Classification Part II

Maximal margin classifier, support vector machines

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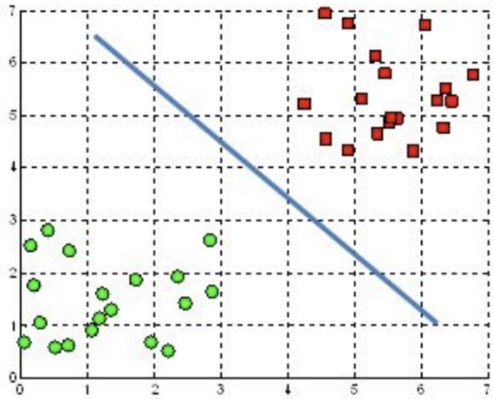
Maximal Margin Classifier

hard margin

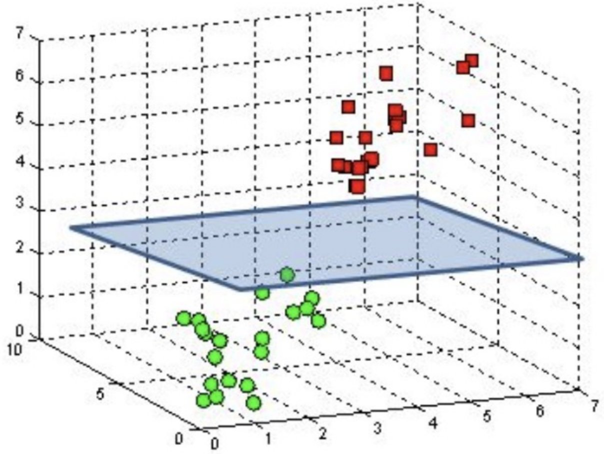
Hyperplane

- *A* **hyperplane in p-dimensional space** *is a flat affine subspace of dimension p-1*

A hyperplane in $\mathbb{R}^2$ is a line



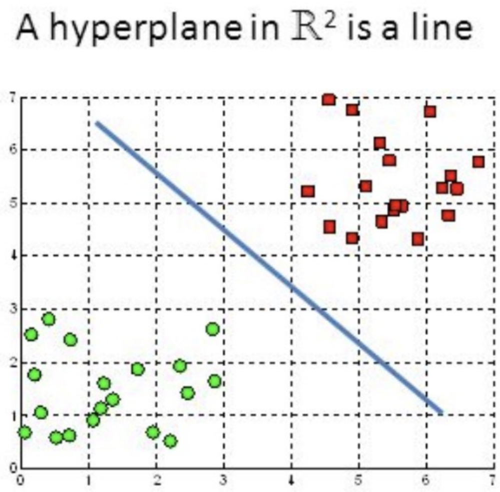
A hyperplane in $\mathbb{R}^3$ is a plane

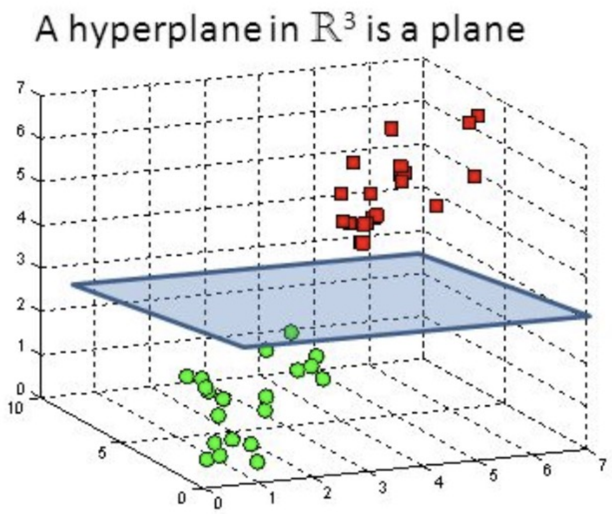


- p-차원에 있는 set 이지만, p-1차원 공간과 본질적으로 같음

Hyperplane

- A **hyperplane in p-dimensional space** is a flat affine subspace of dimension p-1





Given $\beta_0, \beta_1, \ldots, \beta_p$, Hyperplane은 아래와 같이 표현 가능.

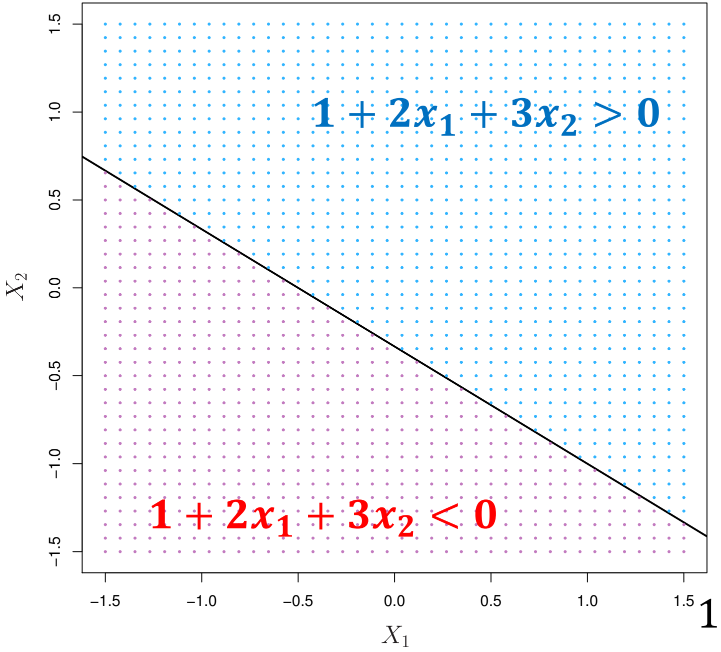
$$Hyperplane = \{(x_1, \ldots, x_p) \in \mathbb{R}^p : \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p = 0\}$$

