Pattern Recognition

SVM 개념 잡기

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What is SVM?

Support Vector Machine → SVM

Traditional Classifier

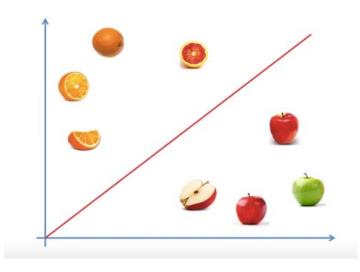
- Until now, favorite classifier to everyone
 - Wondering why? Kernel Trick!!!

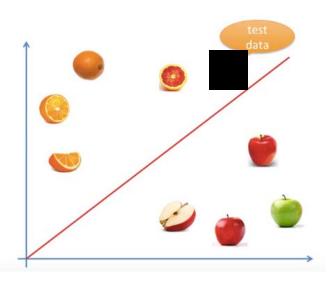
"만약, 문제에 어떠한 알고리즘을 사용할지 모르겠다면, SVM은 좋은 출발선이 될 수 있음"

Classifier

• Classifier is a <u>hypothesis</u> or <u>discrete-valued function</u> that is used to assign (categorical) class labels to particular data points.

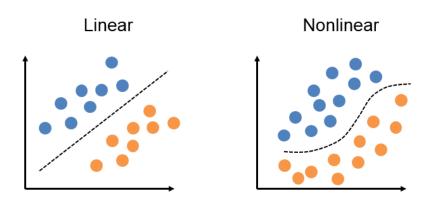
• In the email classification example, this classifier could be a hypothesis for labeling emails as **spam** or **non-spam**.





Classifier

- y = label, x = data, y = f(x), f: classifier
- If decision function is linear, this classifier (f) is linear classifier
- If not, this classifier (f) is non-linear classifier



y = f(x)

데이터를 구획해주는 이 **점선의 함수** (decision boundary)를 우리는 **판별 함** 수 (decision function)라 부른다.

Classifier

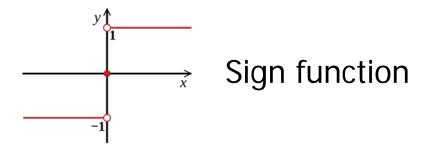
Hyperplane

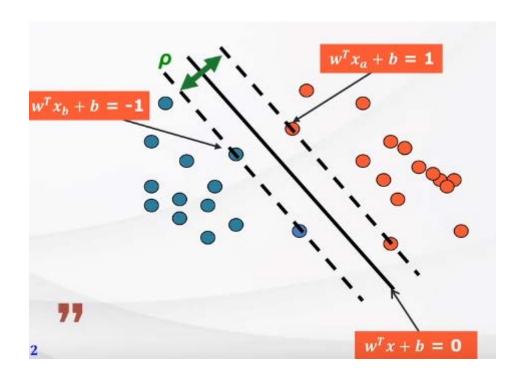
 In geometry, a hyperplane is a subspace whose dimension is one less than that of its ambient space. If a space is 3-dimensional then its hyperplanes are the 2dimensional planes, while if the space is 2-dimensional, its hyperplanes are the 1-dimensional lines.

$$\mathbf{w}^T\mathbf{x}=0$$
 $y=ax+b$ Hyperplane Line

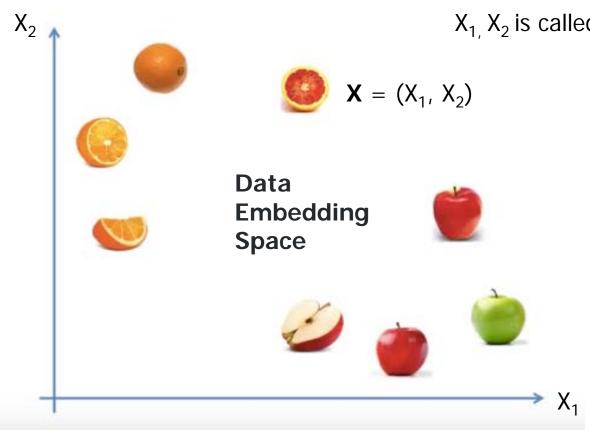
SVM Classifier

- W : vector for hyperplane
- x_i: i_{th} data, y_i: label (class) of i_{th} data
- $Y = sign(W^TX + b) = f(X)$
 - $Y_i = +1$ when $W^T X_i + b > 1$
 - $Y_i = -1$ when $W^T X_i + b < -1$





Data Embedding Space



 X_1 , X_2 is called feature or attribute.

