Machine Learning

Contents

7.1. Characteristics of Support Vector Machine

- **Feed-forward Neural Network(Perceptron, MLP, RBF,..)**
  - Stochastic algorithm
  - Generalizes well but need a lot of tuning
  - Can be learned in incremental fashion
  - To learn complex functions: use multiple hidden layers

- **SVM**
  - Deterministic algorithm
  - Nice Generalization with few parameters to tune
  - Hard to learn – Quadratic programming techniques
  - Using kernel tricks to learn very complex functions

7.2. Linear Separator and Perceptron

Some relevant properties of $L = \{w_0 + \mathbf{w}^T\mathbf{x} = 0\}$

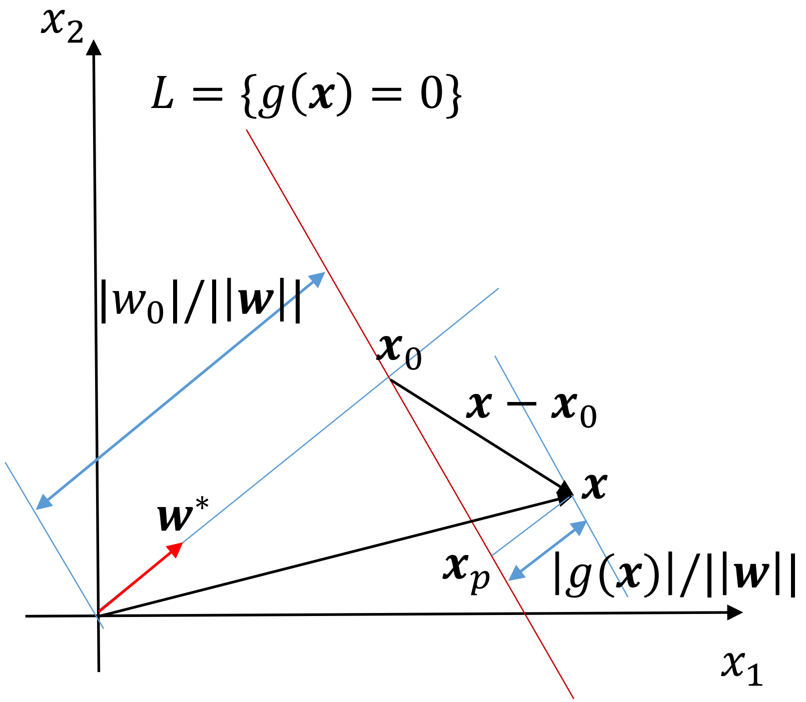
- 1) For any two points $\mathbf{x}_1, \mathbf{x}_2 \in L$,

  $$\mathbf{w}^T(\mathbf{x}_1 - \mathbf{x}_2) = 0$$

  so $\mathbf{w}$ is normal to L

  Define $\mathbf{w}^* = \mathbf{w}/||\mathbf{w}||$ to be the unit normal.
- 2) For any point $\mathbf{x}_0$ in L, $\mathbf{w}^T\mathbf{x}_0 = -w_0$
- 3) The signed distance of any point $\mathbf{x}$ to L is

  $$\mathbf{w}^{*T}(\mathbf{x} - \mathbf{x}_0) = \frac{1}{||\mathbf{w}||}(\mathbf{w}^T\mathbf{x} + w_0)$$



- 4) The geometric margin of example $< \mathbf{x}_i, y_i >$ with respect to hyperplane defined by $w_0, \mathbf{w}$ is

  $$y_i \cdot \frac{1}{||\mathbf{w}||}(\mathbf{w}^T\mathbf{x} + w_0) \qquad y_i \in \{-1, 1\}$$

  A point is misclassified iff its margin is <0.

Perceptron Learning Algorithm

Tries to minimize

$$D(\mathbf{w}, w_0) = -\sum_{\substack{i\in \\ miscalssified}} y_i(\mathbf{w}^T\mathbf{x}_i + w_0)$$

sum of absolute distances of misclassified examples.

Gradient

$$\frac{\partial D(\mathbf{w}, w_0)}{\partial \mathbf{w}} = -\sum_{i\in M} y_i\mathbf{x}_i \qquad \frac{\partial D(\mathbf{w}, w_0)}{\partial w_0} = -\sum_{i\in M} y_i$$

Use stochastic gradient descent to minimize ; estimate the gradient based on a single training examples take a step downhill, repeat.

퍼셉트론 알고리즘

○입력과 목표 값의 쌍으로 구성된 학습패턴 $< \boldsymbol{x}_i, y_i >$를 저장한다.

① 가중치 $\boldsymbol{w}$와 w_0를 임의의 값으로 초기화 시킨다.

② n개의 학습패턴에 대하여 가중치를 다음과 같이 변경시킨다.

$$\text{If } y_i(\boldsymbol{w}^T\boldsymbol{x}_i + w_0) \le 0 \text{ then } \begin{cases} \boldsymbol{w} := \boldsymbol{w} + y_i\boldsymbol{x}_i \\ w_0 := w_0 + y_i \end{cases} \tag{7.2.9}$$

③ 오인식된 학습패턴이 있으면 과정 ②를 다시 수행한다.

④ 새로운 입력 $\boldsymbol{x}$가 주어지면 $g(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + w_0$의 부호로 예측한다.

Perceptron Learning Alg.: Dual Representation

Let α_i be a count of the number of times that example i was mis-classified.

If initial $\omega =< 0, 0, ..., 0 >$, then final weights are sums of the training examples.

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i \qquad w_0 = \sum_{i=1}^{n} \alpha_i y_i$$

Then, our predictor is

$$h(\mathbf{x}) = sign(\mathbf{w}^T \mathbf{x} + w_0) = sign \sum_{i=1}^{n} \alpha_i y_i (\mathbf{x}_i^T \mathbf{x} + 1)$$

퍼셉트론 알고리즘의 이중적 표현

○입력과 목표값의 쌍으로 구성된 학습패턴 $< \boldsymbol{x}_i, y_i >$를 저장한다.

① α_i는 영으로 초기화 시킨다.