Hyperplane : Example

예: $p = 2,\ \ \beta_0 = 1, \beta_1 = 2, \beta_3 = 0$

$$Hyperplane = \{(x_1, x_2) \in \mathbb{R}^2 : 1 + 2x_1 + 3x_2 = 0\}$$

The hyperplane: $1 + 2x_1 + 3x_2 = 0 \ \Leftrightarrow x_2 = -\frac{2}{3}x_1 - \frac{1}{3}$



$1 + 2x_1 + 3x_2 = 0$

Hyperplane 은 공간을 두 부분으로 나눔

Classification : Separating Hyperplane

- Binary Classification Problem
  - X: p−variables
  - y: −1 or 1

- Given $\beta_0, \beta_1, \dots, \beta_p$, Hyperplane은 아래와 같이 표현 가능.

  $$Hyperplane = \{(x_1, \dots, x_p) \in \mathbb{R}^p : \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p = 0\}$$

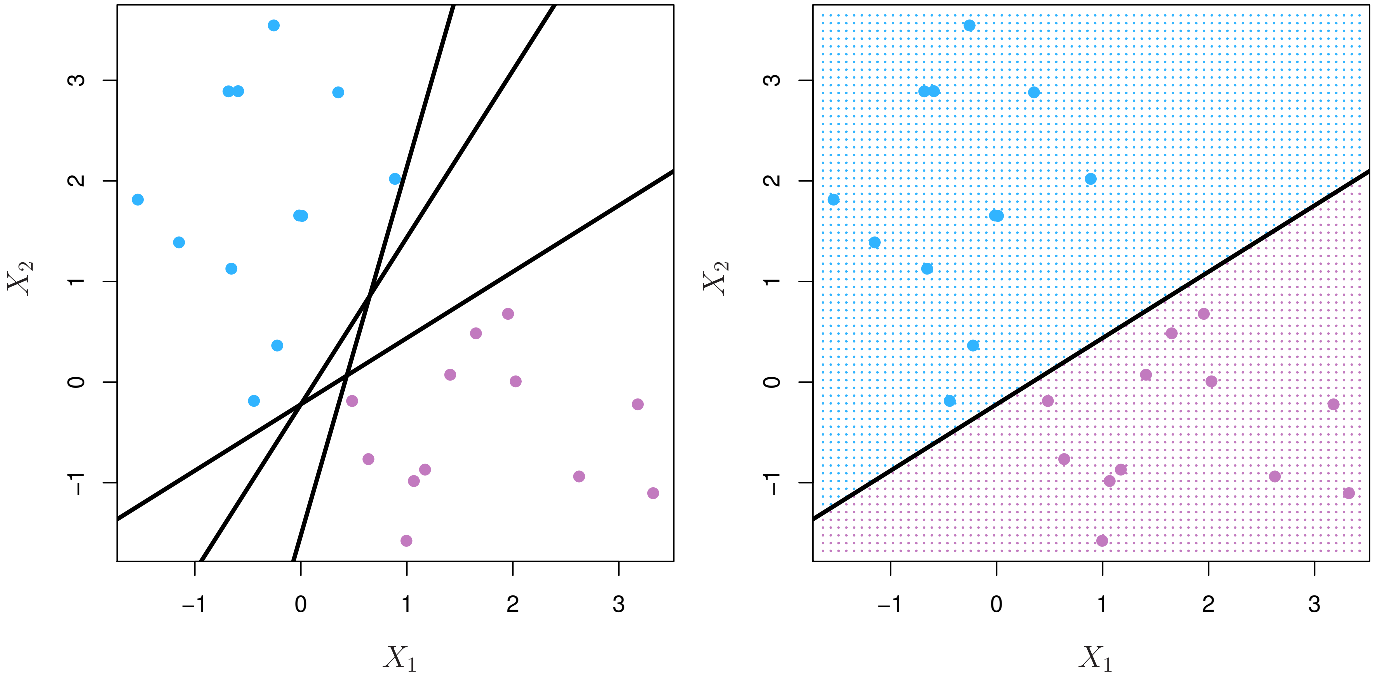
  편의상 $f_\beta(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$ 라고 하면,

- Classifier: Given $\mathrm{X} = x_i$,
  - Assign 1 if $f_\beta(x_i) > 0$
  - Assign −1 if $f_\beta(x_i) < 0$