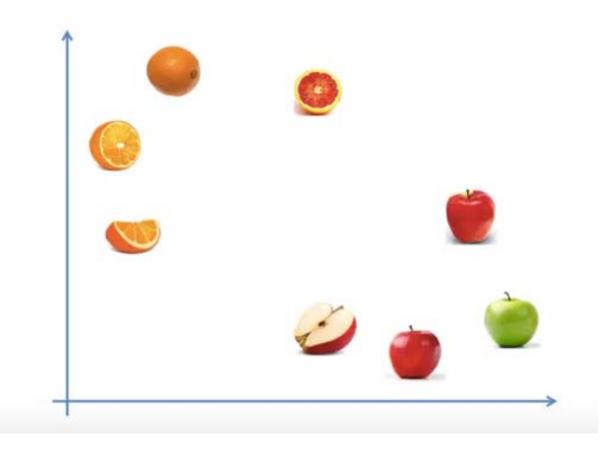
Data Embedding

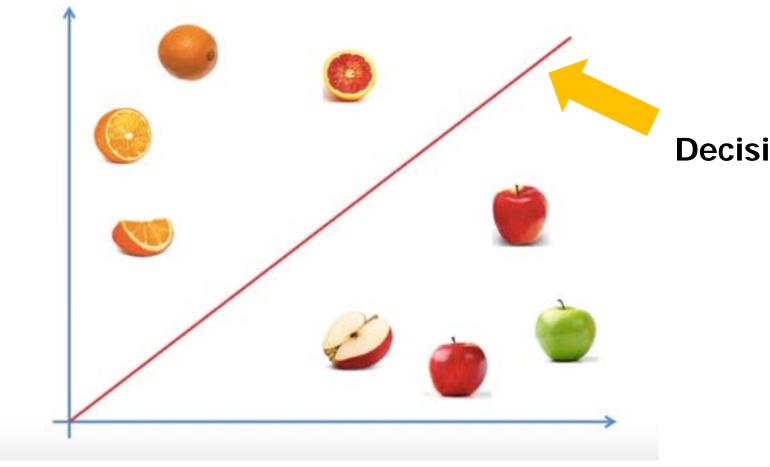
범주형 자료를 **벡터 형태**로 바꾸는 것

Categorical Data

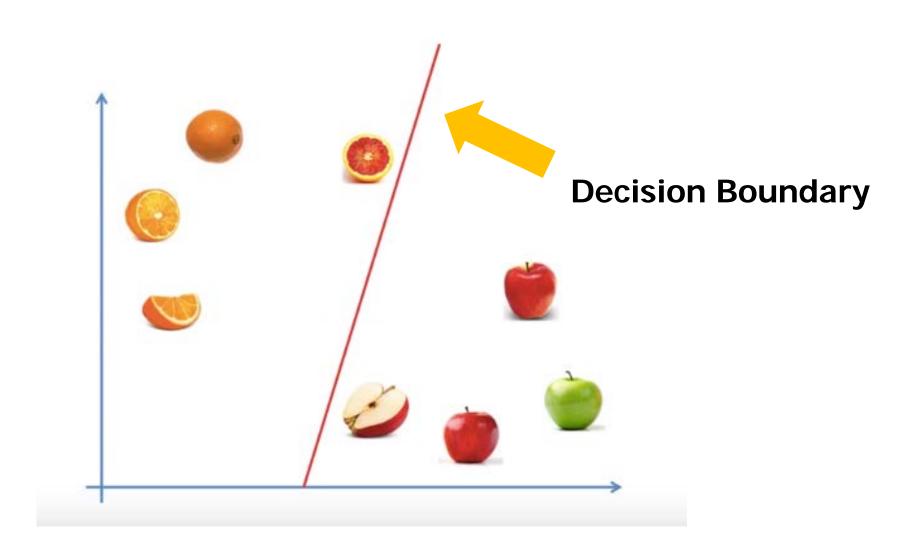
범주형 데이터란 몇 개의 범주로 나누어진데이터 예) 남/여, A/B/O/AB

Which hyperplane can we choose?





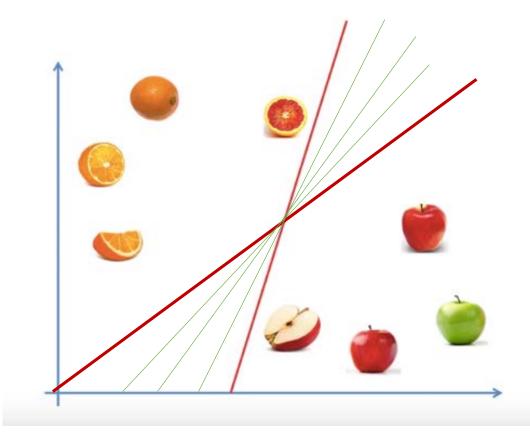
Decision Boundary



- Which one is better?
 - Classifier should have dealt with unseen data

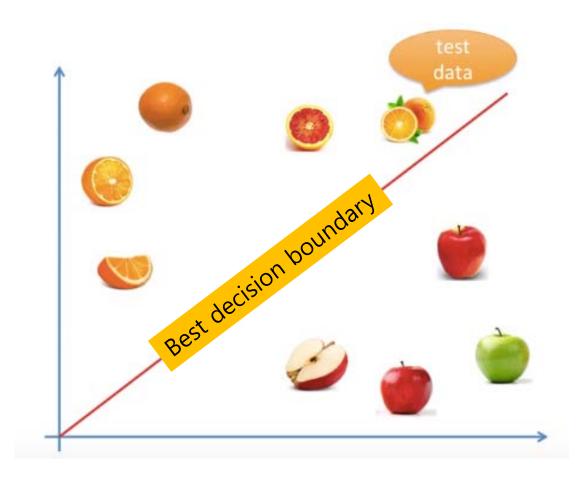
Train sample data → seen data

Test sample data → unseen data



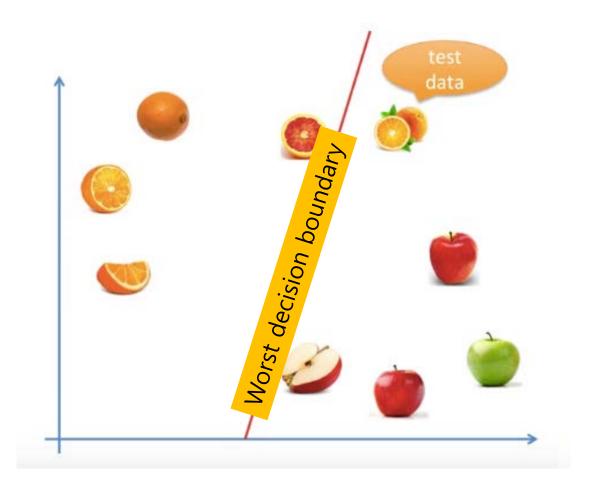
How can we decide decision boundary?

Test data predicted well (O)



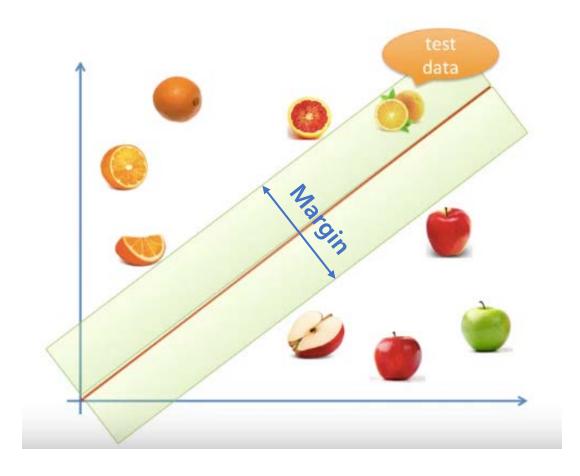
How can we decide decision boundary?

Test data predicted well (X)



How can we decide decision boundary?

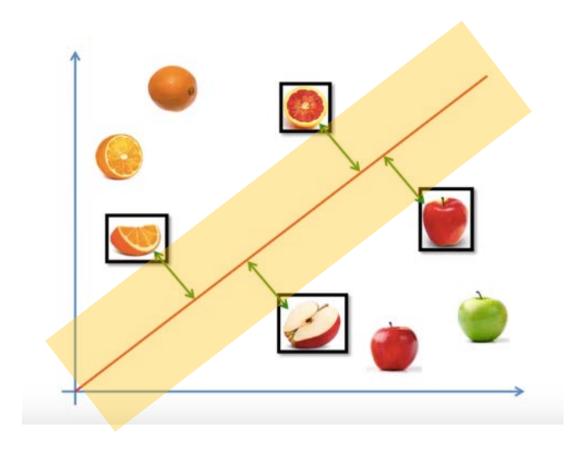
The answer is "Large Margin"!!



