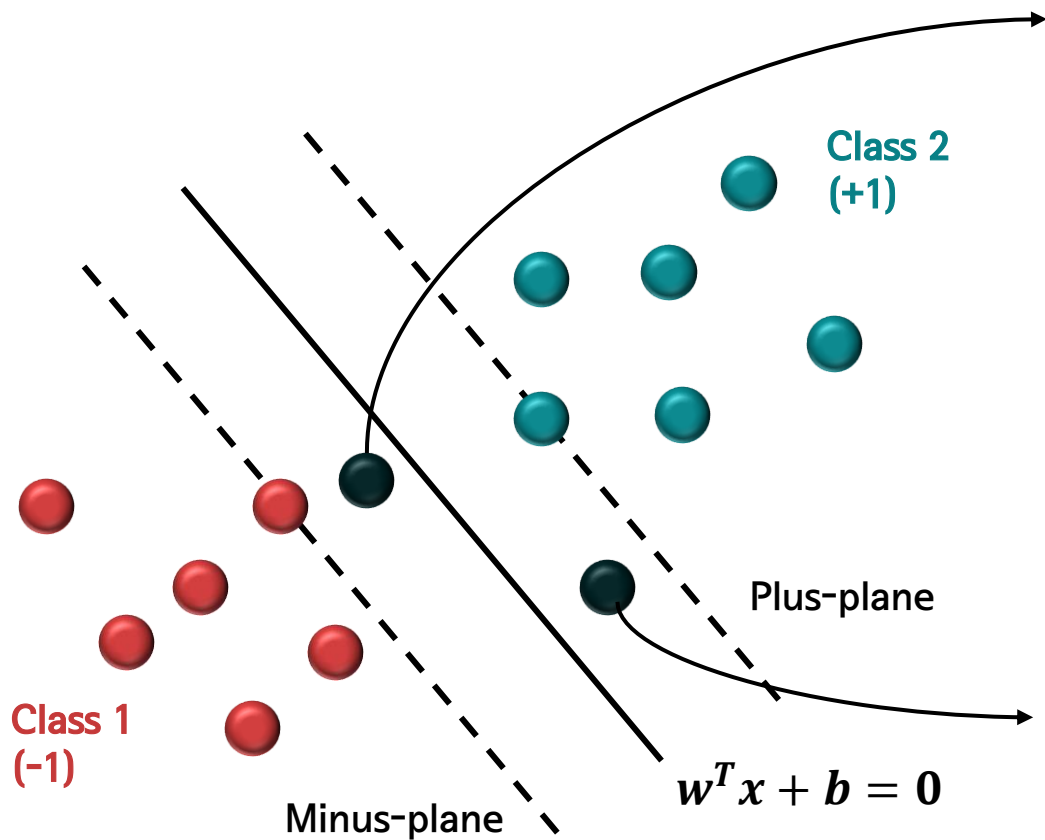
$$w^{*T} + b^* = y_{sv}$$

$$w^{*T} + b^* = \sum_{i=1}^n \alpha_i^* y_i x_i^T x_{sv} + b^* = y_{sv}$$

$$b^* = y_{sv} - \sum_{i=1}^n \alpha_i^* y_i x_i^T x_{sv}$$



Classifying New data Points



새로운 데이터가 optimal separating hyperplane보다 밑에 있음

$$w^{*T} x_{new} + b^* < 0 \Rightarrow \hat{y}_{new} = -1$$



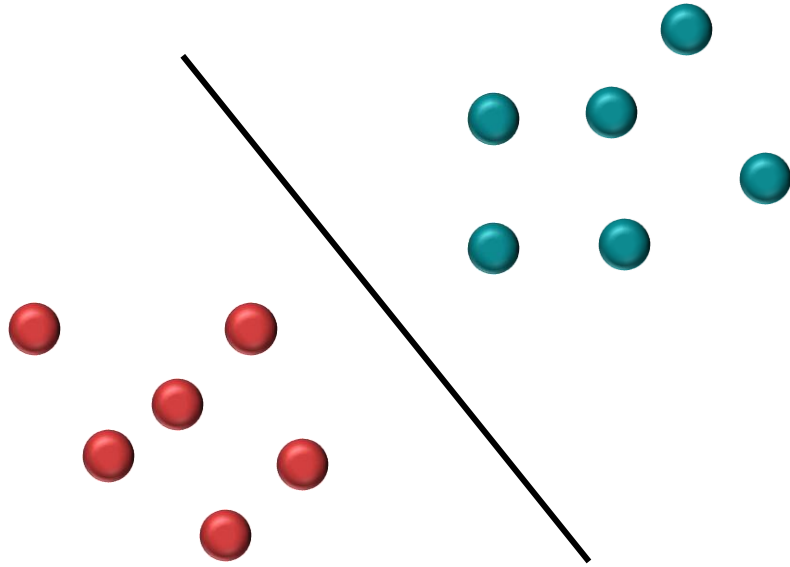
$$\hat{y}_{new} = \text{sign}(w^{*T} x_{new} + b^*) = \text{sign}\left(\sum_{i \in SV} a_i^* y_i x_i^T x_{new} + b^*\right)$$



