Machine Learning

Contents

7.1. Characteristics of Support Vector Machine

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

- **Linear Separator**

$$g(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + w_0 \qquad L = \{\boldsymbol{w}^T\boldsymbol{x} + w_0 = 0\}$$

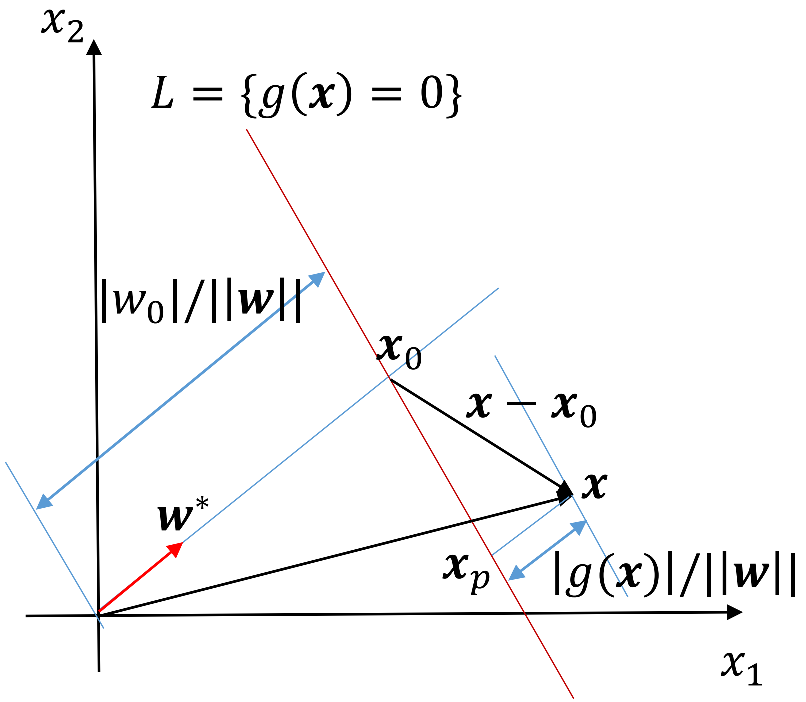
  - For any two points $x_1, x_2 \in L$

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

  - Define unit normal vector $\boldsymbol{w}^* = \boldsymbol{w}/||\boldsymbol{w}||$
  - For any point $x_0 \in L$, $\boldsymbol{w}^T\boldsymbol{x}_0 = -w_0$
  - Distance of any x to L, $\boldsymbol{w}^{*T}(\boldsymbol{x} - \boldsymbol{x}_0) = \dfrac{\boldsymbol{w}^T\boldsymbol{x} + w_0}{||\boldsymbol{w}||}$
  - The geometric margin of example $< \boldsymbol{x}_i, y_i >$ with respect to the hyperplane

$$y_i \frac{\boldsymbol{w}^T\boldsymbol{x} + w_0}{||\boldsymbol{w}||}, \quad y_i \in \{-1, +1\}$$

  - A point is misclassified iff its margin is negative



Perceptron Learning Algorithm

- To minimize

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

- Gradient

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

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.

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

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 Algorithm: Dual Representation

- α_i : a count of the number of times that example i was misclassified
- Initial weights are all zeros
- Then, final weights are

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

- The output of linear predictor is

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

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.