Support Vector

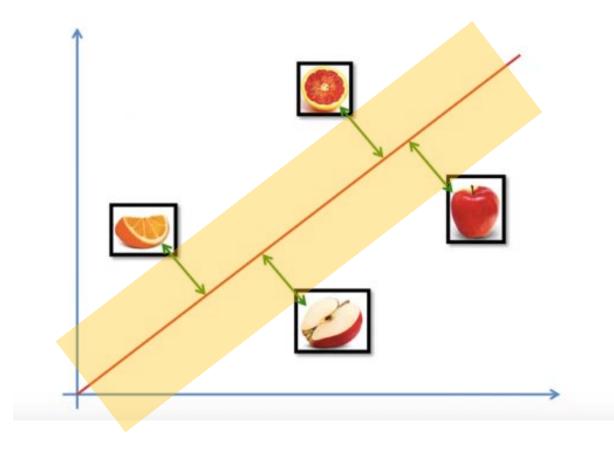
Support Vector

Samples on the margin are called the support vectors.

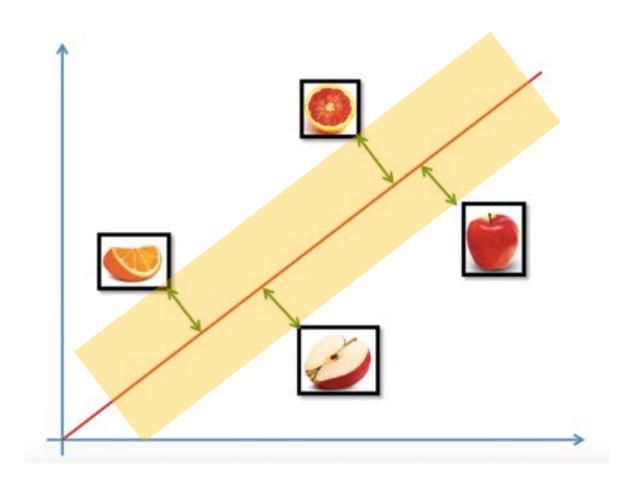


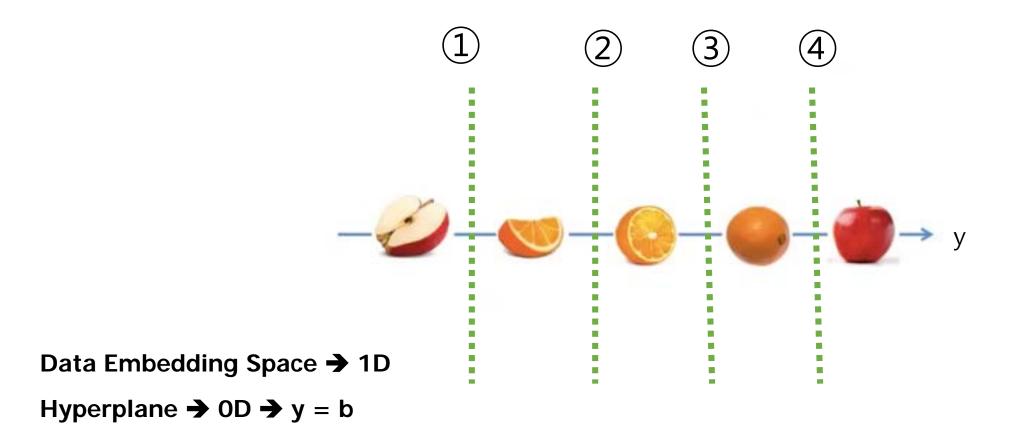
Support Vector

- SVM only uses support vector for prediction
 - Less computation!!!

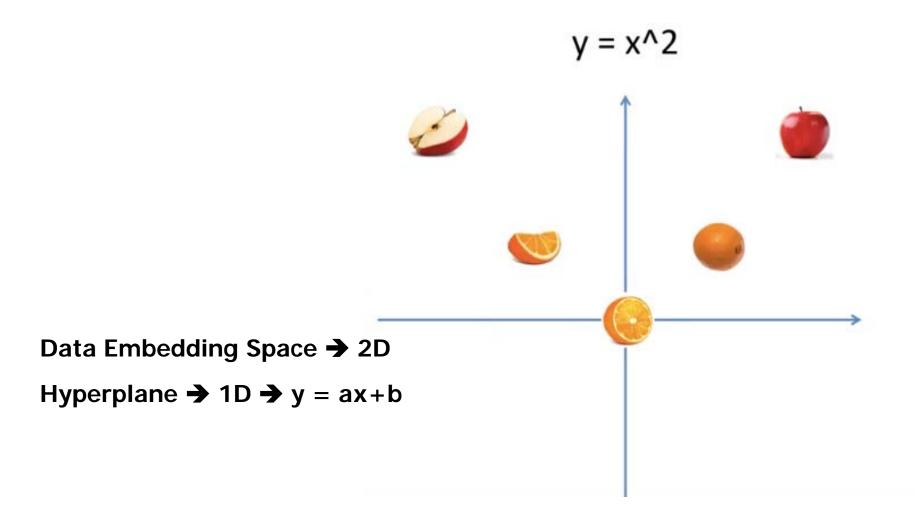


Linearly Separable or not

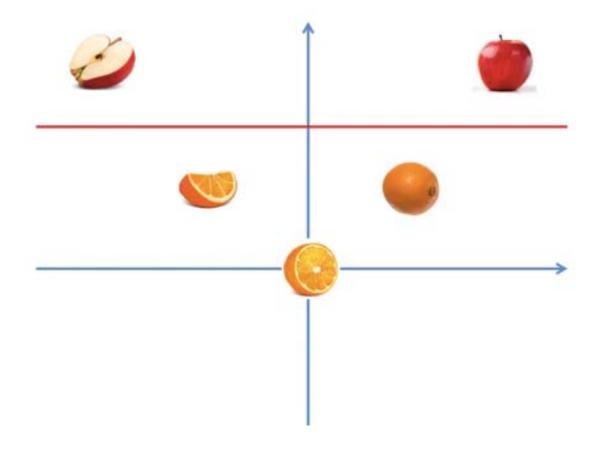




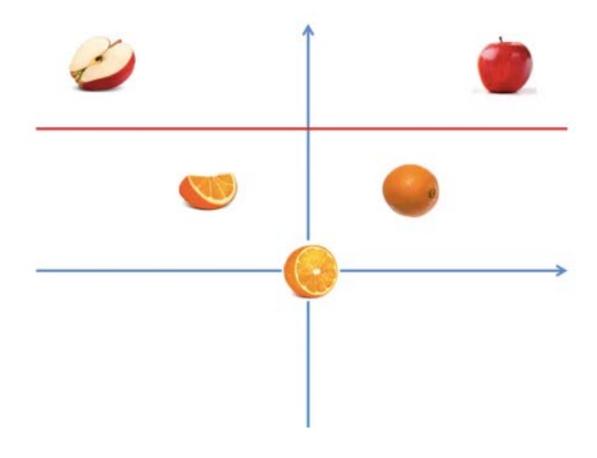
Mapping <u>lower dimension</u> to <u>high dimension</u>



- Now it is linearly separable in higher dimension
 - Mapping to high dimension requires much computation!