② 학습 패턴 n개에 대하여 가중치를 다음과 같이 변경시킨다.

$$\text{If } \sum_{j=1}^{n} y_i \alpha_j y_j (\boldsymbol{x}_j^T \boldsymbol{x}_i + 1) \le 0 \text{ then } \alpha_i := \alpha_i + 1 \tag{7.2.13}$$

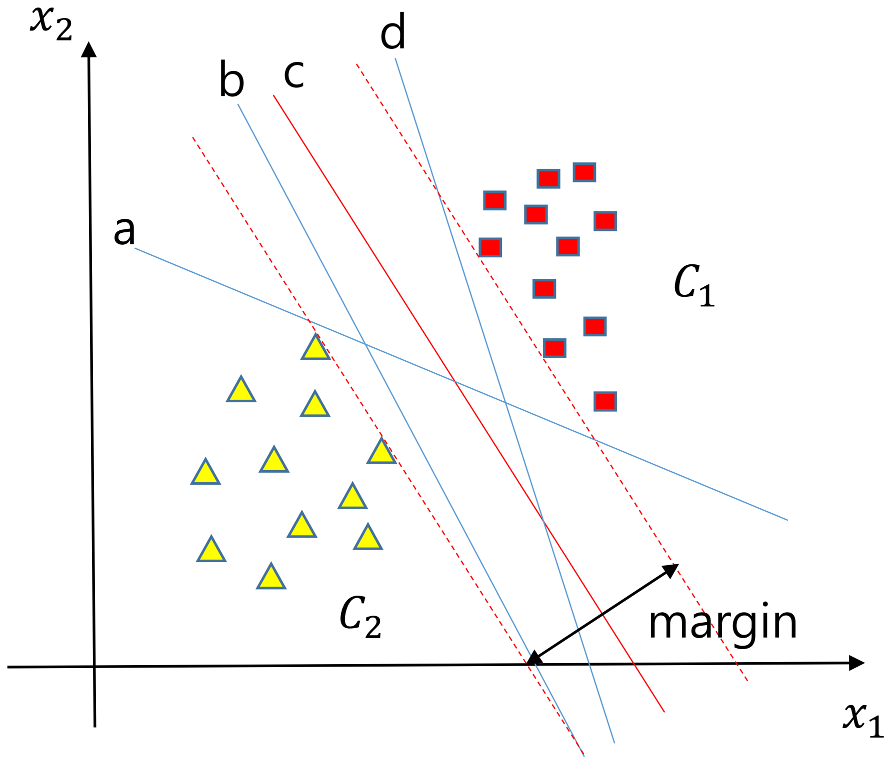
$$\boldsymbol{w} = \sum_{i=1}^{n} \alpha_i y_i \boldsymbol{x}_i \text{ and } w_0 = \sum_{i=1}^{n} \alpha_i y_i$$

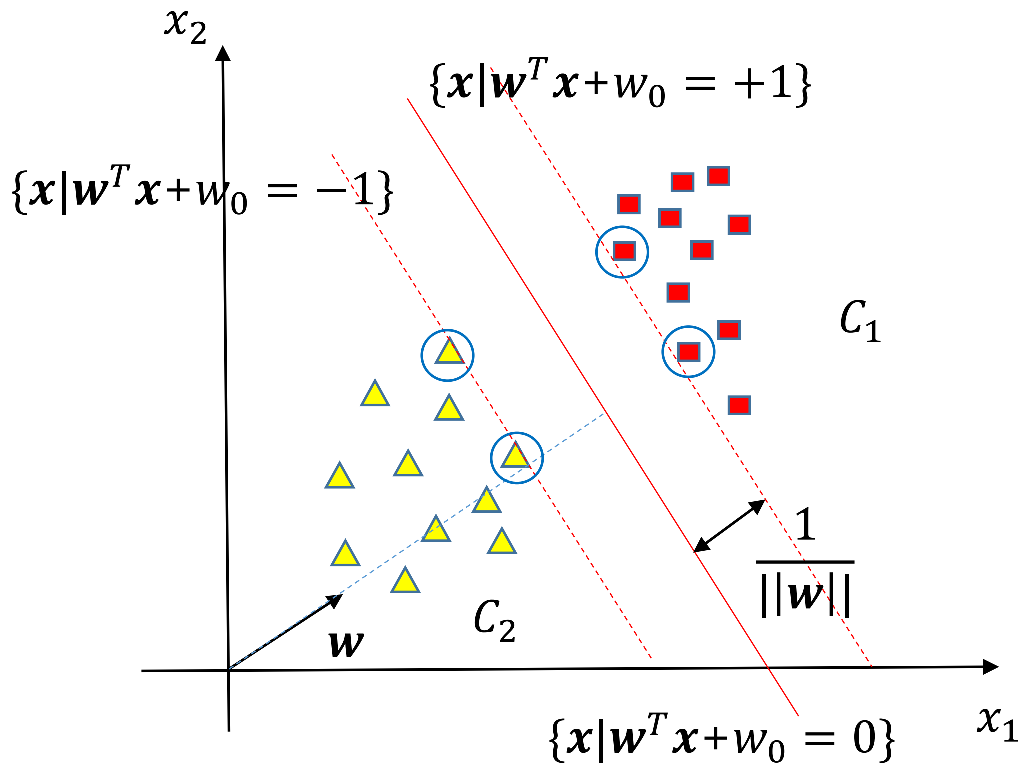
③ 오인식된 학습패턴이 있으면 과정 ②를 다시 수행한다.

④ 새로운 입력 $\boldsymbol{x}$가 주어지면 $h(\boldsymbol{x})$로 예측한다.

7.3. Support Vector Machine

- Maximizing the margin leads to a particular choice of decision boundary. The location of the boundary is determined by a subset of the data points, known as support vectors, which are indicated by the circles.





Support Vector Machine

- **Support vector machines**
  - Names a whole family of algorithms. We'll start with the **maximum margin separator**. The idea is to find the separator with the maximum margin from all the data points. We'll see, later, a theoretical argument that this might be a good idea. Seems a little less haphazard than a perceptron.

Optimization problem :