- Equivalently, the above is

$$y_i f_\beta(x_i) > 0$$

Maximal Margin Classifier

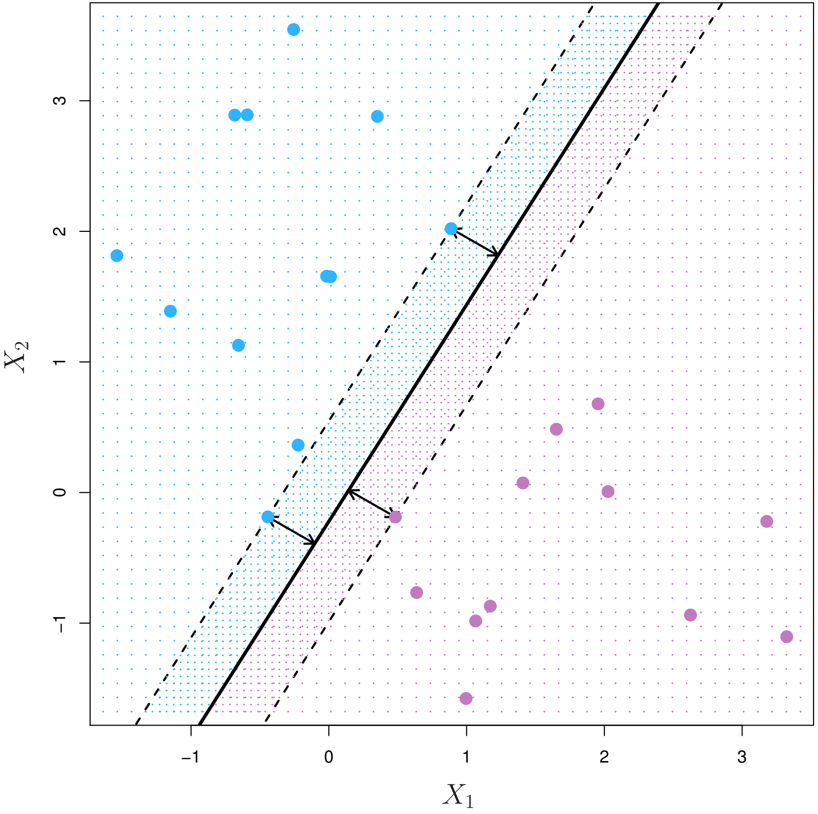


- Which hyperplane will you choose? Any Justification?

Maximal Margin Classifier : Margin

$$f_\beta(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p = 0$$

$\|\beta\| = 1$, 방향만 고려



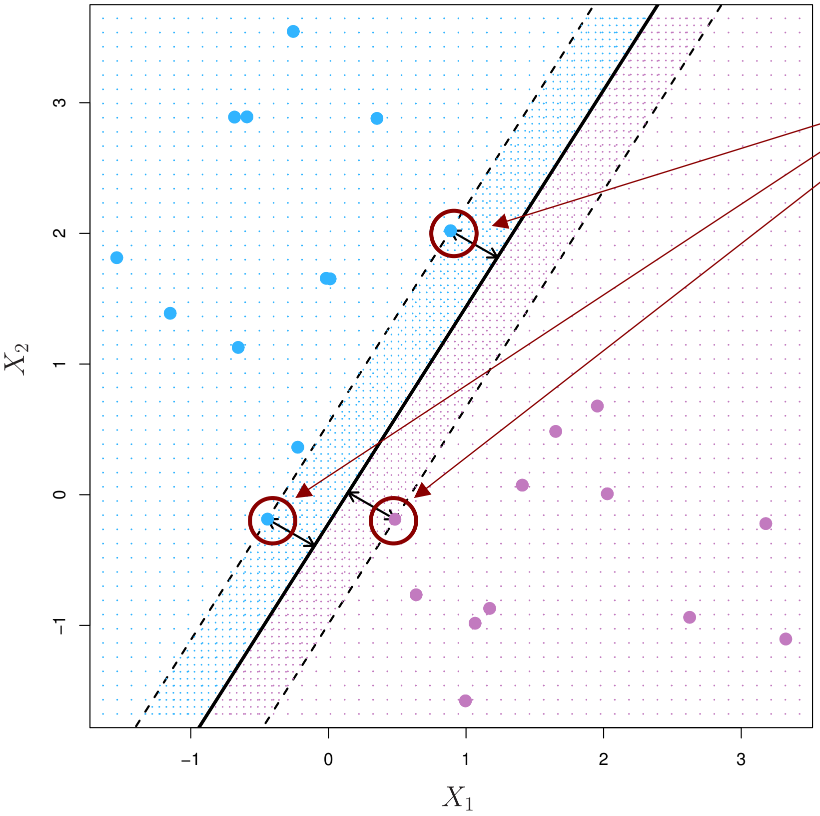
- 직선이 이미 주어졌다고 가정(β)
- 각 data point마다, 직선과의 거리를 계산

$$d_i = |f_\beta(x_i)|$$

- M: margin (or gap): 가장 가까운 점과 직선과의 거리 (거리들 중 가장 작은 거리)
- 거리가 멀다 = more confident
- **Maximal margin classifier**: 이 margin을 가장 크게, gap을 가장 크게, 만드는 hyperplane 찾기 (= β 찾기)