- Kernel trick in SVM do this without explicitly
 - Move data point to higher dimension with low computation!



Kernel Trick

- The **kernel trick** <u>avoids the explicit mapping</u> that is needed to get linear learning algorithms.
- Kernel methods owe their name to the use of kernel functions, which
 enable them to operate in a high-dimensional, <u>implicit</u> feature space
 without ever computing the coordinates of the data in that space, but
 rather by <u>simply computing the inner products</u> between the images
 of all pairs of data in the feature space

Kernel Trick

Kernel Function simply computing the inner products

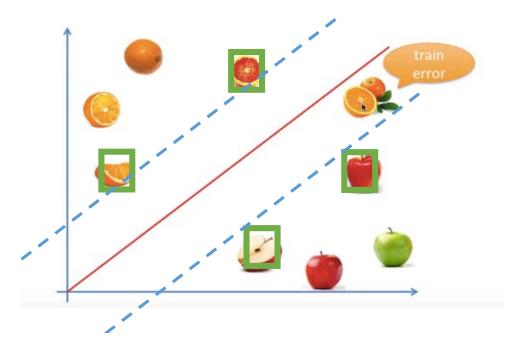
The kernel function can be any of the following:

- linear: $\langle x, x' \rangle$.
- polynomial: $(\gamma\langle x,x'
 angle+r)^d$. d is specified by keyword degree , r by coeff.
- rbf: $\exp(-\gamma ||x-x'||^2)$. γ is specified by keyword gamma, must be greater than 0.
- sigmoid $(anh(\gamma\langle x,x'\rangle+r))$, where r is specified by coeff.

Mapping 함수의 inner-product.. Mapping (m→n)

$$K(x_i, x_j) = \Phi(x_i)^T \Phi(x_j) = x_i^T A^T A x_j$$

• Cost is small == Margin is large



$$\min_{w,b,\zeta} rac{1}{2} w^T w + C \sum_{i=1}^n \zeta_i \qquad ext{subject to } y_i(w^T \phi(x_i) + b) \geq 1 - \zeta_i, \ \zeta_i \geq 0, i = 1, \dots, n$$