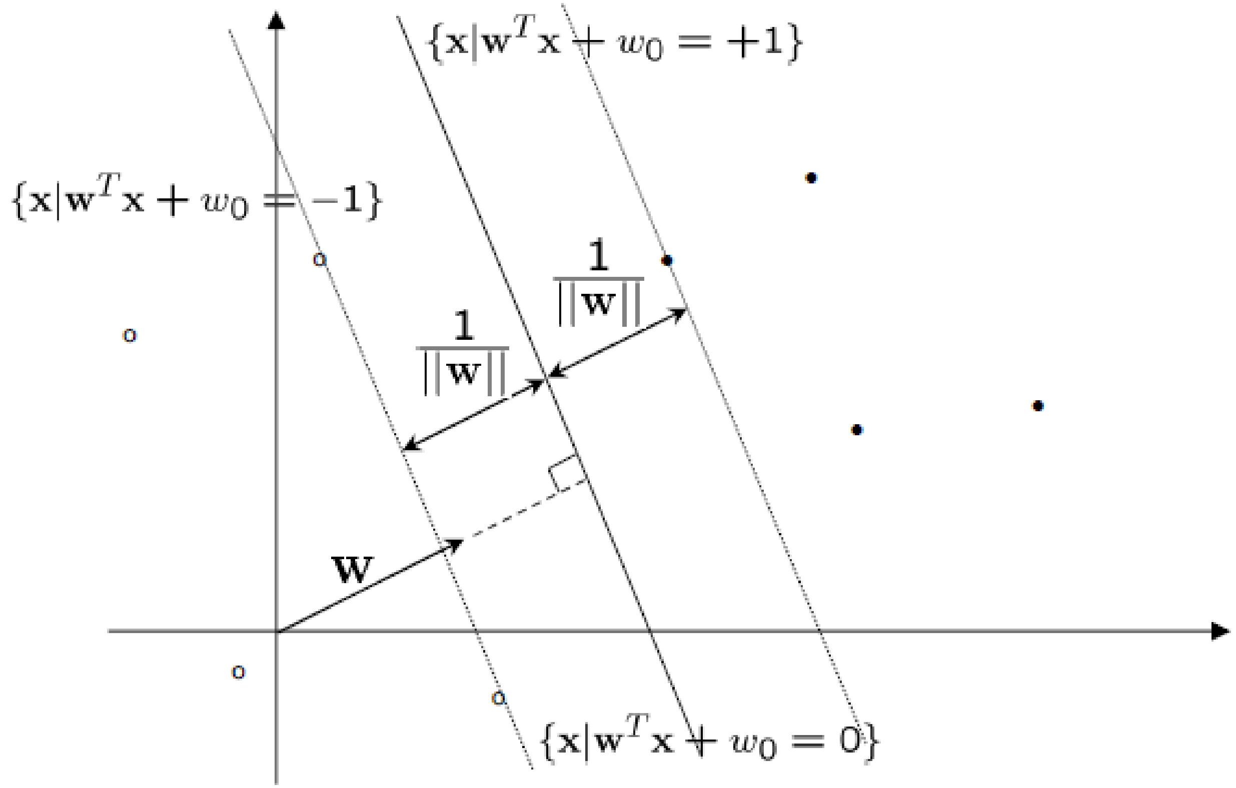
$$\max_{\{w_0,\mathbf{w}\}} C \quad \text{subject to} \quad \frac{1}{||\mathbf{w}||} y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq C \quad i = 1, ..., n$$

Since we have an extra degree of freedom (any scaling of $\mathbf{w}$ specifies the equivalent separator), we can set $||\mathbf{w}||$ to $1/C$.

Support Vector Machine: Formulation

getting the problem

$$\min_{\{w_0,\mathbf{w}\}} \frac{1}{2}(||\mathbf{w}||)^2 \text{ subject to } y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1 \text{ for } i = 1, ..., N$$



Support Vector Machine: Formulation

getting the problem

$$\min_{\{w_0,\mathbf{w}\}} \frac{1}{2}(||\mathbf{w}||)^2 \quad \text{subject to} \quad y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1$$

This is a quadratic optimization (well studied) problem, with a unique solution computable in polynomial time. But looking a little deeper will reveal some important properties.

Lagrangian formulation of constrained optimization :

$$\min_{\{w_0,\mathbf{w}\}} \max_{\alpha \geq \mathbf{0}} L(w_0, \mathbf{w}, \alpha) = \frac{1}{2}||\mathbf{w}||^2 - \sum_{i=1}^{n} \alpha_i [y_i(\mathbf{w}^T\mathbf{x}_i + w_0) - 1]$$

Lagrange multiplier

positive if constraint is satisfied

Support Vector Machine: Kuhn-Tucker Theorem

Kuhn-Tucker theorem :

$$\min_{\{w_0,\mathbf{w}\}} \max_{\alpha} L(w_0,\mathbf{w},\alpha) = \max_{\alpha} \min_{\{w_0,\mathbf{w}\}} L(w_0,\mathbf{w},\alpha)$$

Lagrange showed that, for $L(w_0,\mathbf{w},\alpha)$ convex in $\{w_0,\mathbf{w}\}$, a necessary and sufficient condition for $\{w_0^*,\mathbf{w}^*\}$ to be the solution of $\min L(w_0,\mathbf{w},\alpha)$ is for

$$\frac{\partial L(w_0,\mathbf{w},\alpha)}{\partial \mathbf{w}} = \mathbf{0} \text{ and } \frac{\partial L(w_0,\mathbf{w},\alpha)}{\partial w_0} = 0$$

In our case,

$$\frac{\partial L(w_0,\mathbf{w},\alpha)}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = \mathbf{0}$$

$$\frac{\partial L(w_0,\mathbf{w},\alpha)}{\partial w_0} = \sum_{i} \alpha_i y_i = 0$$

Support Vector Machine: Lagrange Formulation

Substitute these to get L dependent only on α.

$$L(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{j=1}^{n} \sum_{k=1}^{n} \alpha_j \alpha_k y_j y_k (\mathbf{x}_j^T \mathbf{x}_k)$$

Maximize $L(\alpha)$ subject to $\alpha \geq \mathbf{0}$ and $\sum_i \alpha_i y_i = 0$.
Note that $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$ shows weight vector can be represented as weighted sum of data, as in dual perceptron.

Support Vector Machine: Solution

Finding optimal α_i is computationally tractable quadratic programming problem.

An optimal solution must satisfy

$$\alpha_i^*[y_i(\mathbf{w}^{*T}\mathbf{x}_i + w_0) - 1] = 0$$

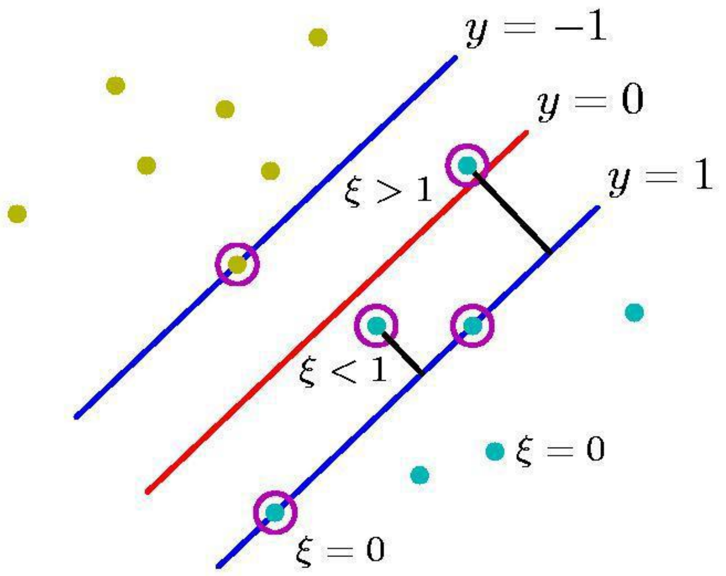
So, α_i are non-zero for points $\mathbf{x}_i$ with margin=1; 0 for all other points. Points with margin=1 are called <u>support vectors</u>.
Finding w_0: let $\mathbf{x}_i$ be a support vector. Then

$$y_i(\mathbf{w}^T\mathbf{x}_i + w_0) = 1$$

So, $w_0 = y_i - \mathbf{w}^T\mathbf{x}_i$

Support Vector Machines

- What if the problem is not linearly separable?