Maximal Margin Classifier : Support Vectors

$$f_\beta(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p = \beta_0 + <\beta, x> = 0$$



- Support Vectors: the points that “support” the maximal margin hyperplane
- 이 (얼마 안되는) Data 포인트들이 조금만 움직여도 hyperplane이 바뀜
- 다른 점들은 hyperplane에 직접적으로 영향을 주지 않음

Maximal Margin Classifier : Optimization

- maximize M
- subject to
  - $\|\beta\| = 1$
  - $d_i = |f_\beta(x_i)| = y_i f_\beta(x_i) \geq M, \quad i = 1, \ldots, n$

- Direct 한 계산이 어렵다.

Maximal Margin Classifier : Optimization

- maximize M
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- Direct 한 계산이 어렵다.

- x_i 와 separating hyperplane $(\{x: f_\beta(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p\})$과의 거리

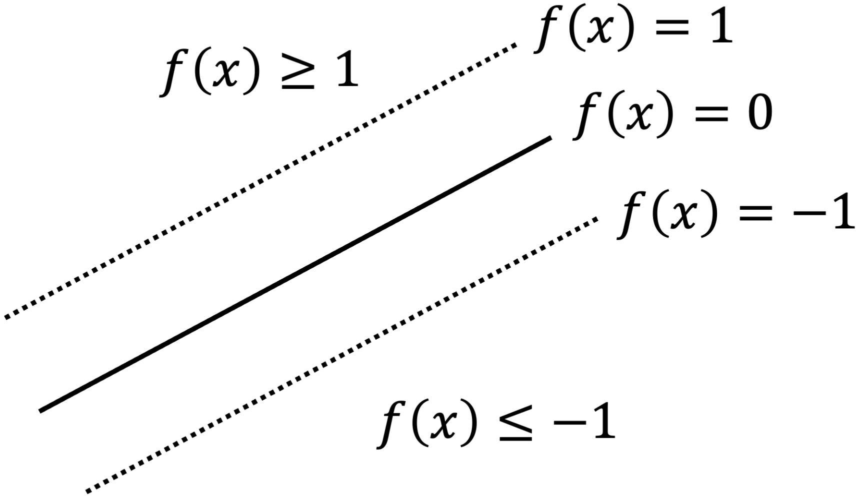
$$\left|\frac{f_\beta(x_i)}{\|\beta\|}\right|$$

Maximal Margin Classifier: Different Formulation

- Margin=1 이라는 조건으로 변경(대신 $\|\beta\| = 1$ 이라는 조건 제외)
- Maximize $\frac{1}{\|\beta\|}$
- Subject to
  - $y_i f_\beta(x_i) \geq 1 \;\; i = 1, \ldots, n$

Equivalently
- Minimize $\|\beta\|^2 = \beta^T \beta$
- Subject to
  - $y_i f_\beta(x_i) \geq 1 \;\; i = 1, \ldots, n$

where $f_\beta(x_i) = \beta_0 + < \beta, x >$



Maximal Margin Classifier : Different Formulation

Equivalently

- Minimize $\frac{1}{2}||\beta||^2 = \frac{1}{2}\beta^T\beta$
- Subject to
  - $y_i f_\beta(x_i) \geq 1 \;\; i = 1, \ldots, n$

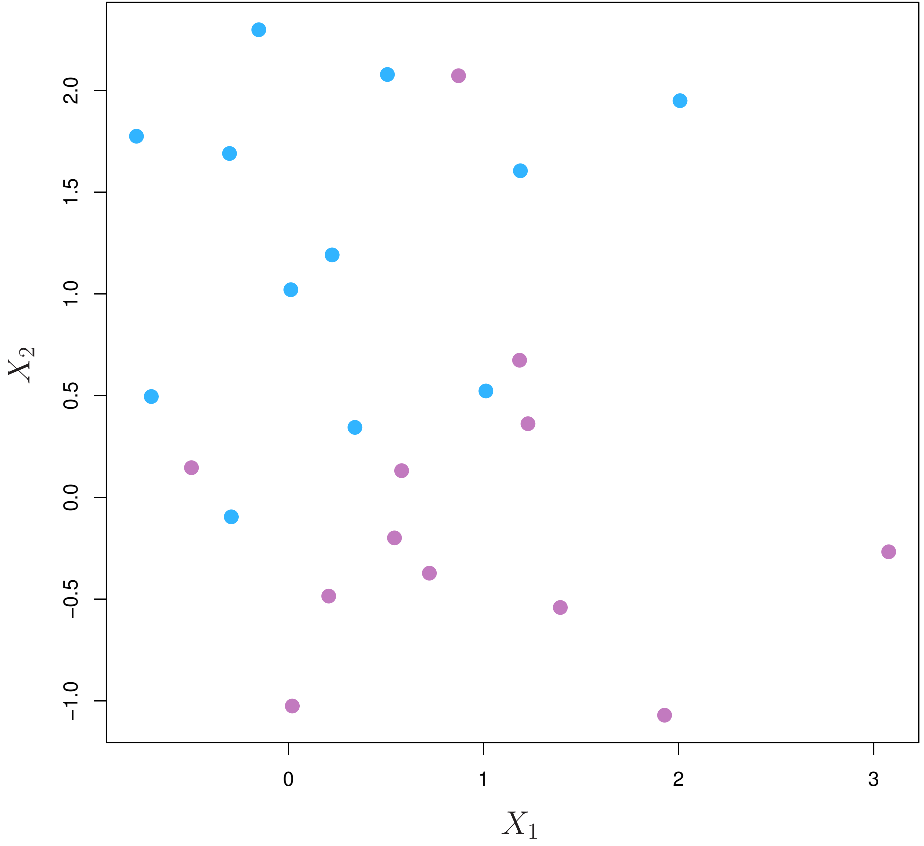
where $f_\beta(x_i) = \beta_0 + < \beta, x >$