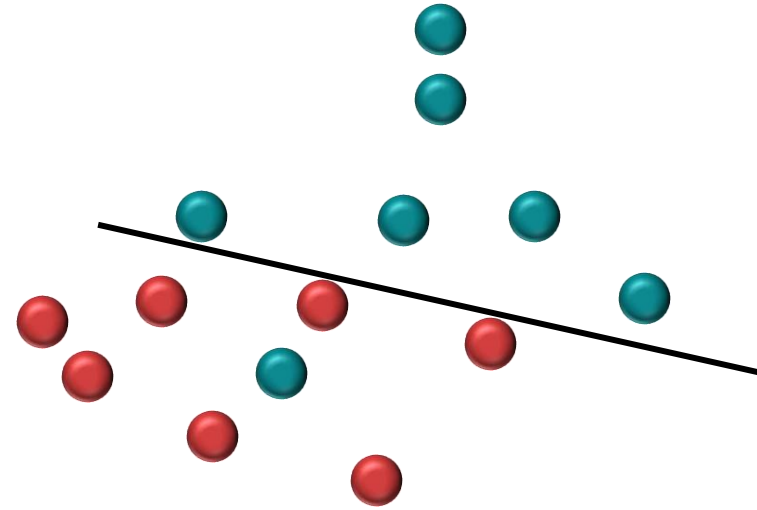
새로운 데이터가 optimal separating hyperplane보다 위에 있음

