Lecture 12: Support Vector Machine II

[SCS4049-02] Machine Learning and Data Science

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Tentative schedule

week	topic	date (수 / 월)
1	Machine Learning Introduction & Basic Mathematics	09.02 / 09.07
2	Python Practice I & Regression	09.09 / 09.14
3	AI Department Seminar I & Clustering I	09.16 / 09.21
4	Clustering II & Classification I	09.23 / 09.28
5	Classification II	(추석) / 10.05
6	Python Practice II & Support Vector Machine I	10.07 / 10.12
7	Support Vector Machine II & Ensemble Learning and Random Forest	10.14 / 10.19
8	(휴강) & **Mid-term exam**	10.21 / **10.26**
9	Neural networks	10.28 / 11.02
10	Backpropagation	11.04 / 11.09
11	Convolutional Neural Network	11.11 / 11.16
12	Model Optimization	11.18 / 11.23
13	Recurrent Neural network	11.25 / 11.30
14	Autoencoders	12.02 / 12.07
15	**Final exam**	(휴강) / **12.14**

Mid-term exam: 비대면

수업시간

- 일시: 10월 26일 (월), 10:00 – 12:00 (2시간, 연장 없음)
- 장소: 비대면 webex (수업 미팅룸)
- 범위
  - 시험 전까지의 모든 강의 ~ 다음주 월요일 수업까지, 수요일 휴강(보강??) 공지할게요.
  - 강의자료, 수업필기, 강의내용, 숙제 등 전부다.
- 방식: 서술형 위주, closed book +단답
  ※ 프로그래밍은 범위에 포함되지 않음
- 준비물
  - webex용 카메라 (웹캠, 노트북, 휴대폰 등)
  - 답안용 A4 용지
  - 스마트폰 스캔앱 (Adobe Scan 등)
  - 카메라, 스마트폰, A4 용지가 필요한 경우 교수에게 문의 (s.park@dgu.edu)

Mid-term exam: 비대면

- 응시 방법
  - 책상, 손, 얼굴이 나오도록 카메라를 설치
  - 모든 수강생이 확인된 후, eclass로 시험지 배포
  - 답안지 첫 페이지: 학번, 학과, 이름, 총 페이지 수를 반드시 기입
  - 답안지 각 페이지: 해당 페이지 수를 반드시 기입
- 제출 방법
  - 시험 종료까지 미팅룸을 먼저 나갈 수 없음
  - 시험시간 종료 후 본인이 작성한 모든 답지를 카메라에 차례로 보여줌
  - 스캔앱으로 답지를 스캔하여 pdf 파일을 메일로 제출 (s.park@dgu.edu)
  - 10월 30일 (금)까지 만해관 210호로 답안지 실물 제출
- 문의 사항: 담당 교수 박성식
  - 이메일: s.park@dgu.edu
  - 사무실: 만해관 210호
  - 전화: 02) 2260-3784

Hard margin SVM: Theory

Maximum margin classifier

We begin our discussion of support vector machines to the two-class classification problem using linear models of the form

$$y(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b \tag{1}$$

where $\phi(\mathbf{x})$ denotes a fixed feature-space transformation, and we have made the bias parameter b explicit.

The training data set comprises N input vectors $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N$, with corresponding target values $t_1, t_2, ..., t_N$ where $t_n \in \{-1, 1\}$, and new data points $\mathbf{x}$ are classified according to the sign of $y(\mathbf{x})$

Maximum margin classifier

We shall assume that the training data set is linearly separable in feature space, so that by definition there exists at least one choice of the parameters $\mathbf{w}$ and b such that a function satisfies $y(\mathbf{x}_n) > 0$ for points having $t_n = +1$ and $y(\mathbf{x}_n) < 0$ for points having $t_n = -1$, so that $t_n y(\mathbf{x}_n) > 0$ for all training data points.