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

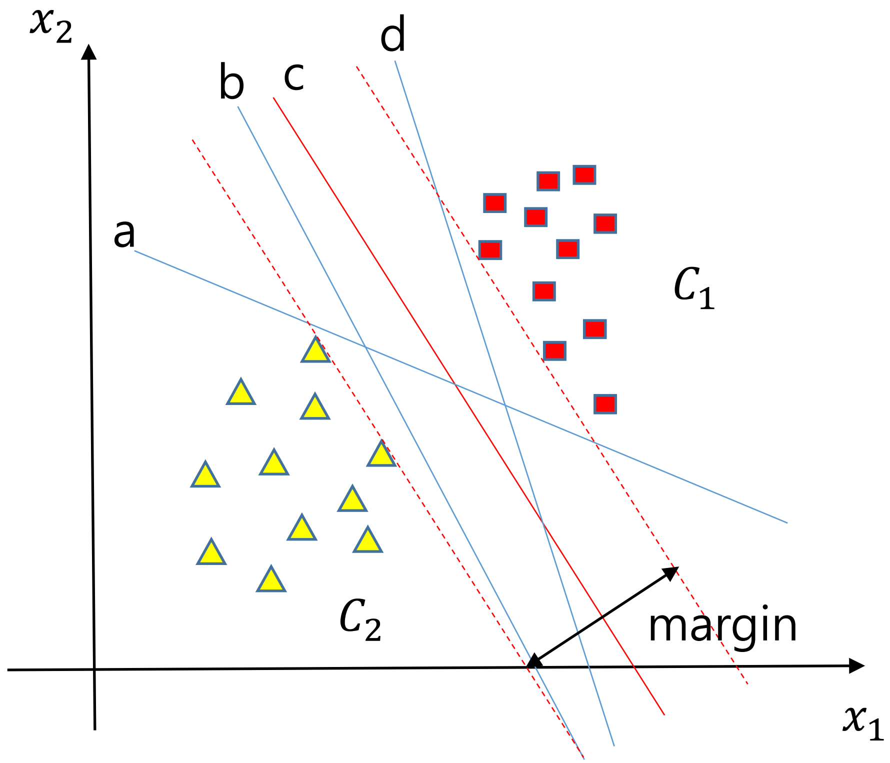
$$\boldsymbol{w} = \sum_{i=1}^{n} \alpha_i y_i \boldsymbol{x}_i \quad \text{and} \quad w_0 = \sum_{i=1}^{n} \alpha_i y_i$$

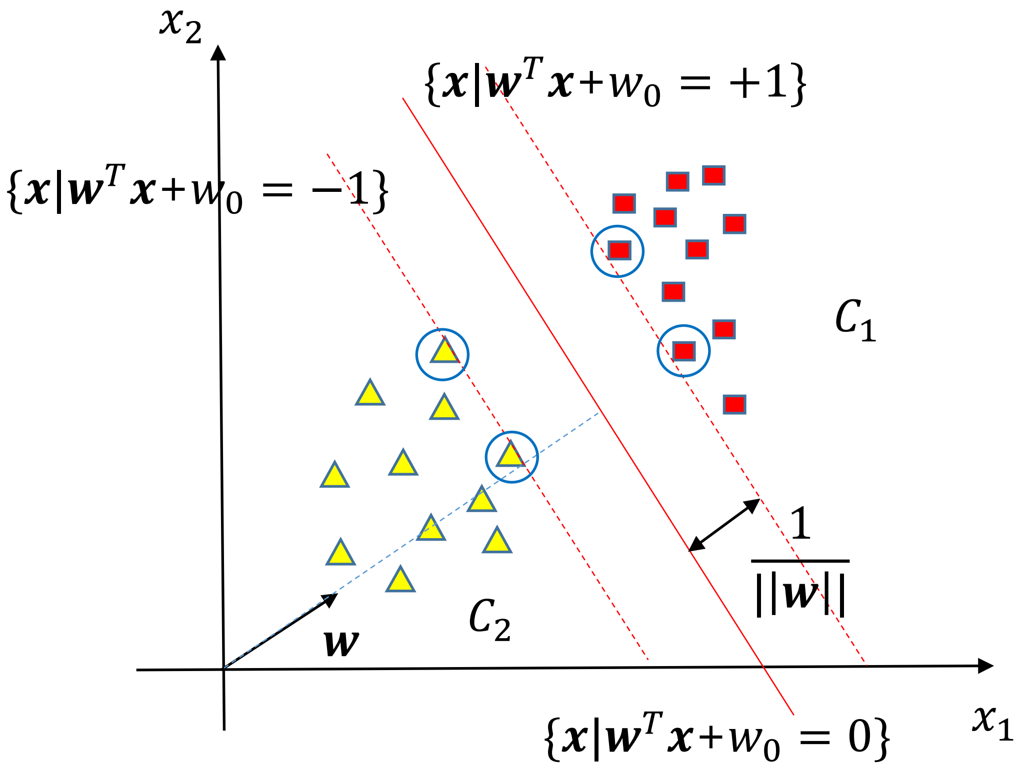
③ 오인식된 학습패턴이 있으면 과정 ②를 다시 수행한다.

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

7.3. Support Vector Machine

- Maximizing the margin
- The decision boundary: determined by a subset of the data points, known as support vectors (indicated by the circles).