$$w^{*T} x_{new} + b^* > 0 \Rightarrow \hat{y}_{new} = +1$$

Linearly Non-separable Problems



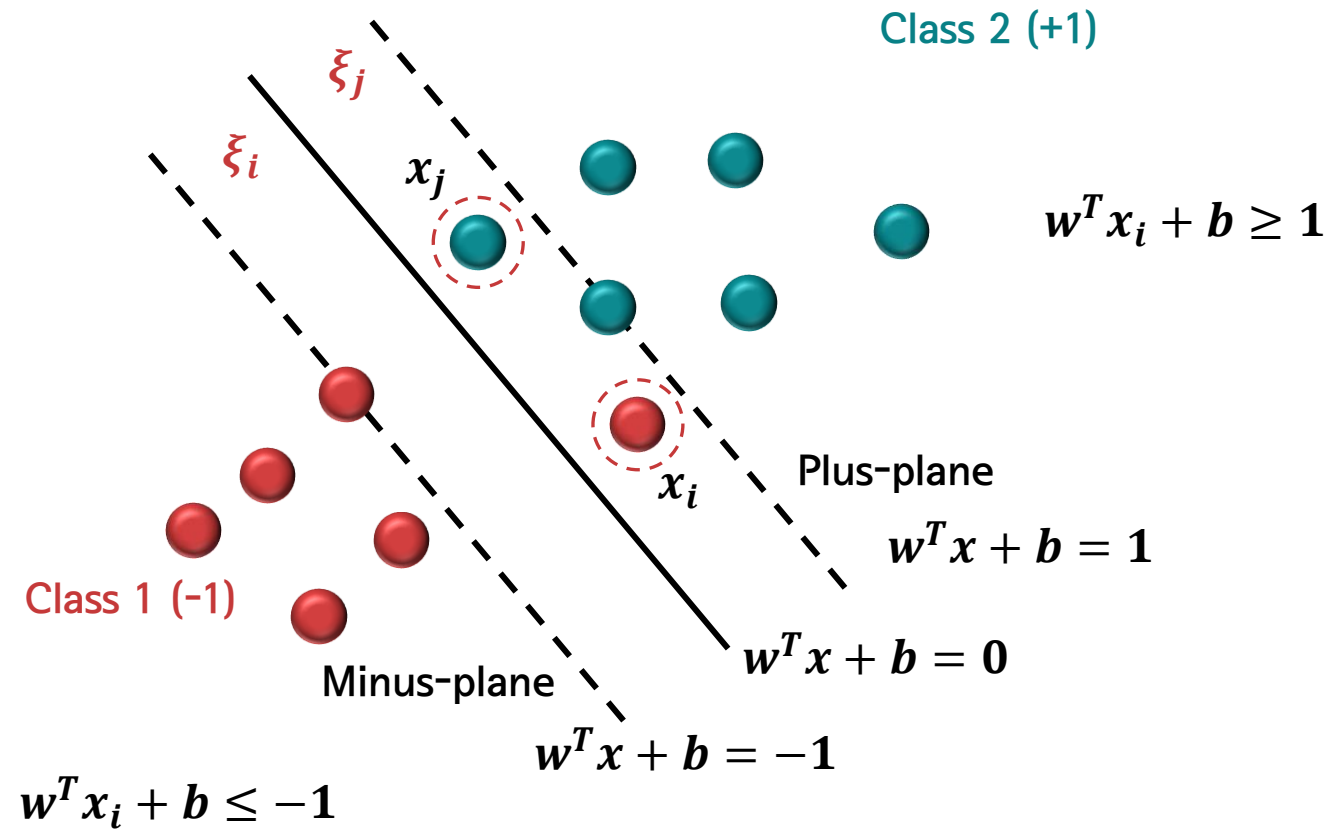
Linearly separable



Linearly non-separable

Linear decision boundary를 이용하여 완벽하게 나누는 것은 불가능 → Error 허용

Linearly Non-separable Problems



Soft Margin

Convex optimization problem

$$\text{minimize } \frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^n \xi_i$$

$$\text{subject to } y_i(w^T x_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0, \quad i = 1, 2, \dots, n$$

- decision variable: w, b, ξ
- slack variable $\xi_i \geq 0$
 - training error를 허용 (마냥 크게 할 수는 없음) $C \uparrow$: training error를 많이 허용하지 않음
 - objective function에 penalty를 추가하여 억제 $C \downarrow$: training error를 많이 허용
- C 는 margin과 training error에 대한 trade-off를 결정하는 hyperparameter
- training data가 linearly separable하지 않아도 해가 존재함

Lagrangian Formulation

Original Problem

$$\text{minimize } \frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^n \xi_i$$

$$\text{subject to } y_i(w^T x_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0, \quad i = 1, 2, \dots, n$$

$$\max_{\alpha, \gamma} \min_{w, b, \xi} \mathcal{L}(w, b, \alpha, \xi, \gamma)$$

$$= \max_{\alpha, \gamma} \min_{w, b, \xi} \frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^n \xi_i - \sum_{i=1}^n \alpha_i (y_i(w^T x_i + b) - 1) - \sum_{i=1}^n \gamma_i \xi_i$$

$$\text{subject to } \alpha_i \cdot \gamma_i \geq 0, \quad i = 1, 2, \dots, n$$

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

$$\text{subject to } \sum_{i=1}^n \alpha_i y_i = 0 \text{ and } 0 \leq \alpha_i \leq C, \quad i = 1, 2, \dots, n$$

Lagrangian
multiplier

Lagrangian
Primal and Dual

Lagrangian Formulation

Lagrangian dual-Soft margin

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

subject to $\sum_{i=1}^n \alpha_i y_i = 0$ and $0 \leq \alpha_i \leq C, i = 1, 2, \dots, n$

Lagrangian dual-Har margin

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

subject to $\sum_{i=1}^n \alpha_i y_i = 0$ and $\alpha_i \geq 0, i = 1, 2, \dots, n$

KKT condition

$$\frac{\partial \mathcal{L}(w, b, \alpha)}{\partial w} = 0 \quad w = \sum_{i=1}^n \alpha_i y_i x_i$$

$$\frac{\partial \mathcal{L}(w, b, \alpha)}{\partial b} = 0 \quad \sum_{i=1}^n \alpha_i y_i = 0$$

$$\frac{\partial \mathcal{L}(w, b, \xi, \alpha, \gamma)}{\partial \xi} = 0 \quad C - \alpha_i - \gamma_i = 0$$