- Introduce slack variables
  - Need to minimize:

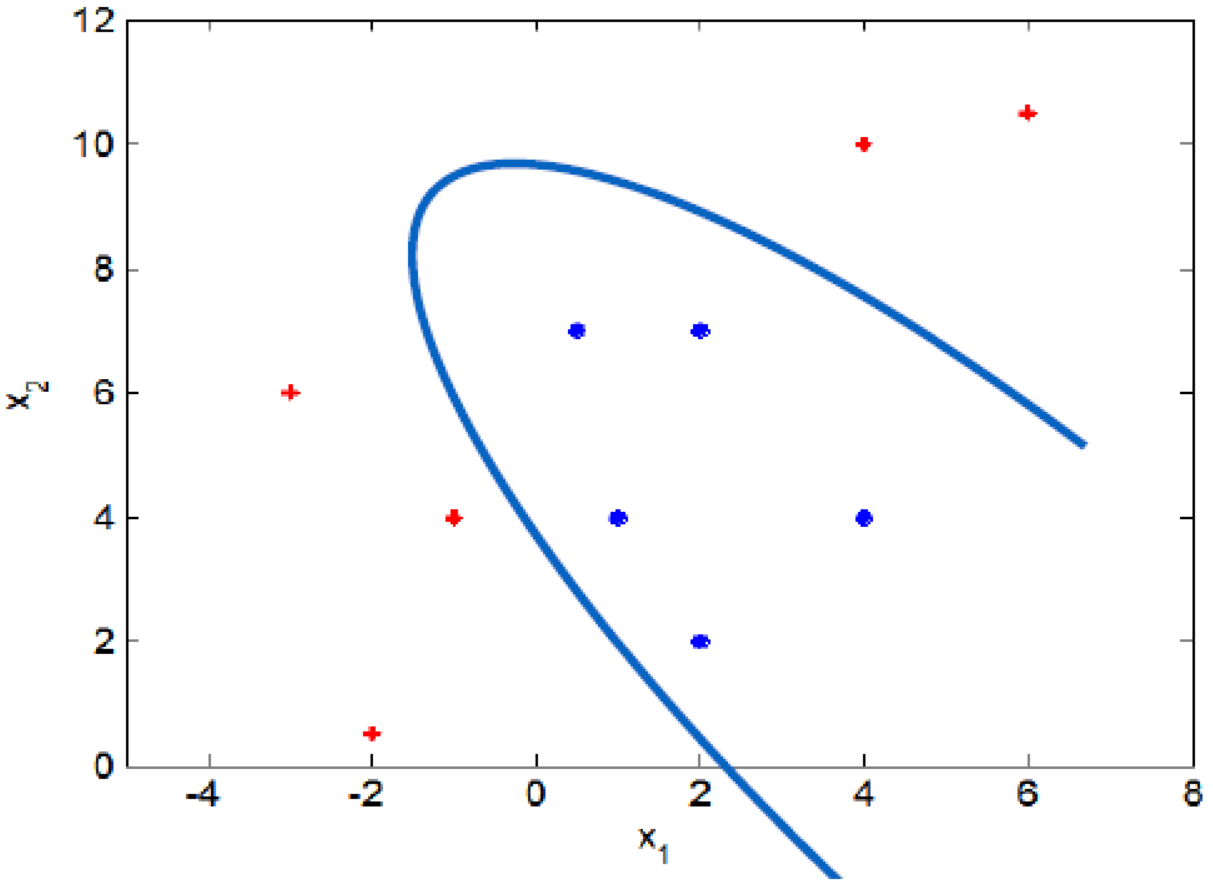
$$L(w,\xi) = \frac{\| \vec{w} \|^2}{2} + C\left(\sum_{i=1}^{m} \xi_i \right)$$

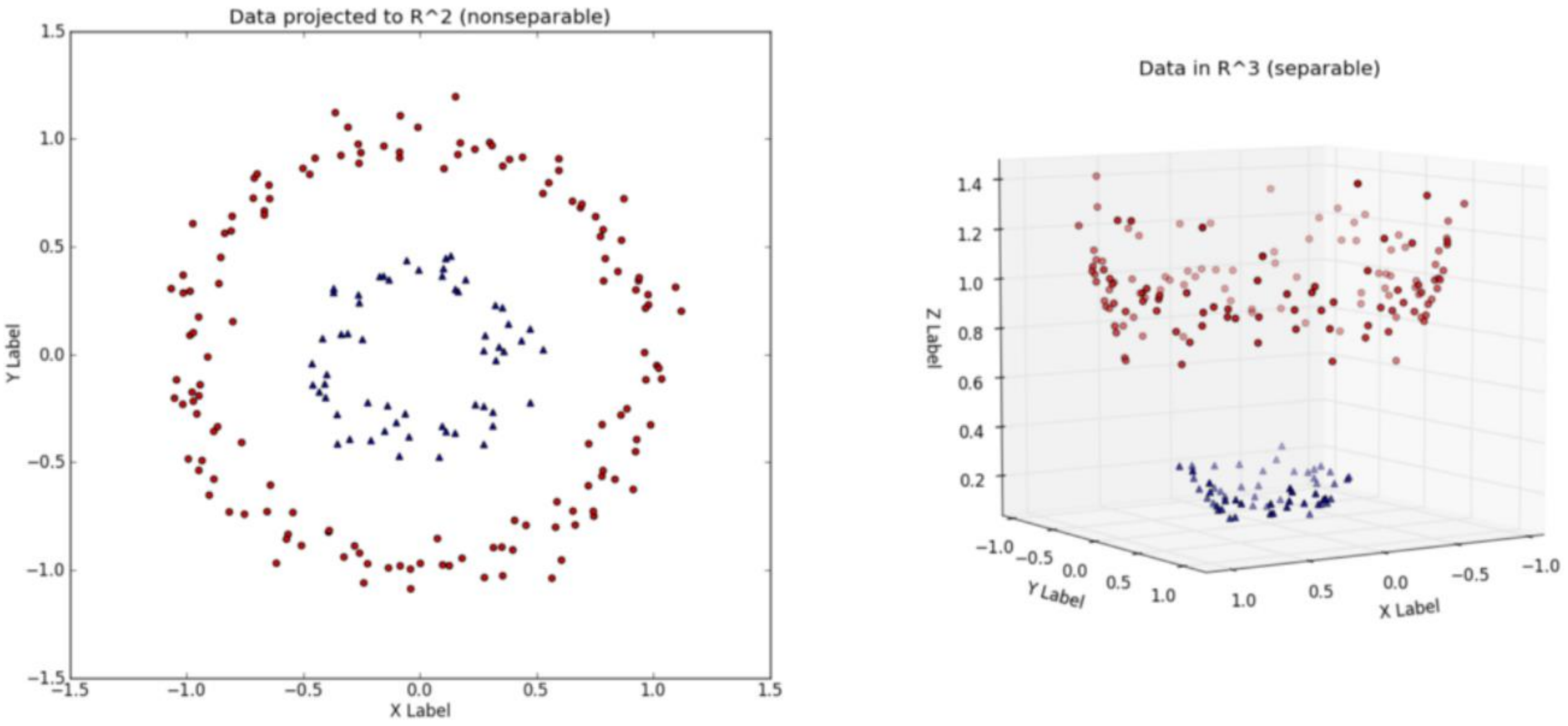
  - Subject to:

$$y_i(\vec{w} \bullet \vec{x}_i + b) \geq 1 - \xi_i, \text{for all } (\vec{x}_i, y_i) \text{ in D}$$