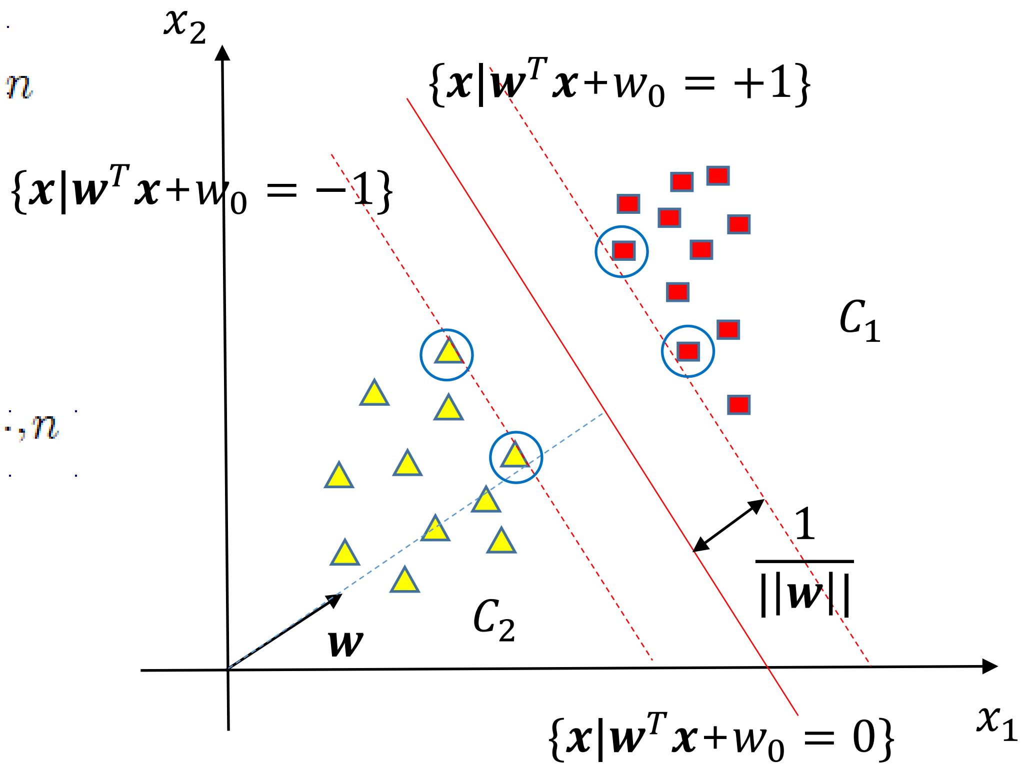
Support Vector Machine

- **Support vector machines**
  - Names a whole family of algorithms of the **maximum margin separator**. The idea is to find the separator with the maximum margin from all the data points.
- Optimization problem

$$\max_{w_0,\boldsymbol{w}} C \quad \text{subject to} \quad \frac{1}{\|\boldsymbol{w}\|} y_i(\boldsymbol{w}^T\boldsymbol{x}_i + w_0) \geq C \quad i = 1,2,..,n$$

- Set $\|\boldsymbol{w}\|$ to $1/C$

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



Support Vector Machine: Formulation

- **Quadratic optimization problem**

$$\min_{w_0,\boldsymbol{w}} \frac{1}{2}(\|\boldsymbol{w}\|)^2 \quad \text{subject to} \quad y_i(\boldsymbol{w}^T\boldsymbol{x}_i + w_0) \geq 1 \;\; i = 1,2,\cdots,n$$

- Lagrangian formulation of constrained optimization

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

- Kuhn-Tucker Theorem $\min_{w_0,\boldsymbol{w}} \max_{\alpha \geq \mathbf{0}} L(w_0,\boldsymbol{w},\alpha) = \max_{\alpha \geq \mathbf{0}} \min_{w_0,\boldsymbol{w}} L(w_0,\boldsymbol{w},\alpha)$

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

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

Support Vector Machine: Formulation & Solution

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

$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

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

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

$$\text{Maximize } L(\alpha) \text{ subject to } \boldsymbol{\alpha} \geq \boldsymbol{0} \text{ and } \sum_i \alpha_i y_i = 0$$