Complementary slackness

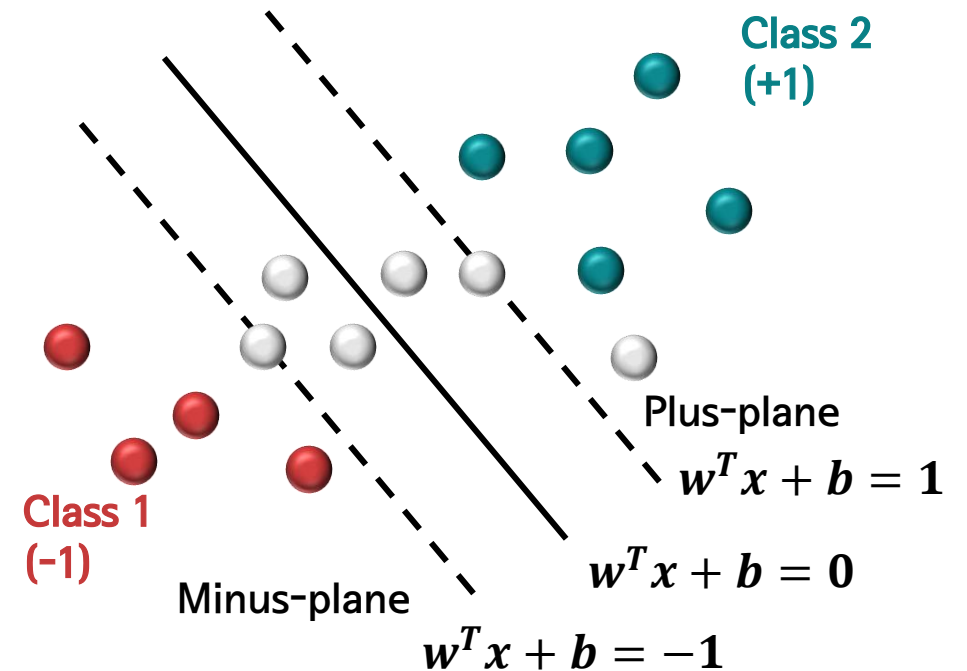
$$\alpha_i (y_i (w^T x_i + b) - 1 + \xi_i) = 0, \gamma_i \xi_i = 0, i = 1, 2, \dots, n$$

Characteristics of the Solutions

$$\alpha_i(y_i(w^T x_i + b) - 1 + \xi_i) = 0, \quad \alpha_i = C - \gamma_i, \quad \gamma_i \xi_i = 0, \quad i = 1, 2, \dots, n$$

$$\begin{aligned} 1) \quad \alpha_i = 0 &\Rightarrow C = \gamma_i \\ &\Rightarrow \xi_i = 0 \\ &\Rightarrow (y_i(w^T x_i + b) - 1) \neq 0 \end{aligned}$$

x_i 가 plus-plane 또는 minus-plane (margin) 위에 있지 않음



Characteristics of the Solutions

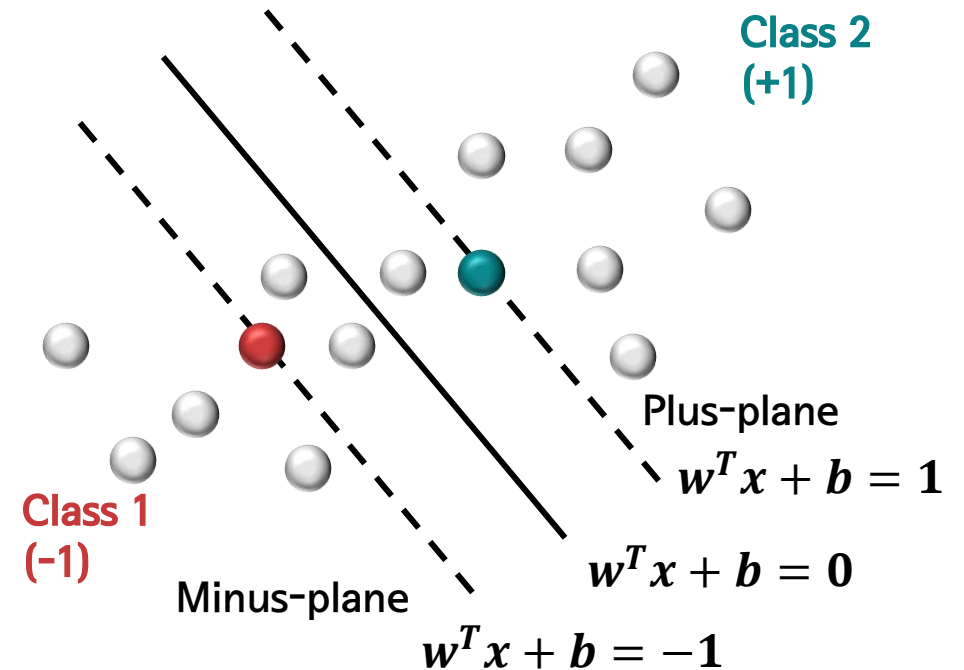
$$\alpha_i(y_i(w^T x_i + b) - 1 + \xi_i) = 0, \quad \alpha_i = C - \gamma_i, \quad \gamma_i \xi_i = 0, \quad i = 1, 2, \dots, n$$

$$2) \quad 0 < \alpha_i < C \Rightarrow \gamma_i > 0$$

$$\Rightarrow \xi_i = 0$$

$$\Rightarrow (y_i(w^T x_i + b) - 1) = 0$$

x_i 가 plus-plane 또는 minus-plane (margin) 위에 있음
(support vector)