C is small

Training error is allowed

Overfitting is not allowed

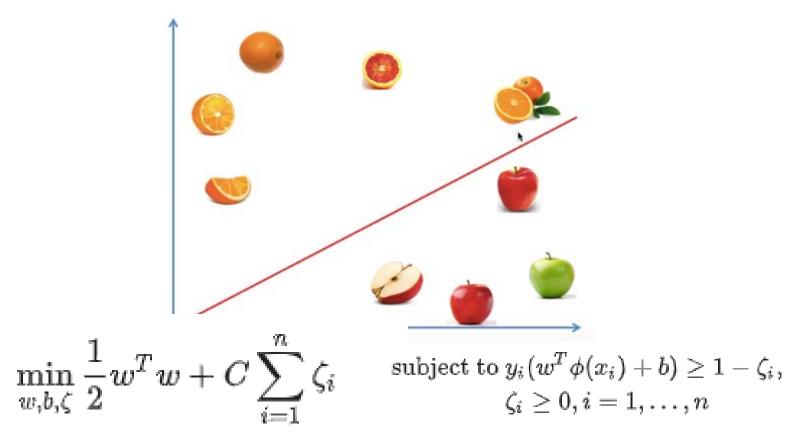
Margin is large

Testing e<mark>rro</mark>r is small

Margin width

misclassification

Cost is large == Margin is small



C is large

Training error is not allowed

Overfitting is allowed

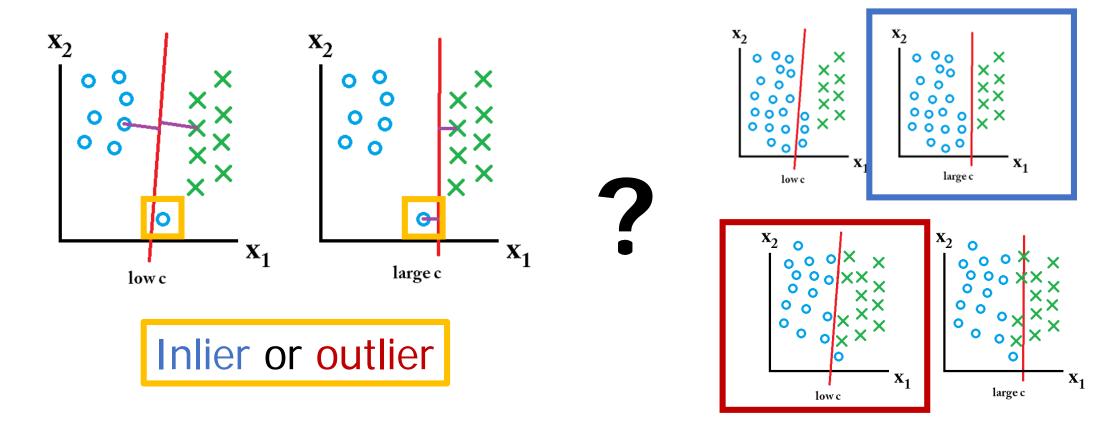
Margin is small

Testing error is large

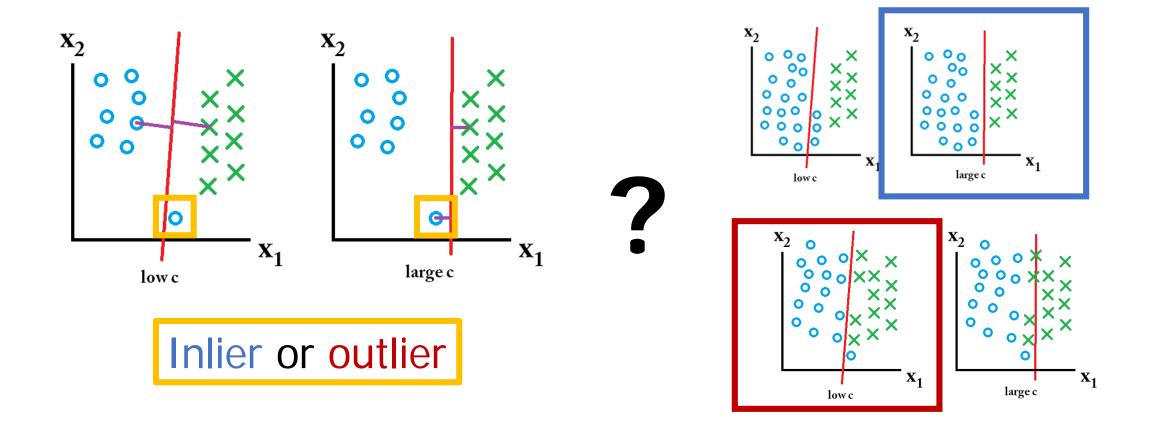
Margin width

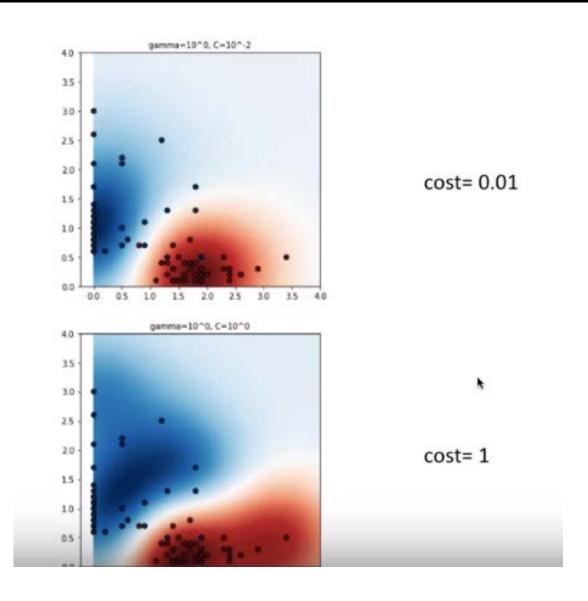
misclassification

- We assume that some samples caused by train error are the outlier.
- Therefore, we generally select a large margin for decision boundary.
- But, if not?



• Therefore, we cannot argue that we should choose large C, but we must make a decision through data analysis.





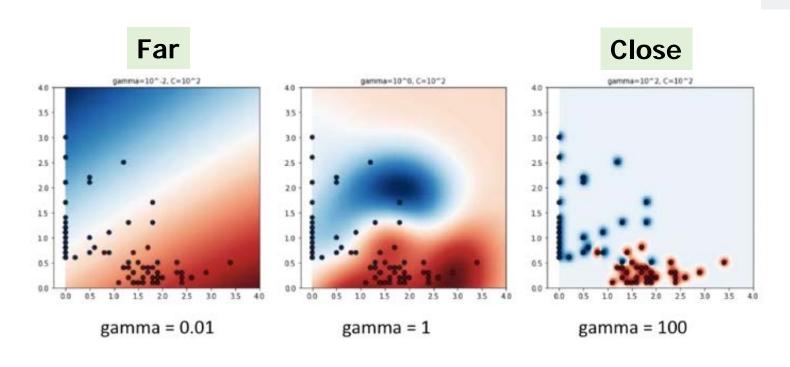
Cost is small
Training error is allowed
Overfitting is not allowed
Decision boundary is simple

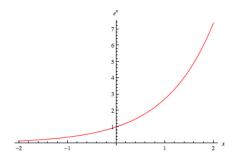
Cost is large
Training error is allowed
Overfitting is allowed
Decision boundary is complex

SVM parameter – Gamma in RBF kernel

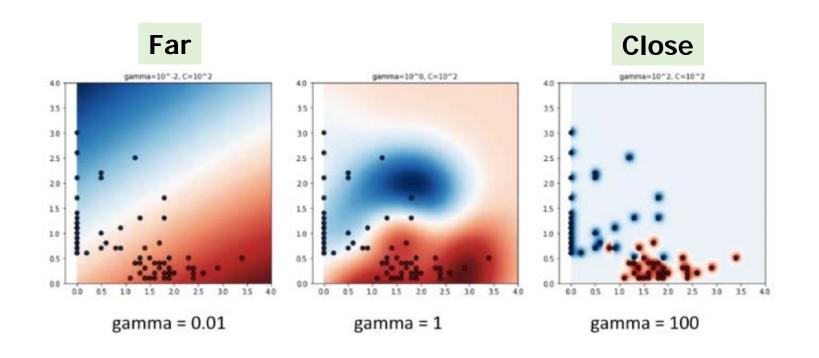
Intuitively, the gamma parameter defines how far the influence of a single training example reaches, with low values meaning 'far' and high values meaning 'close'.
 Radial Base Function (also called Gaussian Kernel)

$$K(x,x') = \exp(-gamma * ||x-x'||^2)$$





SVM parameter – Gamma in RBF kernel



Gamma is small
Influence is large
Margin is large
Similarly to a linear model

Gamma is large Influence is small Margin is small Overfitting is allowed

Find optical parameter – data analysis

Grid Search

• **Grid search** builds a model for **every combination** of hyper-parameters specified and evaluates each model.

					\rightarrow	Gamma
			1	10	100	
cost	1		0.7	0.8	0.7	
	10		0.8	0.8	0.9	
	, 10	0	0.6	0.8	0.8	

Pattern Recognition

SVM 개념 잡기 II

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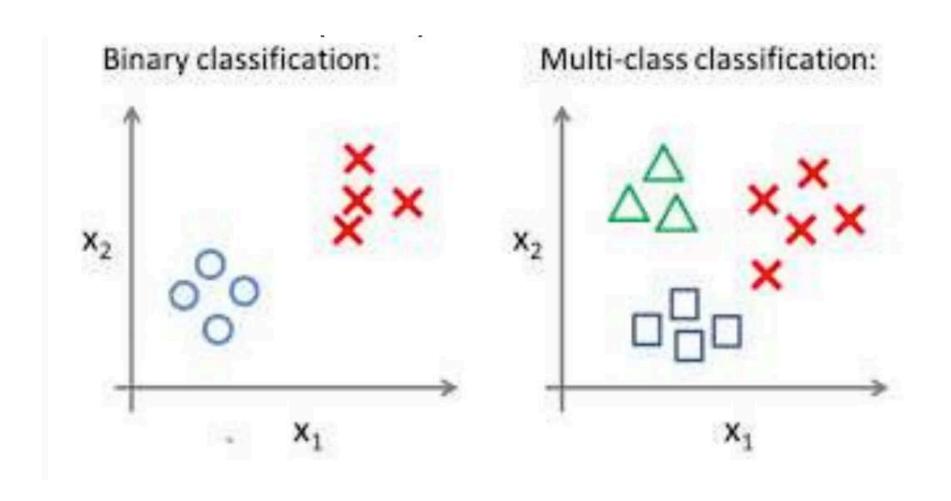
Previous Work