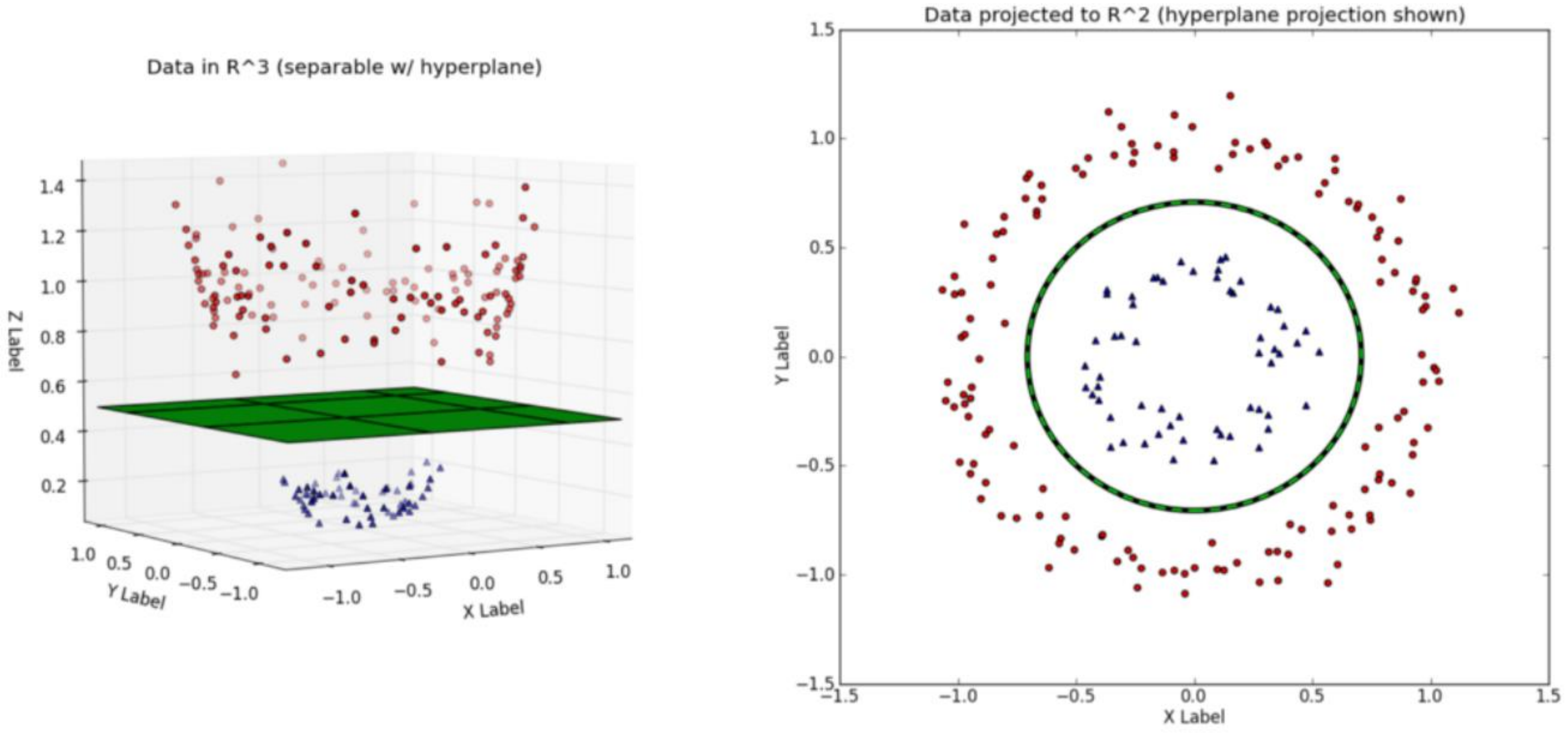
Support Vector Machines

- What if decision boundary is not linear?





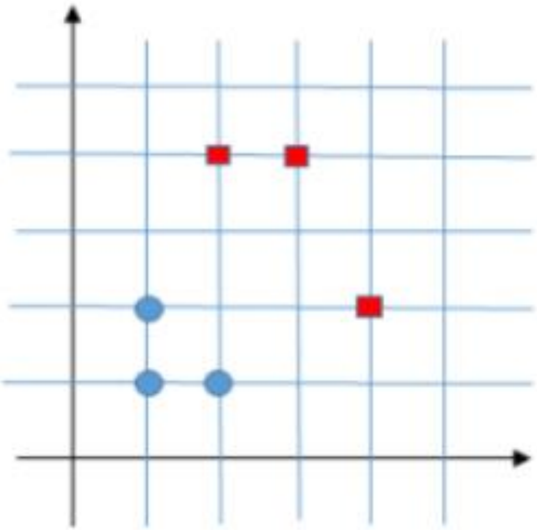
A nonseparable dataset in a two-dimensional space R^2, and the same dataset mapped onto threedimensions with the third dimension being x^2+y^2 (source: http://www.eric-kim.net/eric-kim-net/posts/1/kernel_trick.html)



The decision boundary is shown in green, first in the three-dimensional space (left), then back in the two-dimensional space (right). Same source as previous image.

예제 7.3-1

그림과 같이 2차원 공간상에 두 개의 클래스에 해당하는 점집합이 주어졌다. 사각형 클래스는 $y_i = 1$, 원형 클래스는 $y_i = -1$이라고 두고서 퍼셉트론의 이중적 표현에 의한 학습을 두 epoch 동안 반복하여 보아라. 그리고, Support Vector의 지점을 구하고, 이를 근거로 SVM에 의한 구분자를 구하여라.



내적	$\boldsymbol{x}_1$	$\boldsymbol{x}_2$	$\boldsymbol{x}_3$	$\boldsymbol{x}_4$	$\boldsymbol{x}_5$	$\boldsymbol{x}_6$
$\boldsymbol{x}_1$	20	6	22	10	16	8
$\boldsymbol{x}_2$	6	2	7	3	6	3
$\boldsymbol{x}_3$	22	7	25	11	20	10
$\boldsymbol{x}_4$	10	3	11	5	81	4
$\boldsymbol{x}_5$	16	6	20	8	20	10
$\boldsymbol{x}_6$	8	3	10	4	10	5

7.4. Application of SVM [Suh-Yeon Dong, et al. 2016]

Objective: Discriminate agreement and disagreement to the given self-relevant sentence in the single-trial level.