Characteristics of the Solutions

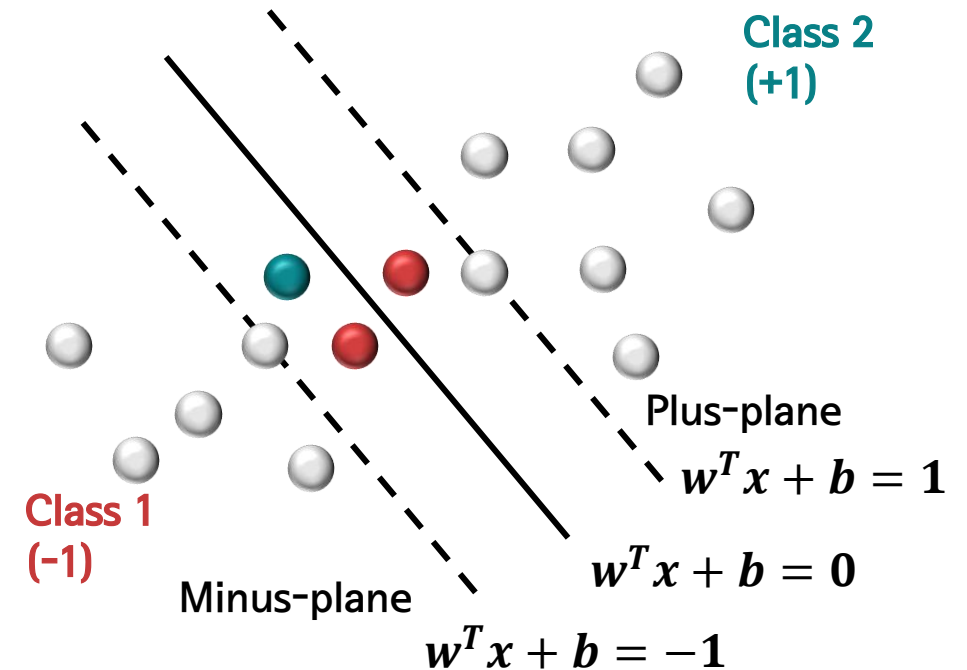
$$\alpha_i(y_i(w^T x_i + b) - 1 + \xi_i) = 0, \quad \alpha_i = C - \gamma_i, \quad \gamma_i \xi_i = 0, \quad i = 1, 2, \dots, n$$

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

$$\Rightarrow \xi_i > 0$$

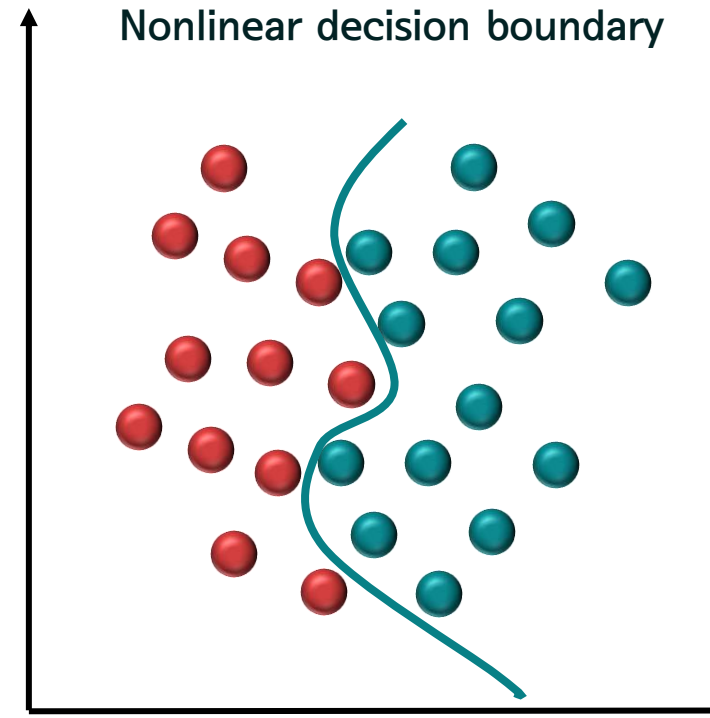
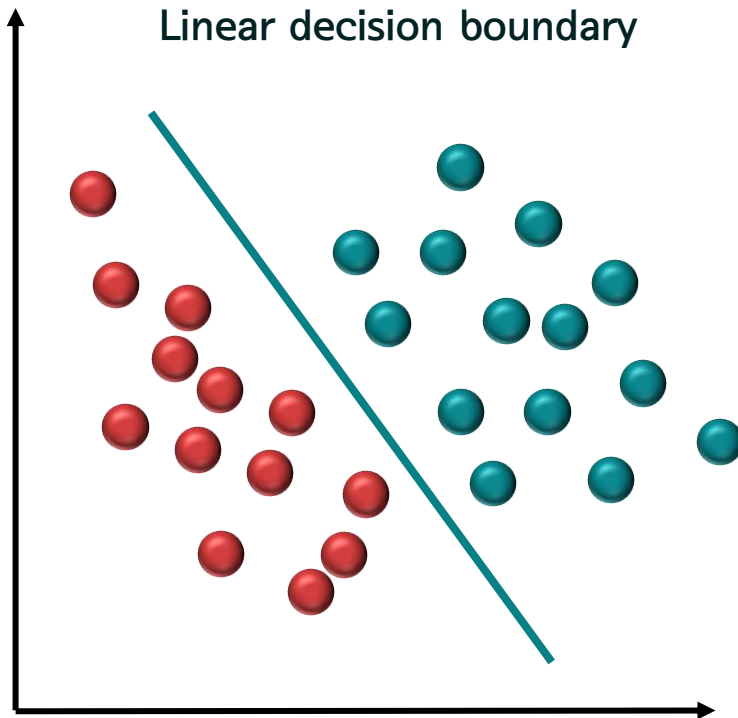
$$\Rightarrow (y_i(w^T x_i + b) - 1) = \alpha_i \xi_i \neq 0$$