- What is a support vector
- What is a best decision boundary
- Hard-SVM
- Soft-SVM
- Parameter C
- Parameter gamma

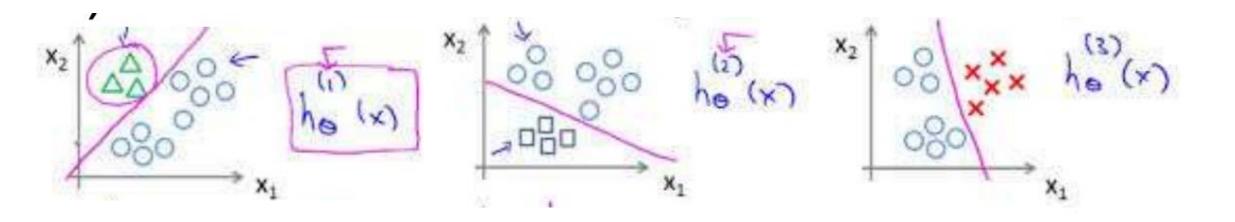
Today Lecture

- Multiclass SVM
 - One vs One
 - One vs Rest (One vs All)
- SVM with Unbalanced Data
- SVM Optimizer

Multiclass Classification



One-vs-Rest (OVR)



One-vs-Rest (OVR)

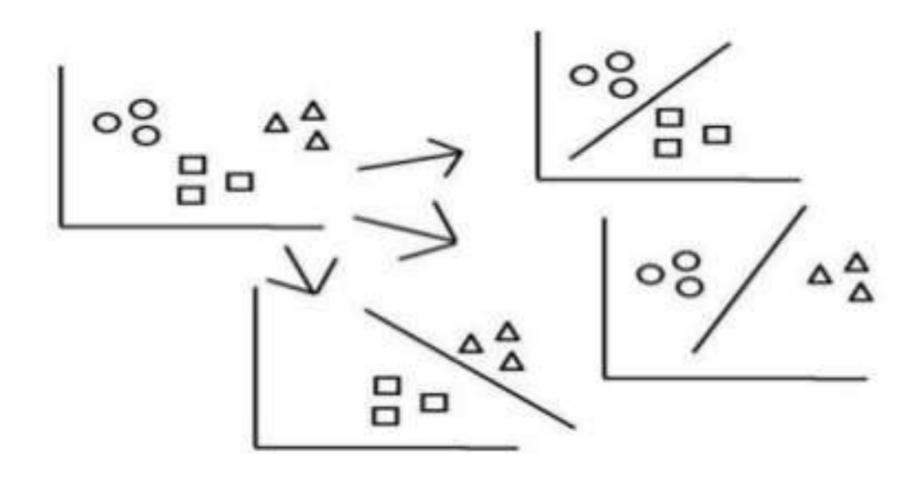
Training: Fits one classifier per class against all other data as a negative class. In total K classifiers.

<u>Prediction:</u> applies K classifiers to a new data point. Selects the one that got a positive class. In case of ties, selects the class with highest confidence.

Pros:

- Efficient
- Interpretable

One vs One (OvO)



One vs One (OvO)

Training: Fits (K-1) classifier per class against each other class. In total K*(K-1)/2 classifiers.

Prediction: applies K*(K-1)/2 classifiers to a new data point. Selects the class that got the majority of votes ("+1"). In case of ties, selects the class with highest confidence.

Pros:

 Used for Kernel algorithms (e.g. "SVM").

Cons:

Not as fast as OVR

Sklearn SVM: OvO vs OvR

```
>>> X = [[0], [1], [2], [3]]
\rightarrow \rightarrow Y = [0, 1, 2, 3]
>>> clf = svm.SVC(gamma='scale', decision_function_shape='ovo')
>>> clf.fit(X, Y)
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape='ovo', degree=3, gamma='scale', kernel='rbf',
    max_iter=-1, probability=False, random_state=None, shrinking=True,
    tol=0.001, verbose=False)
>>> dec = clf.decision_function([[1]])
>>> dec.shape[1] # 4 classes: 4*3/2 = 6
6
>>> clf.decision_function_shape = "ovr"
>>> dec = clf.decision_function([[1]])
>>> dec.shape[1] # 4 classes
>>> lin_clf = svm.LinearSVC()
>>> lin_clf.fit(X, Y)
LinearSVC(C=1.0, class_weight=None, dual=True, fit_intercept=True,
```

```
>>> lin_clf = svm.LinearSVC()
>>> lin_clf.fit(X, Y)
LinearSVC(C=1.0, class_weight=None, dual=True, fit_intercept=True,
    intercept_scaling=1, loss='squared_hinge', max_iter=1000,
    multi_class='ovr', penalty='l2', random_state=None, tol=0.0001,
    verbose=0)
>>> dec = lin_clf.decision_function([[1]])
>>> dec.shape[1]
Similar to SVC with parameter kernel-'linear' be
```

Similar to SVC with parameter kernel='linear', but implemented in terms of liblinear rather than libsym

Sklearn SVM: OvO vs OvR

Colab 실습

• 지난 시간 SVM 열어 확인

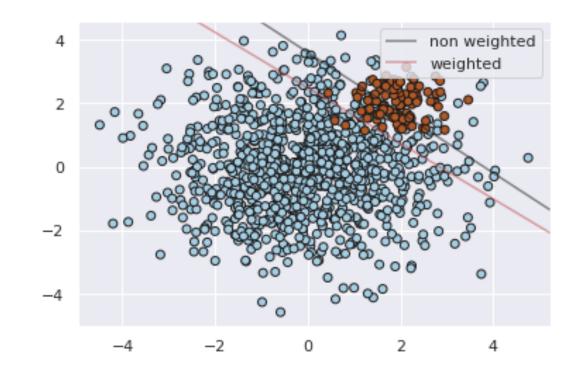
Unbalanced problems

Sklearn: class_weight

```
n_samples_1 = 1000
n_samples_2 = 100

# 1번 클래스에 10배 가중치;;
# 샘플 비율 차이만큼 가중치

wclf = svm.SVC(kernel='linear', class_weight={1: 10})
wclf.fit(X, y)
```



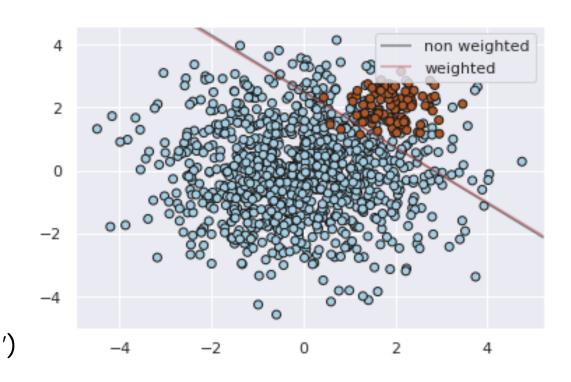
Skearn SVM OvR 에서는 default로 Unbalanced Problem을 해결해주지 않음