with the Lagrangian multiplier, the loss function is

$$L(\beta; \alpha_i) = \frac{1}{2}\beta^T\beta \; + \sum_{i=1}^{n} \alpha_i [y_i(\beta_0 + < \beta, x_i >) \; - 1]$$

$[y_i(\beta_0 + < \beta, x_i >) \; - 1]$ is a form of a **hinge loss** (or **svm loss**)

Non-separable case

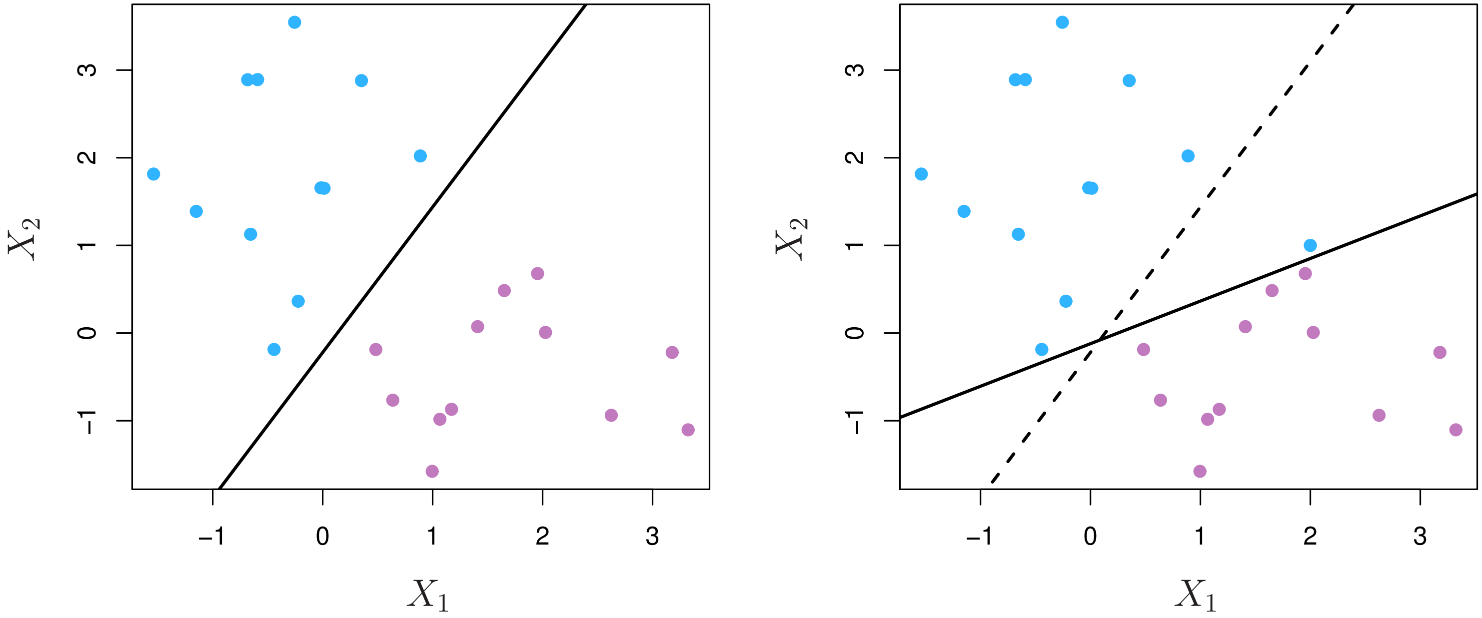


- 많은 경우 Non-separable
- There is no maximal margin classifier
- Instead of the hard margin,
- Use soft margin (일부 오류 허용)

Support Vector Classifier

soft margin

Maximal Margin Classifier



- A change in a single observation −〉 affect the classifier a lot
- Potential overfitting

Support Vector Classifiers

- Find a hyperplane that **does not perfectly separate** the two classes.

- Separate almost all the data correctly, allow **a few** mis-classification.