x_i 가 plus-plane 또는 minus-plane (margin) 사이에 있음
(support vector)



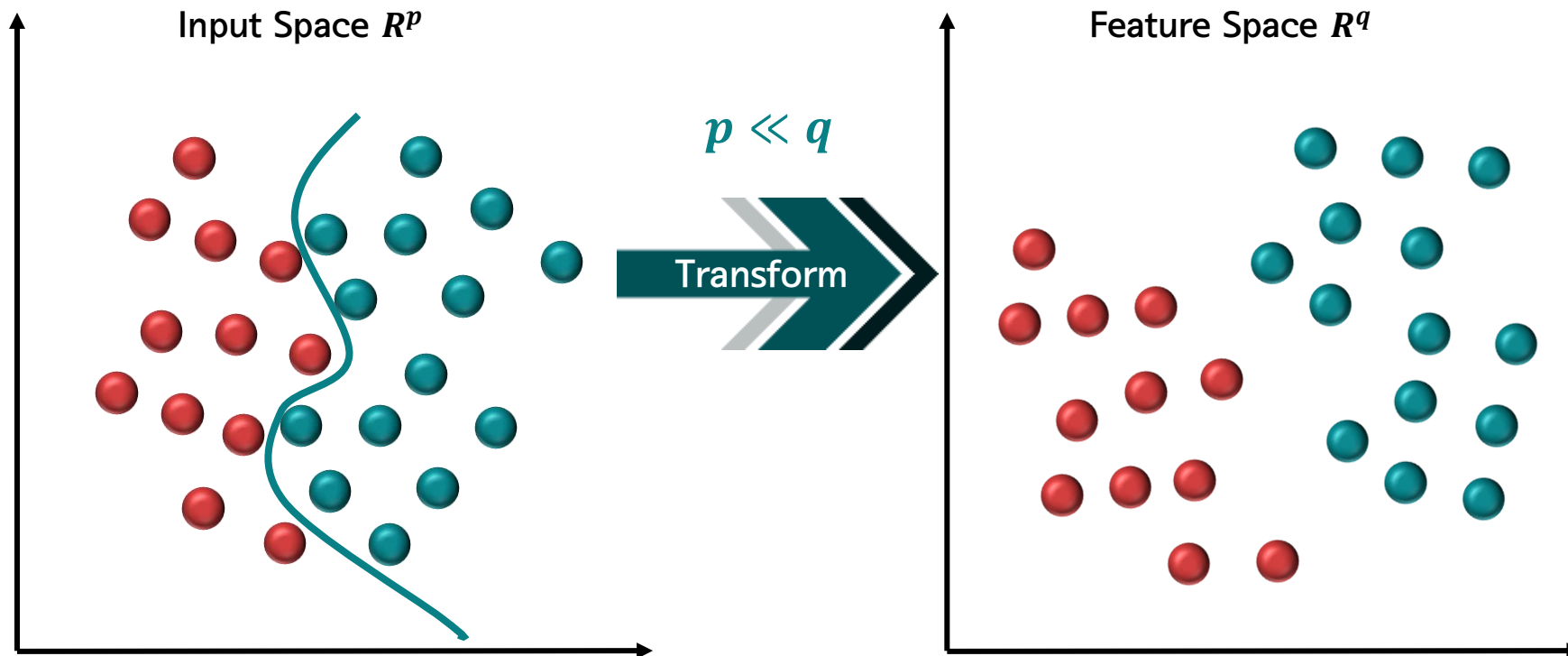
Nonlinear Decision Boundary

데이터에 비선형성이 있을 때는 어떻게 분류할까?