Unbalanced problems

Sklearn: class_weight

```
n_samples_1 = 1000
n_samples_2 = 100

# 1번 클래스에 10배 가중치;;
# 샘플 비율 차이만큼 가중치
wclf = svm.SVC(kernel='linear', class_weight='balanced')
wclf.fit(X, y)
```



Skearn SVM 옵션으로 class_weight='balanced'

Colab 실습

• 지난 시간 SVM 열어 확인

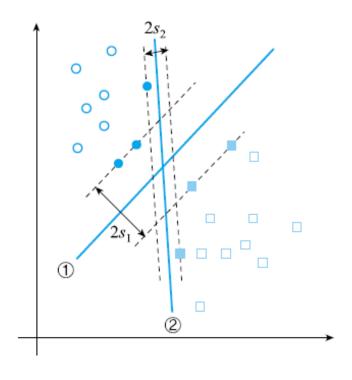


그림 5.3 선형 분리 가능한 상황

$$J(\mathbf{w}) = \frac{1}{2} \|\mathbf{w}\|^2$$
$$t(\mathbf{w}^{\mathsf{T}} \mathbf{x} + b) \ge 1$$

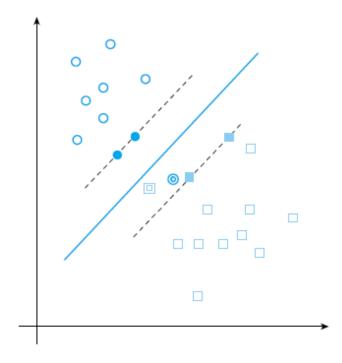


그림 5.6 선형 분리 불가능한 상황의 SVM

$$J(\mathbf{w}, \boldsymbol{\xi}) = \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^{N} \xi_i$$
$$t(\mathbf{w}^{\mathsf{T}} \mathbf{x} + b) \ge 1 - \xi$$

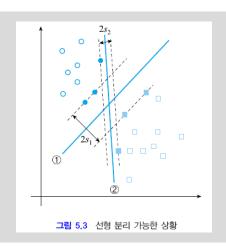
❖ 여백은 아래와 같이 공식화

여백 =
$$2h = \frac{2|d(\mathbf{x})|}{\|\mathbf{w}\|} = \frac{2}{\|\mathbf{w}\|}$$
 (5.4)

❖ 이제 문제를 **조건부 최적화 문제**로 공식화

• 조건부 최적화 문제

아래 조건 하에, $\mathbf{w}^{\mathrm{T}}\mathbf{x}_{i} + b \geq 1, \forall \mathbf{x}_{i} \in \omega_{1}$ $\mathbf{w}^{\mathrm{T}}\mathbf{x}_{i} + b \leq -1, \forall \mathbf{x}_{i} \in \omega_{2}$ $\frac{2}{\|\mathbf{w}\|}$ 를 최대화하라.



❖ 훈련 집합 X={(x₁,t₁),...,(xŊ,tŊ)}

- ❖ (5.5)를 간단한 형태로 변형하면,
 - 조건부 최적화 문제

아래 조건하에,
$$t_i(\mathbf{w}^T\mathbf{x}_i + b) - 1 \ge 0, i = 1, \dots, N$$

$$J(\mathbf{w}) = \frac{1}{2} \|\mathbf{w}\|^2 \triangleq 최소화하라.$$
 (5.6)

$$\mathbf{w}^{\mathsf{T}}\mathbf{x}_{i} + b \ge 1, \forall \mathbf{x}_{i} \in \omega_{1}$$

 $\mathbf{w}^{\mathsf{T}}\mathbf{x}_{i} + b \le -1, \forall \mathbf{x}_{i} \in \omega_{2}$ \mathbf{t}_{i} 를 통해 합쳐 쓰고

최대화 문제를 최소화 문제로 변경

- ❖문제의 특성
 - ❖ 해의 유일성
 - ❖ (5.6)은 볼록이므로 해는 유일하다.
 - ❖ 따라서 구한 해는 전역 최적 점을 보장한다. (Convex Optimization!!)
 - ❖ 문제의 난이도
 - ❖ N개의 선형 부등식을 조건으로 가진 2차 함수의 최적화 문제
 - ❖ 조건부 최적화 문제는 라그랑제 승수로 푼다. (11.2.3 절)

- ❖ 라그랑제 승수 방법
 - ❖ 목적 함수와 조건을 하나의 식 (즉 라그랑제 함수 ∠)으로 만들고,
 - ❖ KKT조건을 이용하여 라그랑제 함수를을 최적화하는 해를 구한다. (a,는 라그랑제 승수)

$$L(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2} \left\| \mathbf{w} \right\|^2 - \sum_{i=1}^{N} \underline{\alpha_i} (\underline{t_i} (\mathbf{w}^{\mathsf{T}} \mathbf{x}_i + b) - 1)$$

❖ KKT 조건이란?

라그랑제 함수 $L(\mathbf{\theta}, \lambda) = J(\mathbf{\theta}) - \sum_{i=1,N} \lambda_i f_i(\mathbf{\theta})$ 에 대한 KKT 조건은

(5.7)

②
$$\lambda_i \geq 0, i = 1, \dots, N$$

$$3 \quad \lambda_i f_i(\mathbf{\theta}) = 0, i = 1, \dots, N$$

❖ (5.7)의 KKT 조건

$$\frac{\partial L(\mathbf{w}, b, \alpha)}{\partial \mathbf{w}} = \mathbf{0} \quad \to \quad \mathbf{w} = \sum_{i=1}^{N} \alpha_i t_i \mathbf{x}_i \tag{5.8}$$

$$\frac{\partial L(\mathbf{w}, b, \alpha)}{\partial b} = 0 \quad \to \quad \sum_{i=1}^{N} \alpha_i t_i = 0 \tag{5.9}$$

$$\alpha_i \ge 0, i = 1, \dots, N \tag{5.10}$$

$$\alpha_{i}(t_{i}(\mathbf{w}^{T}\mathbf{x}_{i}+b)-1)=0, i=1,\dots,N$$
 (5.11)

- $2 \quad \lambda_i \geq 0, i = 1, \dots, N$
- \Im $\lambda_i f_i(\mathbf{\theta}) = 0, i = 1, \dots, N$

- ❖ (5.11)에 의하면 모든 샘플이 a = 0 또는 t(w x + b)-1=0이어야 함. a ≠ 0인 샘플이 서포트 벡터임
- ❖ (5.8)에 의하면, **라그랑제 승수 a, 알면 w 구할 수 있음 (결정 초평면을 구한 셈)**
 - ❖ 이제부터 'w 구하는 대신 라그랑제 승수 구하는' 문제로 관심 전환
- **❖** (5.11)로 *b* 구할 수 있음

- ❖ 문제의 볼록 성질을 이용하여 풀기 쉬운 형태로 변환
 - ❖ 볼록 성질을 만족하는 조건부 최적화 문제는 Wolfe 듀얼로 변형할 수 있다.