Finding optimal α_i : computationally tractable quadratic programming problem

Support Vector: points with margin=1

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

Support Vector Machines

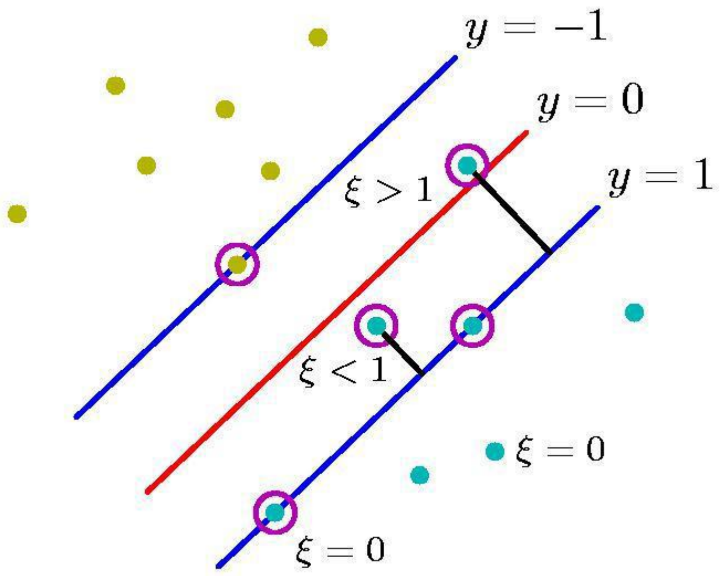
- What if the problem is not linearly separable?

- Introduce slack variables
  - Need to minimize:

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

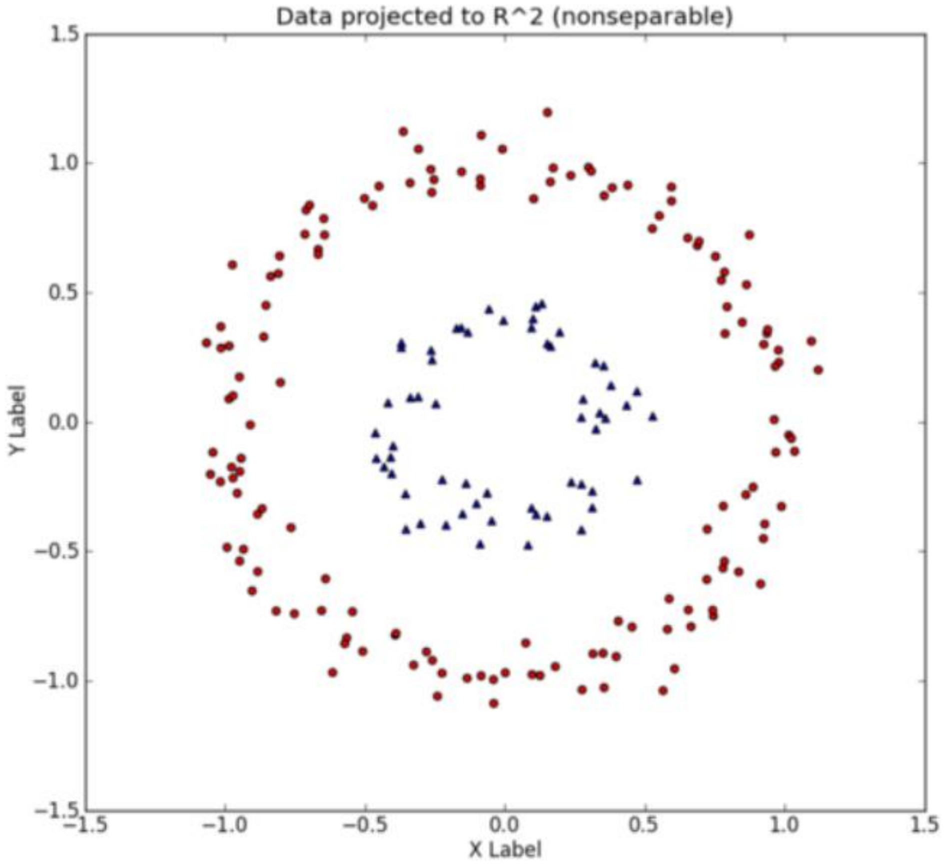
  - Subject to:

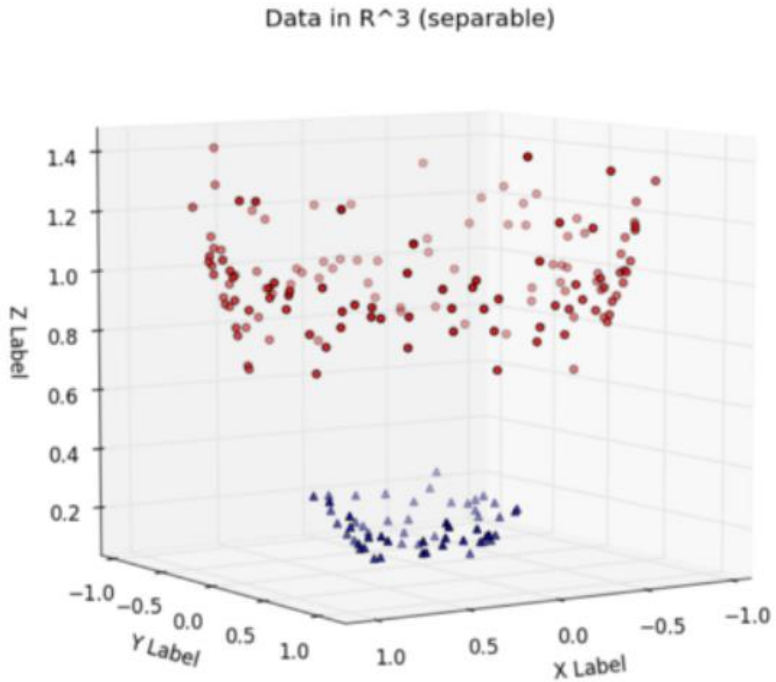
$$y_i(\vec{w} \bullet \vec{x}_i + b) \geq 1 - \xi_i, \text{ for all } (\vec{x}_i, y_i) \text{ in D}$$