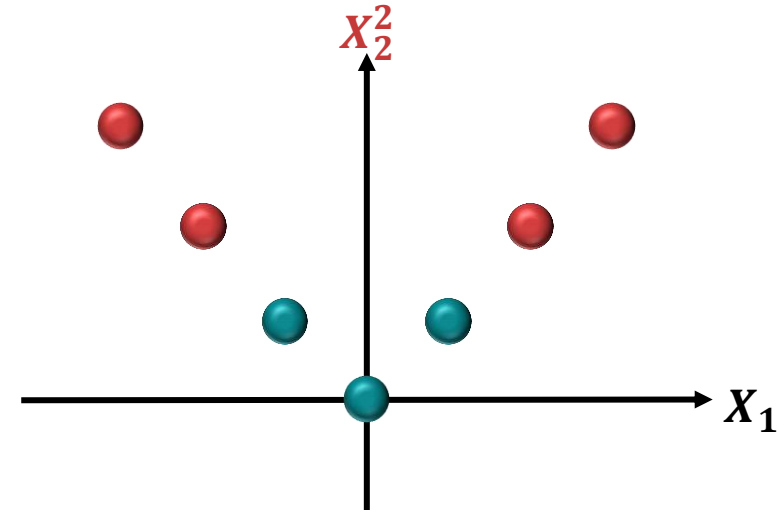
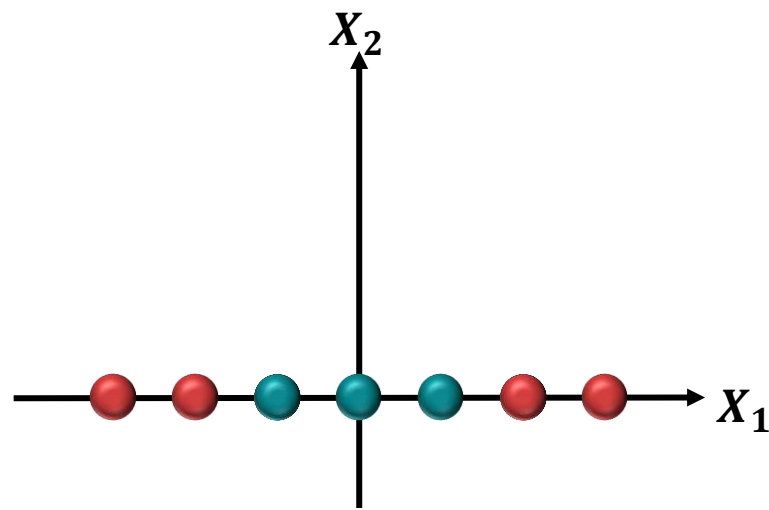


Transforming Data

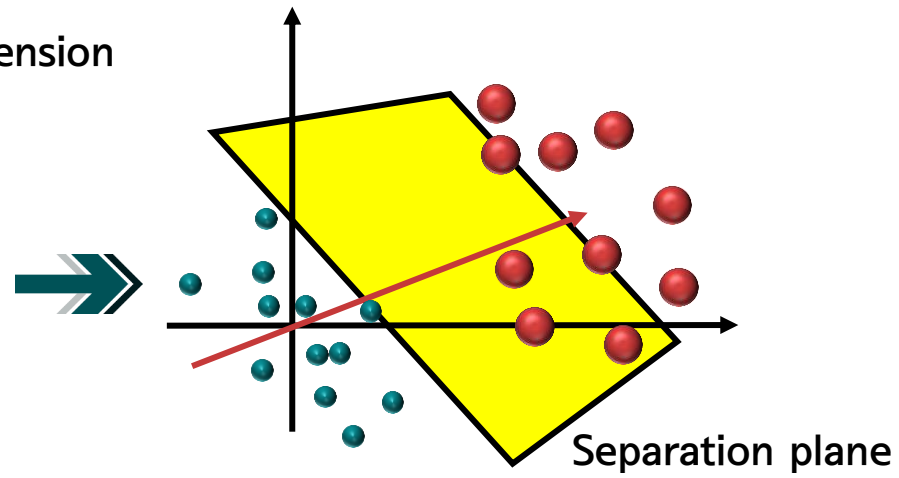
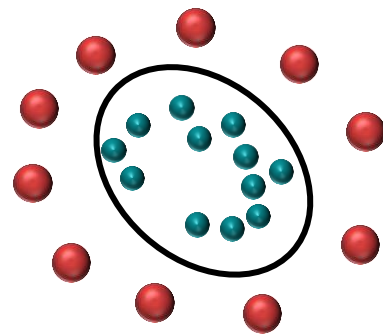
$$\mathbf{x} = (x_1, x_2, \dots, x_n) \rightarrow \phi(\mathbf{x}) = \mathbf{z} = (z_1, z_2, \dots, z_n)$$