- **Stimuli:** 74 Korean sentences from the Minnesota Multiphasic Personality inventory-II (MMPI-II). Sentence contents are related to personal experience.
- **Presentation:** Considering the Subject-object-verb (SOV) typology of the Korean language, each sentence was separated into two parts: the verb (sentence ending) and the remainder of the sentence (contents).

(a) Positive ending	**Contents**	**Sentence ending**
Stimulus sentence (Korean)	돈에 대해 걱정한 적이	있다
English translations in SOV form	The experience of worrying over money	Does exist
Original English MMPI-2 sentence	I worry a great deal over money.	
(b) Negative ending	**Contents**	**Sentence ending**
Stimulus sentence (Korean)	기절한 적이	없다
English translations in SOV form	The experience of having a fainting spell	Does not exist
Original English MMPI-2 sentence	I have never had a fainting spell.	

Experiment Design

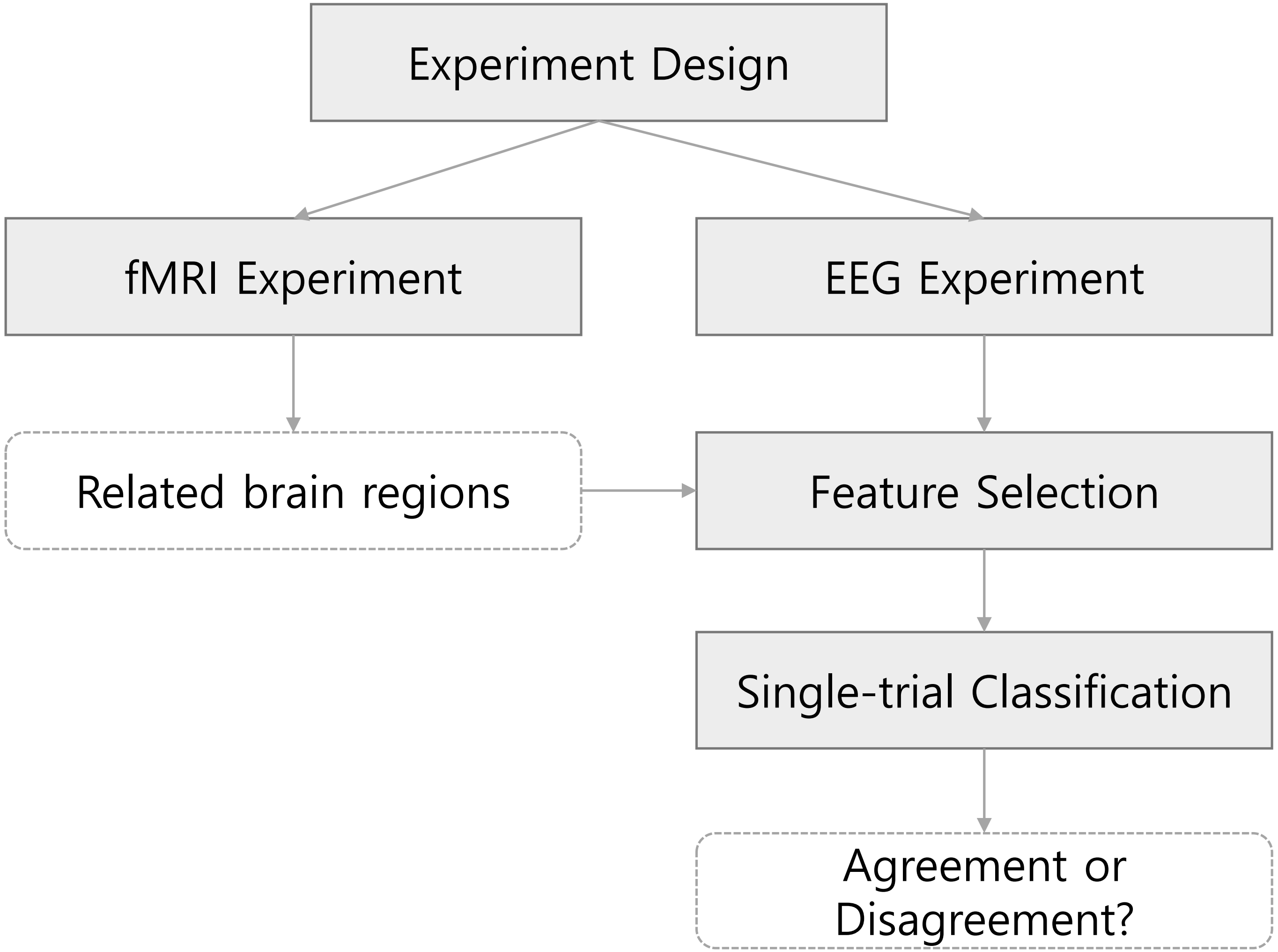
Objective: Discriminate agreement and disagreement to the given self-relevant sentence in the single-trial level.

- The relationship between “yes/no” and “agree/disagree” in Korean.

예) 가족과 말다툼한 적이 있다/없다.
The experience of having quarrels with members of my family does/does not exist.

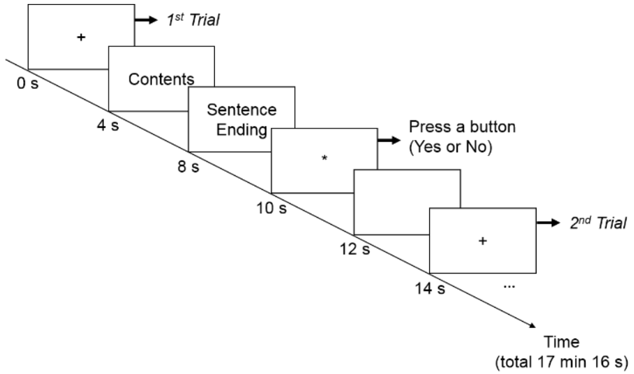
Example sentence		User response	
		User with experience	User without experience
The experience of having quarrels with members of my family (가족과 말다툼한 적이)	Does exist (있다)	Yes	No
	Does not exist (없다)	No	Yes
Categorization for the classification		**Agree**	**Disagree**

Experiment Procedure



Experiment Procedure

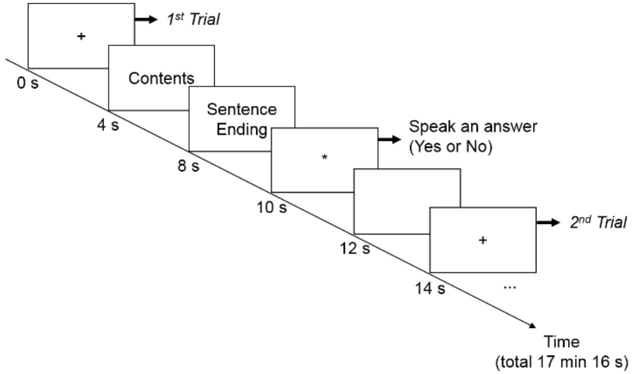
- **fMRI Experiment (19 subjects)**



- **Image acquisition**
  - 3T MR scanner (Siemens Magnetom Vero, Germany)
  - MR-compatible goggle (NordicNeuroLab Visual systmes, Norway)
  - Gradient-echo echo-planar imaging (EPI) sequence (36 slices; thickness = 4 mm; no gap between slices; FOV = 220 × 220 mm; matrix = 64 × 64; TE = 28 ms; TR = 2.0 s; flip angle = 90 °; voxel size 3.4 mm × 3.4 mm × 4 mm)