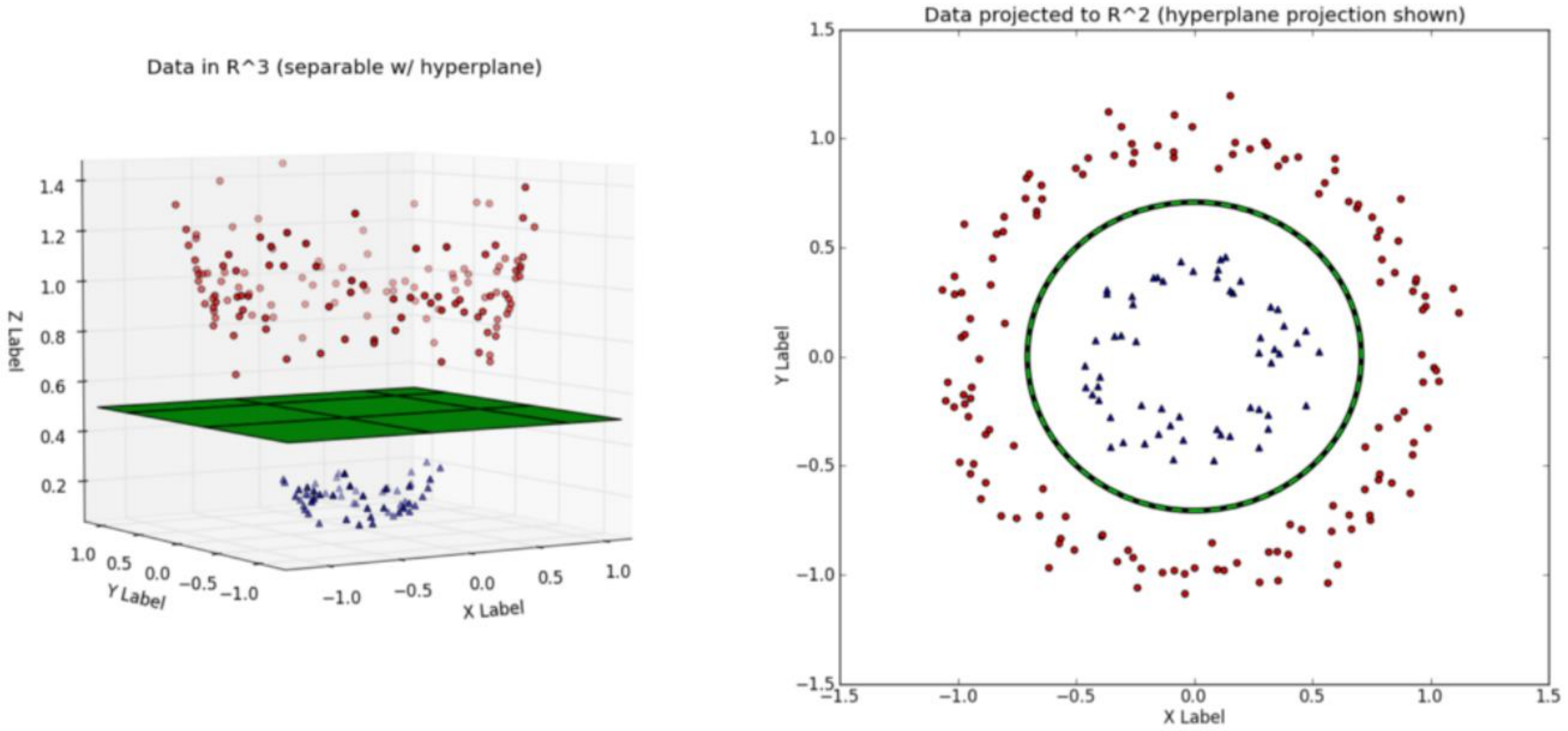
Support Vector Machines

- What if decision boundary is not linear?