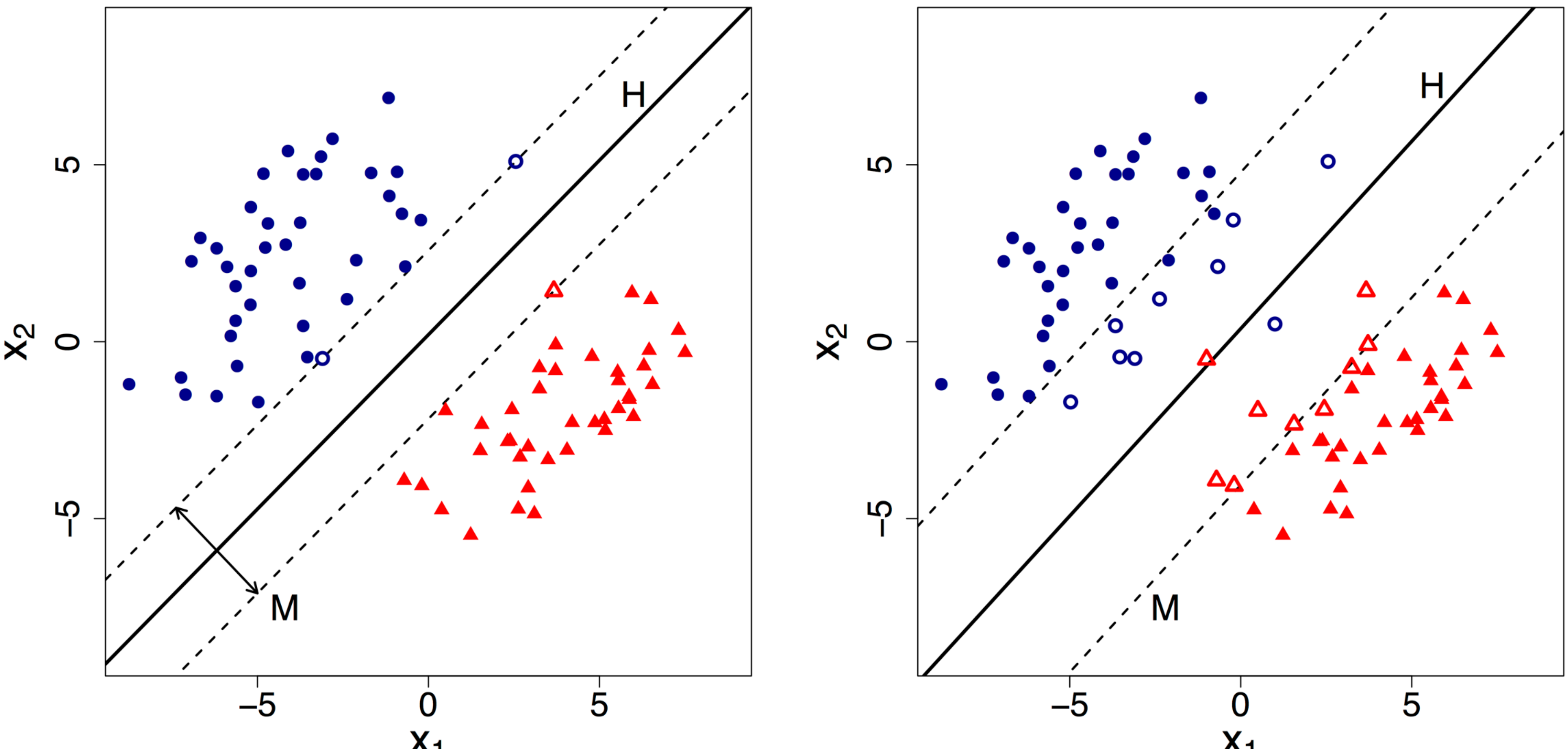
- Gain:
  - **Robustness** to individual observations
  - **Better** classification of **most** of the training observations

Support Vector Classifiers

- maximize M
- subject to
  - ✓ $\|\beta\| = 1$
  - ~~✓~~ $\cancel{d_i = |f_\beta(x_i)| = y_i f_\beta(x_i) \geq M, \ \ i = 1, \dots, n}$
  - ✓ $y_i f_\beta(x_i) \geq M(1 - \epsilon_i), \quad i = 1, \dots, n$
  - ✓ $\epsilon_i \geq 0\,, \sum \epsilon_i \leq B$

where $f_\beta(x) = \beta_0 + < \beta, x >$, B: a budget

Support Vector Classifiers



Support Vector Classifier : Optimization

Maximal Margin Classifier

- Minimize $\frac{1}{2}\|\beta\|^2 = \frac{1}{2}\beta^T\beta$
- Subject to
  - $y_i f_\beta(x_i) \geq 1 \;\; i = 1, \dots, n$

where $f_\beta(x_i) = \beta_0 + < \beta, x >$

Support Vector Classifier

- Minimize $\frac{1}{2}\|\beta\|^2 = \frac{1}{2}\beta^T\beta + C\sum_{i=1}^{n}\epsilon_i$
- Subject to
  - $y_i f_\beta(x_i) \geq 1 - \epsilon_i \qquad i = 1, \dots, n$
  - $\epsilon_i \geq 0$