- **Preprocessing**
  - (SPM8) Realign, coregister, segmentation, normalize, and smooth [11]

- **EEG Experiment (9 subjects)**

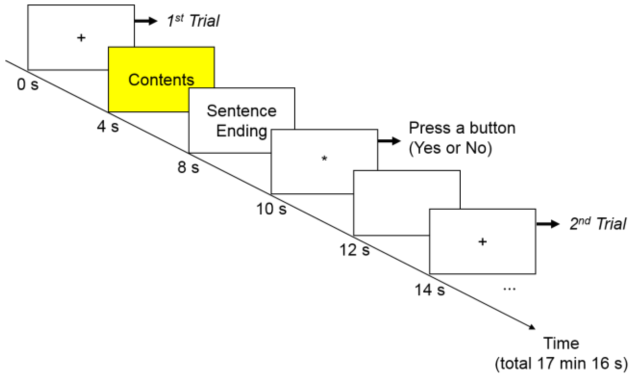


- **Data acquisition**
  - BrainAmp system (Brain Products GmbH, Germany)
  - 32-channel EEG cap (BrainCap)
  - Eyetracker x120 (Tobii Technology, Sweden)

- **Preprocessing**
  - 60Hz notch filtering and 1Hz high-pass filtering
  - Offline re-referencing to average (except EOG and ECG) [12]
  - Artifact Removal: EOG and ECG-related independent components
  - Trial rejection: Reject trials whose absolute amplitude is over 70 μV

fMRI Data Analysis

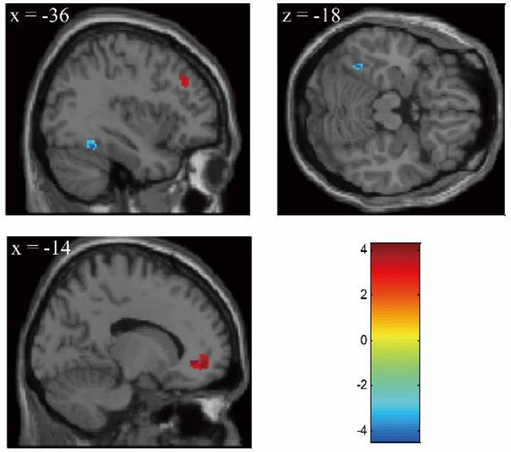
- **Activation during reading 'contents'**



- **Activated regions and their functions**

- Agree>disagree: Dorsolateral prefrontal cortex (BA 9), anterior cingulate (BA32)
  -> decision-making
  -> self-descriptive trait judgment, and empathic judgments[14]

- Disagree>agree: Left fusiform gyrus
  -> written word recognition[16][17]
  -> unfamiliar stimuli[18]



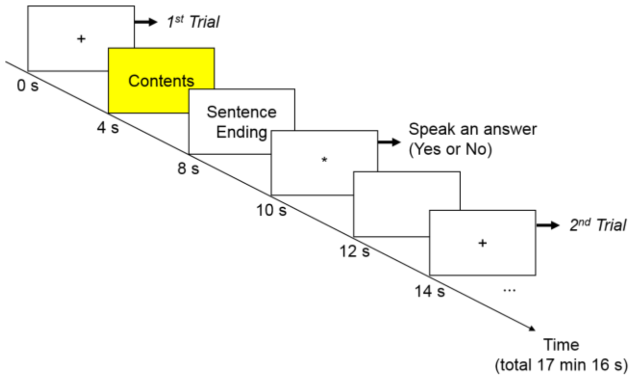
Peak coordinate region	Number of voxels	Peak intensity	Peak MNI Coordinate X	y	z
(A) Agree > Disagree					
L Superior frontal gyrus	43	4.2654	-38	34	36
L Anterior cingulate	105	4.1851	-14	48	-6
R Anterior cingulate	30	3.8177	4	40	8
R Cingulate gyrus	53	3.7786	12	4	30
R Paracentral lobule	50	3.6175	8	-38	76
R Supplementary motor area	36	3.5777	2	-20	68
L Postcentral gyrus	35	3.3399	-32	-46	70
R Paracentral lobule	24	3.2484	12	-36	52
(B) Disagree > Agree					
L Fusiform gyrus	28	4.414	-36	-50	-18

Notes. Contrasts were thresholded at an uncorrected p-value 0.005, corresponding to a t-statistic of 2.8784 and cluster size of 20 voxels. L = left. R = right

EEG Data Analysis

- Referring to the fMRI results, responses at frontal channels are considered.

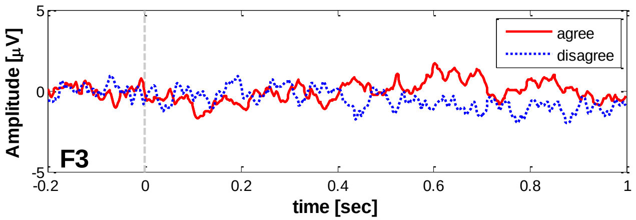
- **EEG patterns during reading ‘contents’**

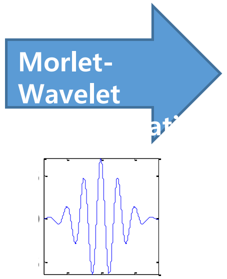


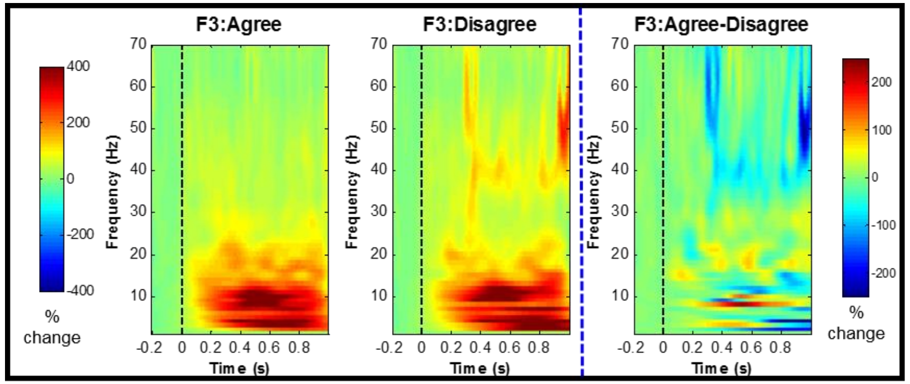
- **Oscillatory responses in sentence processing**
  - Grammatical or semantic violation affects EEG oscillatory responses.[3]-[7] -> *disagreement*
  - Gamma: increase at frontocentral
  - Theta: increase at frontal midline and temporo-parietal