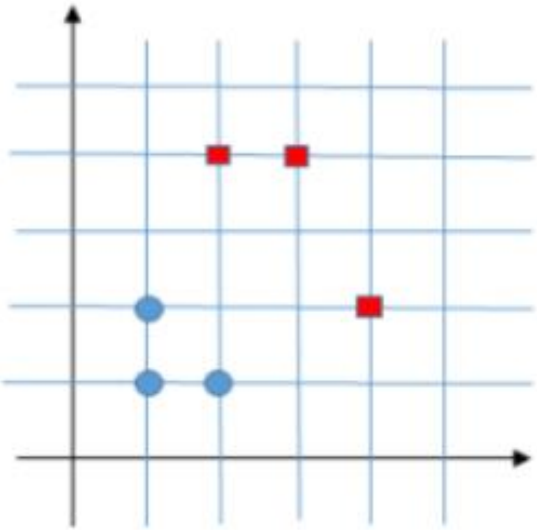
A nonseparable dataset in a two-dimensional space R^2, and the same dataset mapped onto threedimensions with the third dimension being x^2+y^2 (source: http://www.eric-kim.net/eric-kim-net/posts/1/kernel_trick.html)



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

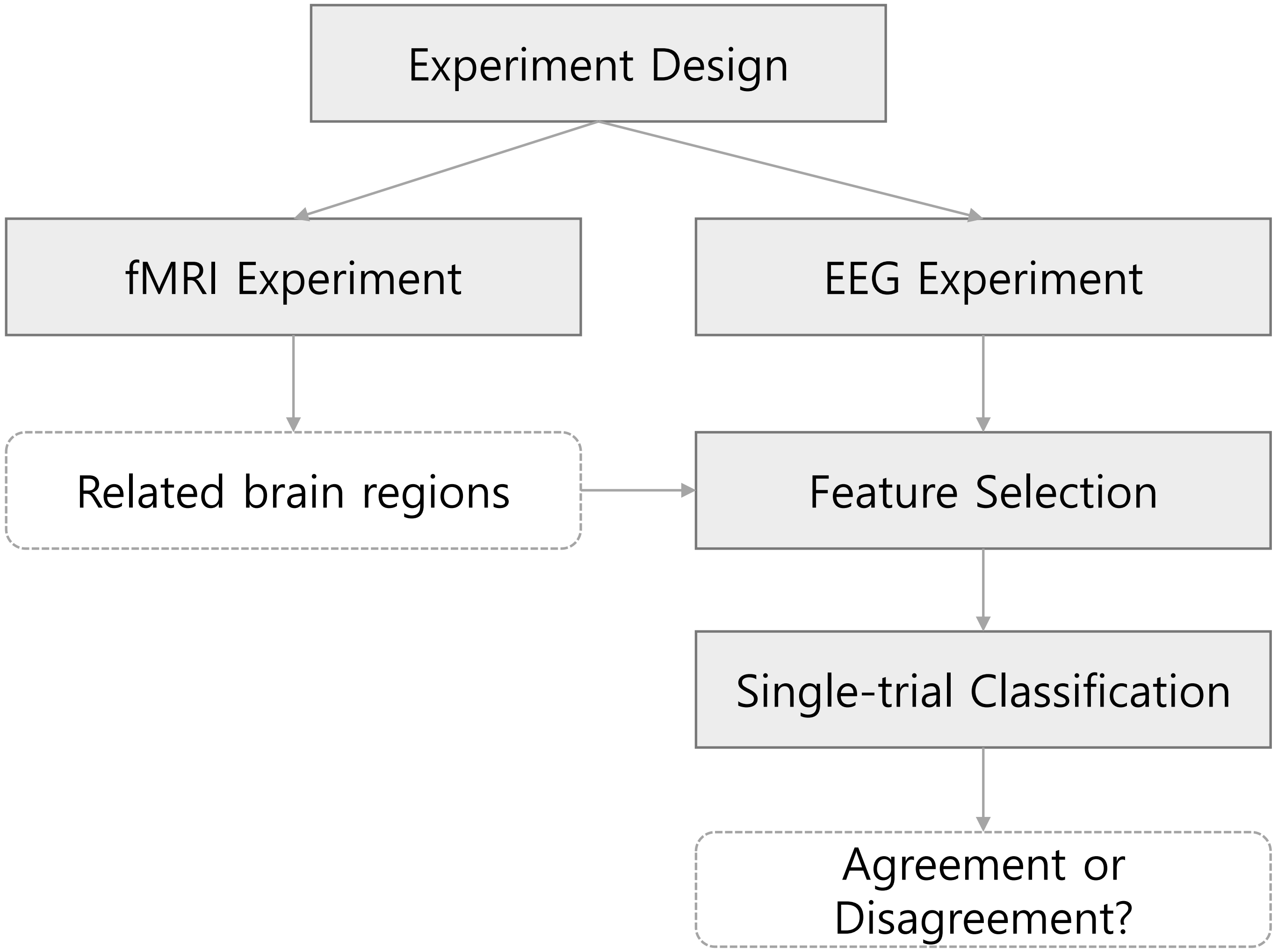
7.4. Application of SVM[10] [Suh-Yeon Dong, et al. 2016]