where $f_\beta(x_i) = \beta_0 + < \beta, x >$

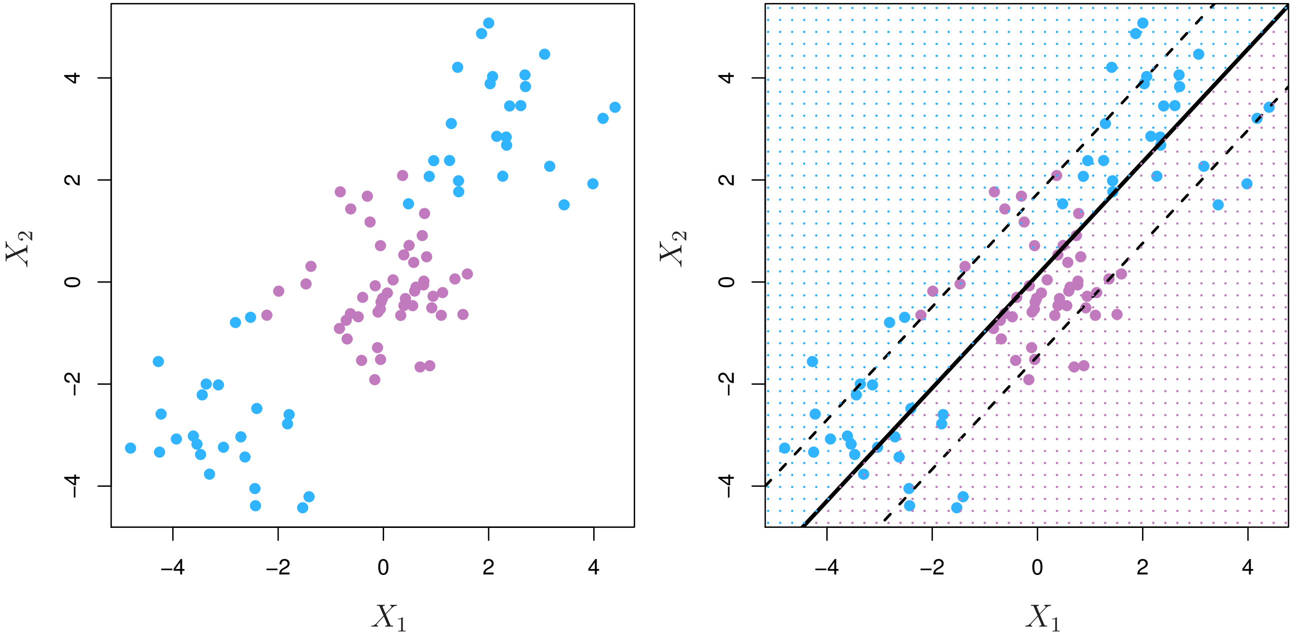
C: penalty on $\sum_{i=1}^{n}\epsilon_i$

- cost of violation
- C 무한대 ~ maximal margin classifier (ϵ_i=0)

The Support Vector Machines

Nonlinear classifier

Linear Boundary Can Fail



(Optional) SVM Optimization Detail

The linear SVM is

minimize $\frac{1}{2}\beta^T\beta + C\sum_{i=1}^{n}\epsilon_i$

Subject to $y_i(\beta_0 + < \beta, x_i >) \geq 1 - \epsilon_i$ for all $i = 1, .., n$.

Or, $\epsilon_i \geq 1 - y_i(\beta_0 + < \beta, x_i >)$ tells

minimize $\frac{\lambda}{2} \| \beta \|^2 + \sum_{i=1}^{n} \max(0, 1 - y_i f(x_i))$

Subject to $\mathrm{f(x)} = \beta_0 + < \beta, x >$

Considering $\frac{\lambda}{2} = C^{-1}$

(Optional) SVM Optimization Detail

With the linear constraints

minimize $\frac{\lambda}{2} \parallel \beta \parallel^2 + \sum_{i=1}^{n} \max(0, 1 - y_i f(x_i))$

Subject to $\mathrm{f(x)} = \beta_0 + < \beta, x >$

Removing the **linear constraints**,

minimize $\frac{\lambda}{2} \parallel f \parallel_{\mathcal{H}}^2 + \sum_{i=1}^{n} \max(0, 1 - y_i f(x_i))$

Subject to $f \in \mathcal{H}$

How? Feature Mapping!