Example of Transforming Data



Complex structure of low dimension



Simple structure of high dimension

Example of Transforming Data

$$\phi: x \mapsto z = \phi(x)$$

$$\phi: (x_1, x_2) \mapsto (x_1, x_2, x_1^2, x_2^2, x_1, x_2)$$

$$\begin{array}{cc} 2\text{D} & 6\text{D} \\ \text{(original space)} & \text{(feature space)} \end{array}$$

- original space를 feature space로 변환하여 학습에 활용
- original space에서 nonlinear decision boundary \rightarrow feature space에서 linear decision boundary
- 고차원 feature space에서 관측치 분류가 더 쉬울 수 있음
 - 고차원 feature space를 효율적으로 계산할 수 있는 방법 존재 (Kernel mapping, kernel trick)

Kernel Mapping

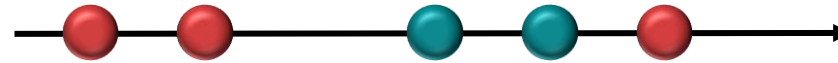
$$\hat{y}_{new} = \text{sign} \left(\sum_{i \in SV} a_i^* y_i \mathbf{x}_i^T \mathbf{x}_{new} + b^* \right)$$

$$\hat{y}_{new} = \text{sign} \left(\sum_{i \in SV} a_i^* y_i \phi(\mathbf{x}_i) \phi(\mathbf{x}_{new}) + b^* \right)$$

$$= \text{sign} \left(\sum_{i \in SV} a_i^* y_i K \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_{new}) \rangle + b^* \right)$$

Example of Nonlinear SVM using Kernel Function

x	y
1	+1
2	+1
4	-1
5	-1
6	+1



- 1-dimensional data 분류 문제
- $C=100$
- Linearly non-separable problem → kernel function 사용

$$K(x, y) = (xy + 1)^2$$

Example of Nonlinear SVM using Kernel Function

Solution

x	y
1	+1
2	+1
4	-1
5	-1
6	+1

$$\max_{\alpha} \sum_{i=1}^5 \alpha_i - \frac{1}{2} \sum_{i=1}^5 \alpha_i \alpha_j y_i y_j (x_i x_j + 1)^2$$

subject to $\sum_{i=1}^5 \alpha_i y_i = 0$ and $0 \leq \alpha_i \leq 100$

α_1	α_2	α_3	α_4	α_5
0	2.5	0	7.333	4.833

$$f(x) = \sum_{i \in SV} \alpha_i^* y_i K\langle \phi(x_i), \phi(x_{new}) \rangle + b$$

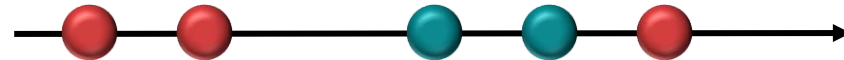
Example of Nonlinear SVM using Kernel Function

Solution

$$\begin{aligned} f(x) &= 2.5(+1)(2x + 1)^2 + 7.333(-1)(5x + 1)^2 + 4.833(+1)(6x + 1)^2 + b \\ &= 0.667x^2 - 5.333x + b \end{aligned}$$

$$\begin{aligned} x = 2 &\Rightarrow f(2) = 0.667 * 2^2 - 5.333 * 2 + b = 1 \\ b &= 8.993 \end{aligned}$$

$$f(x) = 0.667x^2 - 5.333x + 8.993$$



Choosing Kernel Functions

SVM 사용시 kernel을 결정하는 것은 어려운 문제 (기준은 없음)

사용하는 kernel에 따라 feature space의 특징이 달라지기 때문에 데이터의 특성에 맞는 kernel 결정해야 함

일반적으로 RBF kernel, sigmoid kernel, low degree polynomial kernel 등이 사용됨

- linear kernel $K\langle x_1, x_2 \rangle = \langle x_1, x_2 \rangle$
- polynomial kernel $K\langle x_1, x_2 \rangle = (a\langle x_1, x_2 \rangle + b)^d$
- sigmoid kernel $K\langle x_1, x_2 \rangle = \tanh(a\langle x_1, x_2 \rangle + b)$
- RBF kernel (Gaussian kernel, Radial basis function) $K\langle x_1, x_2 \rangle = \exp\left(\frac{-\|x_1 - x_2\|_2^2}{2\sigma^2}\right)$

End of slide