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).

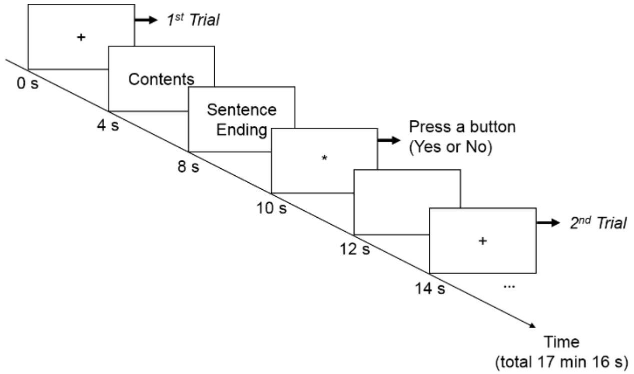
(a) Positive ending	Contents	Sentence ending
Stimulus sentence (Korean)	돈에 대해 걱정한 적이	있다
English translations in SOV form	The experience of worrying over mon ey	Does exist
Original English MMPI-2 sentence	I worry a great deal over money.	
(b) Negative ending	**Contents**	**Sentence ending**
Stimulus sentence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

Experiment Procedure



Experiment Procedure

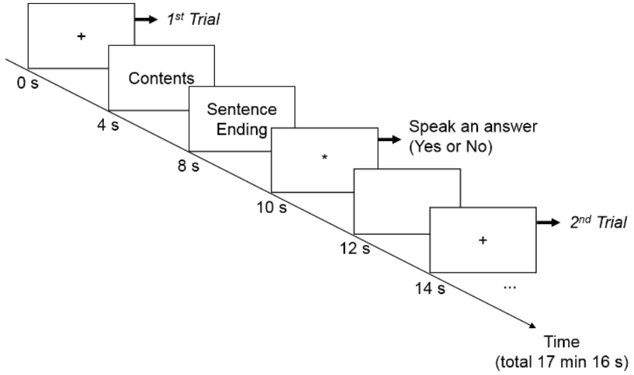
- **fMRI Experiment (19 subjects)**



- **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 [1]

- **EEG Experiment (9 subjects)**



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

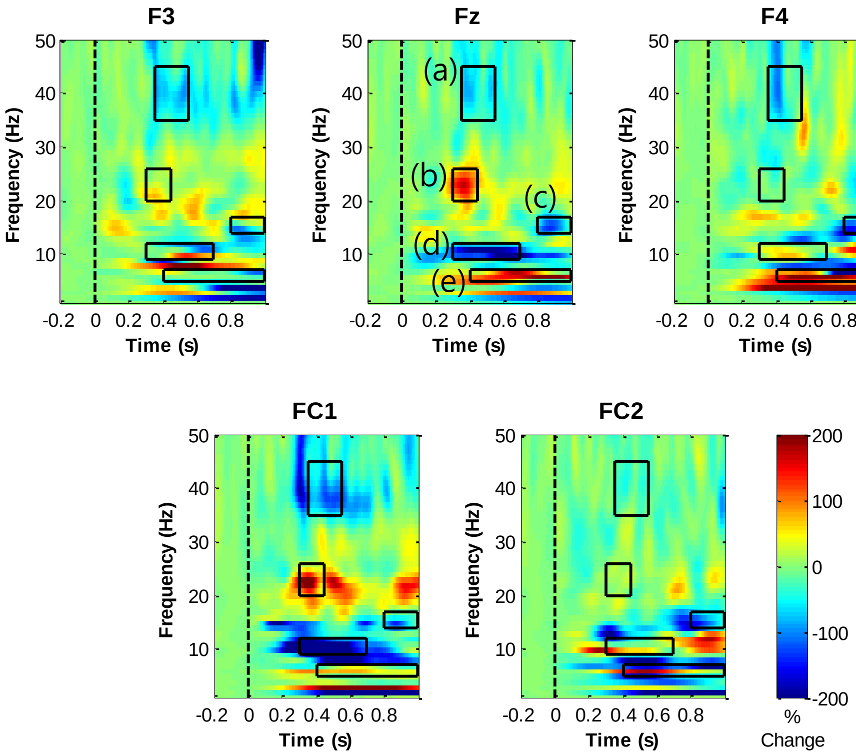
- **Preprocessing**
- 60Hz notch filtering and 1Hz high-pass filtering
- Offline re-referencing to average (except EOG and ECG) [2]
- Artifact Removal: EOG and ECG-related independent components
- Trial rejection: Reject trials whose absolute amplitude is over 70 μV