- **Time-frequency Representations (TFRs)**

Event-related potential





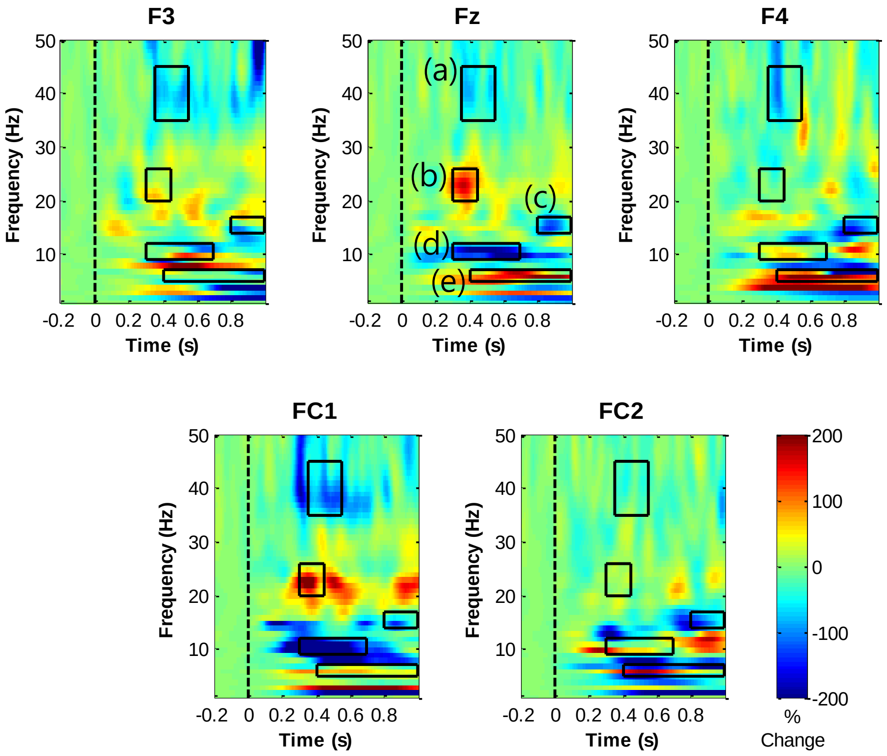


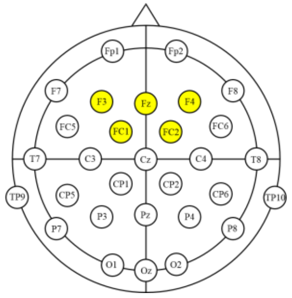
Feature Selection

- Referring to the fMRI results, responses at frontal channels are considered.

▪ **Time-frequency Representations (TFRs)**

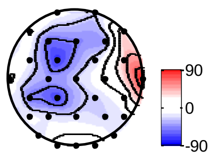
Average TFR difference: Agree - Disagree



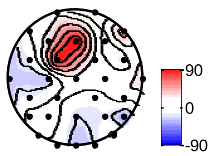


Select 5 feature candidates
(a) gamma 35-45Hz 350-550ms
(b) beta2 20-26Hz 300-450ms
(c) beta1 14-17Hz 800-1,000ms
(d) alpha 9-12Hz 300-700ms
(e) theta 5-7Hz 400-1,000ms

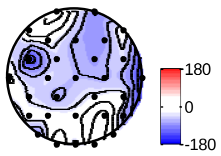
(a) Gamma 35-45Hz 350-550ms



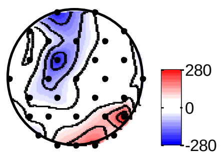
(b) Beta2 20-26Hz 300-450



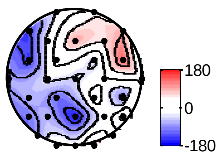
(c) Beta1 14-17Hz 800-1,000ms



(d) Alpha 9-12Hz 300-700n

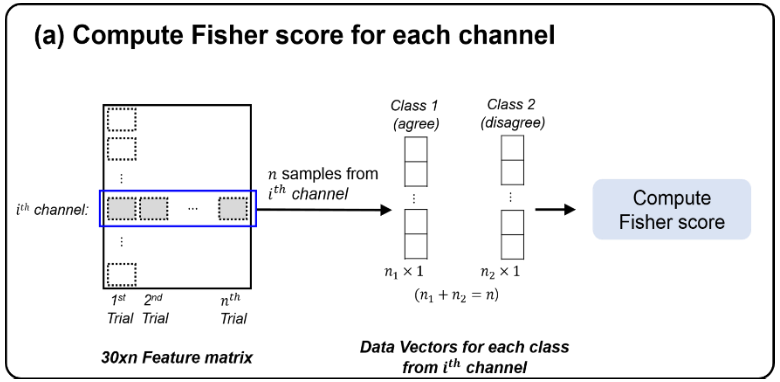


(e) Theta 5-7Hz 400-1,000ms



Channel Selection

- Channel selection using the Fisher score



The Fisher score for the i^{th} channel: [19]

$$F_i = \frac{\sum_{k=1}^{c} n_k \left(\mu_k^i - \mu^i\right)^2}{\sum_{k=1}^{c} n_k \left(\sigma_k^i\right)^2}$$

n_k: sample size of k^{th} class
μ_k^i: mean of k^{th} class in the i^{th} channel
σ_k^i: std of k^{th} class in the i^{th} channel
μ^i: mean of entire data in the i^{th} channel
c: Total number of classes (here, c = 2)

Rank	Theta		Alpha		Beta1		Beta2		Gamma	
	Channel	Fisher score	Channel	Fisher score	Channel	Fisher score	Channel	Fisher score	Channel	Fisher score
1	C3	0.028	C3	0.028	P7	0.034	C3	0.030	F3	0.040
2	CP5	0.027	Fz	0.027	T8	0.026	CP5	0.029	T8	0.030
3	CP2	0.025	CP1	0.026	F4	0.022	FC1	0.026	FC5	0.027
4	P7	0.025	FC1	0.025	FC1	0.022	Fp2	0.025	FC2	0.024
5	P3	0.023	F4	0.025	F3	0.020	Fp1	0.025	CP5	0.023

Classification

- Subject-dependent classification with increasing the number of selected channels
- Average accuracy using 5-fold cross validation
- SVM classifier with linear and RBF kernels (LIBSVM)

Component	Classifier	
	Linear SVM	**RBF SVM**
Theta	67.03% (30)	70.89% (2)
Alpha	66.39% (30)	73.86% (4)
Beta1	62.88% (30)	71.30% (4)
Beta2	65.07% (30)	73.49% (3)
Gamma	67.01% (20)	**75.54% (5)**