볼록 성질을 만족하는 조건부 최적화 문제는 Wolfe 듀얼 문제로 변형할 수 있다. 원래 문제가 $f_i(\theta)$ $\geq 0, i=1,\cdots,N$ 이라는 조건 하에 $J(\theta)$ 를 최소화하는 것이라 하자. 이때 Wolfe 듀얼 문제는 $\partial L(\theta,\alpha)/\partial \theta=0$ 과 $\alpha_i\geq 0, i=1\cdots,N$ 이라는 두 가지 조건 하에 $L(\theta,\alpha)=J(\theta)-\sum_{i=1,N}\alpha_i f_i(\theta)$ 를 최대 화하는 것이다. 부등식 조건이 등식 조건으로 바뀌었고 최소화 문제가 최대화 문제로 바뀌었다.

- ❖ (5.6)을 Wolfe 듀얼로 바꾸어 쓰면,
 - 조건부 최적화 문제

아래 조건 하에, $\mathbf{w} = \sum_{i=1}^{N} \alpha_i t_i \mathbf{x}_i$ $\stackrel{\bullet}{\mathbf{v}} = \sum_{i=1}^{N} \alpha_i t_i \mathbf{x}_i$ $\sum_{i=1}^{N} \alpha_i t_i = 0$ $\alpha_i \ge 0, i = 1, 2, ..., N$ $L(\mathbf{w}, b, \boldsymbol{\alpha}) 를 최대화하라.$



(5.12)

• 조건부 최적화 문제

아래 조건하에,

$$t_i(\mathbf{w}^{\mathsf{T}}\mathbf{x}_i + b) - 1 \ge 0, i = 1, \dots, N$$

$$J(\mathbf{w}) = \frac{1}{2} \|\mathbf{w}\|^2$$
을 최소화하라.

$$\frac{\partial L(\mathbf{w}, b, \alpha)}{\partial \mathbf{w}} = \mathbf{0} \quad \to \quad \mathbf{w} = \sum_{i=1}^{N} \alpha_i t_i \mathbf{x}_i$$
 (5.8)

$$\frac{\partial L(\mathbf{w}, b, \boldsymbol{\alpha})}{\partial b} = 0 \quad \to \quad \sum_{i=1}^{N} \alpha_i t_i = 0 \tag{5.9}$$

$$\alpha_i \ge 0, i = 1, \dots, N \tag{5.10}$$

$$\alpha_i(t_i(\mathbf{w}^T\mathbf{x}_i + b) - 1) = 0, i = 1, \dots, N$$
 (5.11)

❖ 부등식 조건이 등식 조건이 되어 풀기에 유리함

Wolfe 듀얼

$$L(\mathbf{\theta}, \boldsymbol{\alpha}) = J(\mathbf{\theta}) - \sum_{i=1,N} \alpha_i f_i(\mathbf{\theta})$$

- ❖ 간단한 수식 정리를 하면,
 - 조건부 최적화 문제

$$\sum_{i=1}^{N} \alpha_i t_i = 0$$

$$\alpha_i \geq 0, i = 1, \dots, N$$

$$\tilde{L}(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j t_i t_j \mathbf{x}_i^{\mathrm{T}} \mathbf{x}_j 를 최대화하라.$$

최소화 문제 → 최대화 문제

$$L(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^{N} \alpha_i (t_i (\mathbf{w}^T \mathbf{x}_i + b) - 1)$$
(5.7)

 $L(\mathbf{w}, b, \boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i (t_i (\mathbf{w}^{\mathrm{T}} \mathbf{x}_i + b) - 1) - \frac{1}{2} \|\mathbf{w}\|^2$ (5.7)

(5.13)

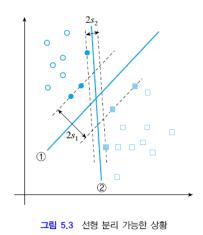
$$\frac{\partial L(\mathbf{w}, b, \alpha)}{\partial \mathbf{w}} = \mathbf{0} \quad \rightarrow \quad \mathbf{w} = \sum_{i=1}^{N} \alpha_i t_i \mathbf{x}_i$$
 (5.8)

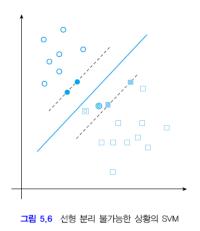
$$\frac{\partial L(\mathbf{w}, b, a)}{\partial b} = 0 \quad \to \quad \sum_{i=1}^{N} \alpha_i t_i = 0 \tag{5.9}$$

$$\alpha_i \ge 0, i = 1, \dots, N \tag{5.10}$$

$$\alpha_i (t_i (\mathbf{w}^T \mathbf{x}_i + b) - 1) = 0, i = 1, \dots, N$$
 (5.11)

- ❖ 흥미로운 특성들
 - ❖ 2차 함수의 최대화 문제임
 - ❖ w와 b가 사라졌다. (a를 찾는 문제가 되었다.)
 - ❖ 특징 벡터 x/가 내적 형태로 나타난다. (비선형으로 확장하는 발판)
 - ❖ 목적 함수의 두번째 ∑항은 Nº개의 항을 갖는다. (여전히 풀기 어려운 문제)





• 조건부 최적화 문제

아래 조건하에,
$$\sum_{i=1}^{N} \alpha_i t_i = 0$$

$$\alpha_i \ge 0, i = 1, \cdots, N$$

$$\tilde{L}(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j t_i t_j \mathbf{x}_i^{\mathsf{T}} \mathbf{x}_j 를 최대화하라.$$

조건부 최적화 문제 (선형 SVM)

아래 조건하에,
$$\sum_{i=1}^{N} \alpha_i t_i = 0$$

$$0 \le \alpha_i \le C, \quad i = 1, \cdots, N$$

$$\tilde{L}(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j t_i t_j \mathbf{x}_i^{\mathsf{T}} \mathbf{x}_j 를 최대화하라.$$

(5.27)

쉬운 방정식으로 변경했으나, N이 크면 여전히 분석적으로 최적화 하기는 어렵다. 결국 수치적(Gradient Descent, etc.)으로 풀어야 한다.