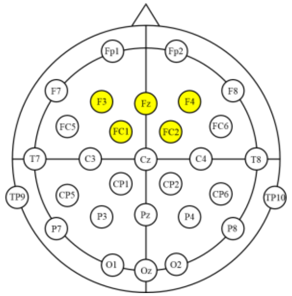
Feature Selection

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

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

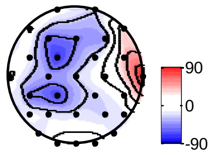
Average TFR difference: Agree - Disagree



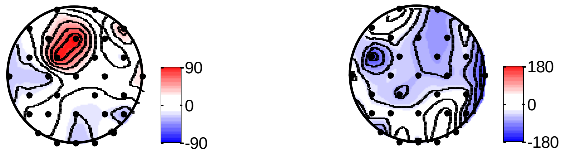


Select 5 feature candidates
(a) gamma 35-45Hz 350-550ms
(b) beta2 20-26Hz 300-450ms
(c) beta1 14-17Hz 800-1,000ms
(d) alpha 9-12Hz 300-700ms
(e) theta 5-7Hz 400-1,000ms

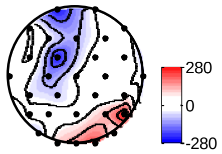
(a) Gamma 35-45Hz 350-550ms

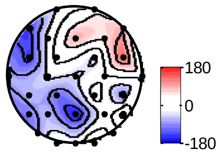


(b) Beta2 20-26Hz 300-450 (c) Beta1 14-17Hz 800-1,000ms



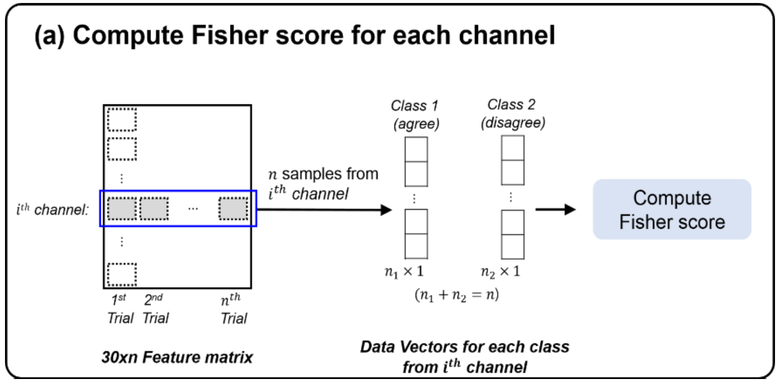
(d) Alpha 9-12Hz 300-700n (e) Theta 5-7Hz 400-1,000ms

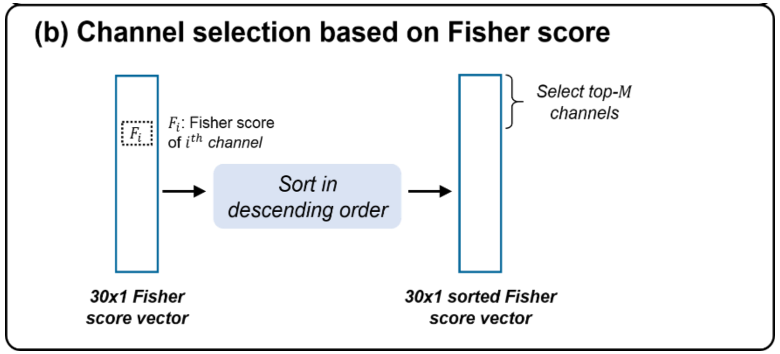




Channel Selection

- 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)**