Recall: Feature Mapping

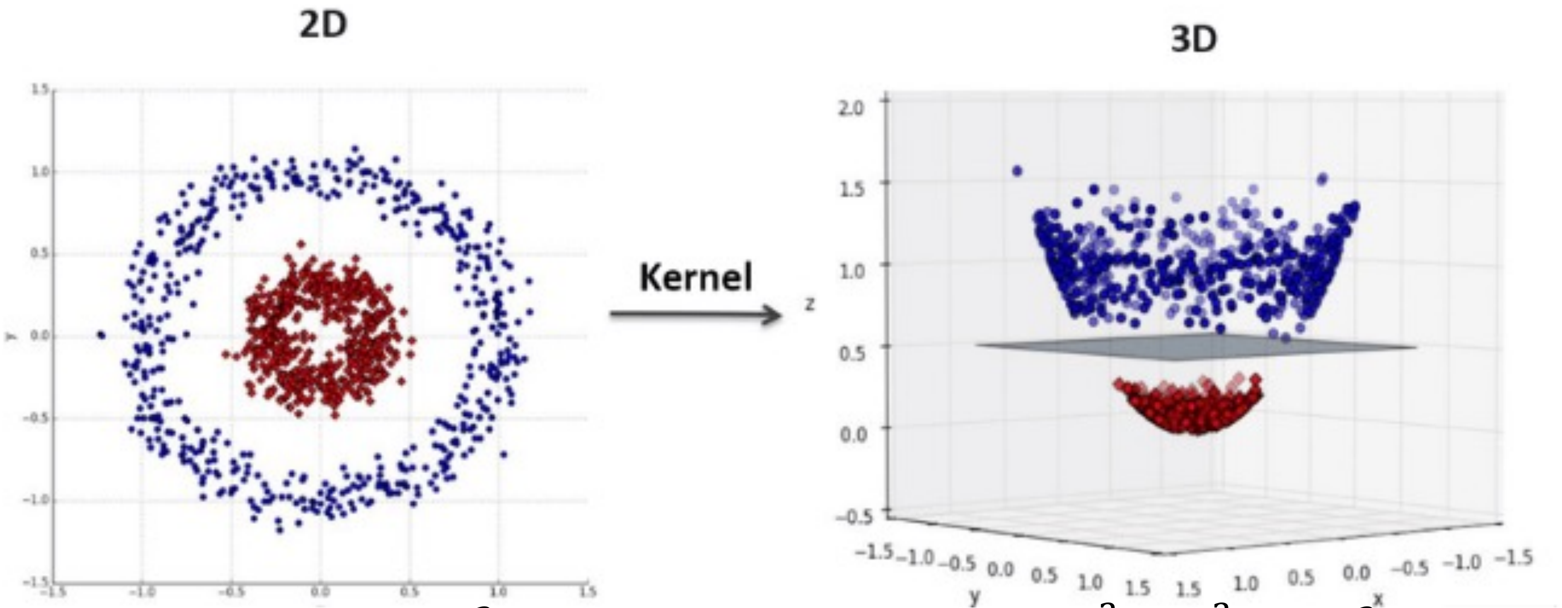
- $\hat{y} = \hat{A}(x)$ 라는 선형방법론이 있다고 가정
- $\hat{A}$ 은 데이터 $(x_1, y_1), \dots, (x_n, y_n)$을 통해 만들어짐.

Feature Mapping: ϕ: $\mathbb{R}^p \rightarrow \mathcal{H}$ 가 원래 데이터를 더 고차원으로 보내는 mapping일 때

$$(\phi(x_1), y_1), \dots, (\phi(x_n), y_n)$$

을 이용하여 만든다면, 최종 $\hat{A}$ 은 $\phi(x_1), \dots, \phi(x_n)$와 선형관계. x에 대한 비선형 함수!

Recall: Feature Mapping



$$(X_1, X_2) \in \mathbb{R}^2 \quad \rightarrow \quad (X_1, X_2, {X_1}^2 + {X_2}^2) \in \mathbb{R}^3$$

Decision boundary: becomes **nonlinear** in terms of x_1, x_2.

$$\beta_0 + \beta_1 x_1 + \beta_2 x_2 = 0, \qquad v.s. \qquad c_0 + c_1 x_1 + c_2 x_2 + c_3({x_1}^2 + {x_2}^2) = 0$$

Kernel SVM

- Feature Mapping: ϕ: $\mathbb{R}^p \rightarrow \mathcal{H}$ 에서 $\mathcal{H}$가 특별한 성질을 만족하는 함수공간

- Reproducing kernel Hilbert Space (RKHS) with a reproducing kernel

$$\phi(x_i) = \kappa(\cdot, x_i)$$

$$< \kappa(\cdot, x_i), \kappa\left(\cdot, x_j\right) > = \kappa(x_i, x_j)$$

Gaussian Radial Basis Function(GRBF)

$$\varkappa(x_1, x_2) = \exp(-\gamma \parallel x_1 - x_2 \parallel^2)$$

Polynomial Kernel

$$\varkappa(x_1, x_2) = (a + < x_1, x_2 >)^2$$

The Support Vector Machine

- The **Support Vector Machine (SVM)** is an extension of the support vector classifier that results from enlarging feature space to be a RKHS.

- It is well known that RKHS generated by the **GRBF kernel** is rich enough space to cover any nonlinear function of x.

- Note
  - Why do we use the kernel functions? What is the RKHS?
  - Choice of kernel?
  - What is the role of γ? in the kernel function?

Summary

- SVM: Find a separating hyperplane with a soft-margin

- Hyperparameters
  - Cost parameter: 얼마나 hard하게 soft-margin 구성?
  - Kernel function: Gaussian RBF, Polynomial, Brownian, …
  - Parameter of the kernel: Gaussian: γ, Polynomial: degree

- 다른 Classifiers (두번째 모듈)
  - Tree-based models (decision trees)
  - Ensemble of trees
    - parallel: Random Forest
    - sequential: adaboost
  - GBM계열: GBM, XGBoost, LightGBM, CatBoost, …