Maximum margin classifier: optimality criterion

Thus the distance of a point $\mathbf{x}_n$ to the decision surface is given by

$$\frac{t_n y(\mathbf{x}_n)}{\|\mathbf{w}\|} = \frac{t_n(\mathbf{w}^T\phi(\mathbf{x}_n) + b)}{\|\mathbf{w}\|}. \tag{2}$$

The margin is given by the perpendicular distance to the closest point $\mathbf{x}_n$ from the data set, and we wish to optimize the parameters $\mathbf{w}$ and b in order to maximize this distance. Thus the maximum margin solution is found by solving

$$\arg\max_{\mathbf{w},b} \left\{ \frac{1}{\|\mathbf{w}\|} \min[t_n(\mathbf{w}^T\phi(\mathbf{x}_n) + b)] \right\} \tag{3}$$

where we have taken the factor $1/\|\mathbf{w}\|$ outside the optimization over n because $\mathbf{w}$ does not depend on n.

Dual problem for convex optimization

Primal optimization problem for hard SVM

$$\text{maximize} \quad \frac{1}{\|\mathbf{w}\|} \min[t_n(\mathbf{w}^T\phi(\mathbf{x}_n) + b)] \tag{4}$$

$$\text{subject to} \quad t_n(\mathbf{w}^T\phi(\mathbf{x}_n) + b) \geq 0 \tag{5}$$

$$\tag{6}$$

Equivalently,

$$\text{minimize} \quad \frac{1}{2}\|\mathbf{w}\|^2 \tag{7}$$

$$\text{subject to} \quad t_n(\mathbf{w}^T\phi(\mathbf{x}_n) + b) \geq 1 \tag{8}$$

Direct solution of this optimization problem would be very complex, so we shall convert it into an equivalent problem that is much easier to solve.

Lagrangian function with constraint

In order to solve this constrained optimization problem, we introduce Lagrange multipliers $a_n \geq 0$, with one multiplier a_n for each of the constraints, giving the Lagrangian function

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n\{t_n(\mathbf{w}^T\phi(\mathbf{x}_n) + b) - 1\} \tag{9}$$

where $\mathbf{a} = (a_1, ..., a_N)^T$. Note the minus sign in front of the Lagrange multiplier term, because we are minimizing with respect to $\mathbf{w}$ and b, and maximizing with respect to $\mathbf{a}$.

Setting the derivatives of $L(\mathbf{w}, b, \mathbf{a})$ with respect to $\mathbf{w}$ and b equal to zero, we obtain the following two conditions

$$\mathbf{w} = \sum_{n=1}^{N} a_n t_n \phi(\mathbf{x}_n) \tag{10}$$

$$0 = \sum_{n=1}^{N} a_n t_n \tag{11}$$

Lagrangian function with constraint

Eliminating $\mathbf{w}$ and b from $L(\mathbf{w}, b, \mathbf{a})$ using these conditions then gives the *dual representation* of the maximum margin problem in which we maximize

$$\tilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m) \tag{12}$$

with respect to $\mathbf{a}$ subject to the constraints

$$a_n \geq 0, \qquad n = 1, ..., N \tag{13}$$

$$\sum_{n=1}^{N} a_n t_n = 0. \tag{14}$$

Here the kernel function is defined by $k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T \phi(\mathbf{x}')$.

Prediction for a new sample: support vector machine

In order to classify new data points using the trained model, we evaluate the sign of $y(\mathbf{x})$. This can be expressed in terms of the parameter $\{a_n\}$ and the kernel function by substituting for $\mathbf{w}$ to give

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}, \mathbf{x}_n) + b \tag{15}$$

KKT condition: complementary slackness

We show that a constrained optimization of this form satisfies the *Karush-Kuhn-Tucker* (KKT) conditions, which in this case require that the following three properties hold

$$a_n \geq 0 \tag{16}$$

$$t_n y(\mathbf{x}_n) - 1 \geq 0 \tag{17}$$

$$a_n \{t_n y(\mathbf{x}_n) - 1\} = 0 \tag{18}$$

Thus for every data point, either $a_n = 0$ or $t_n y(\mathbf{x}_n) = 1$. Any data point for which $a_n = 0$ will not appear in the sum and hence plays no role in making predictions for new data points. The remaining data points are called *support vectors*, and because they satisfy $t_n y(\mathbf{x}_n) = 1$, they correspond to points that lie on the maximum margin hyperplanes in feature space.

KKT condition: complementary slackness

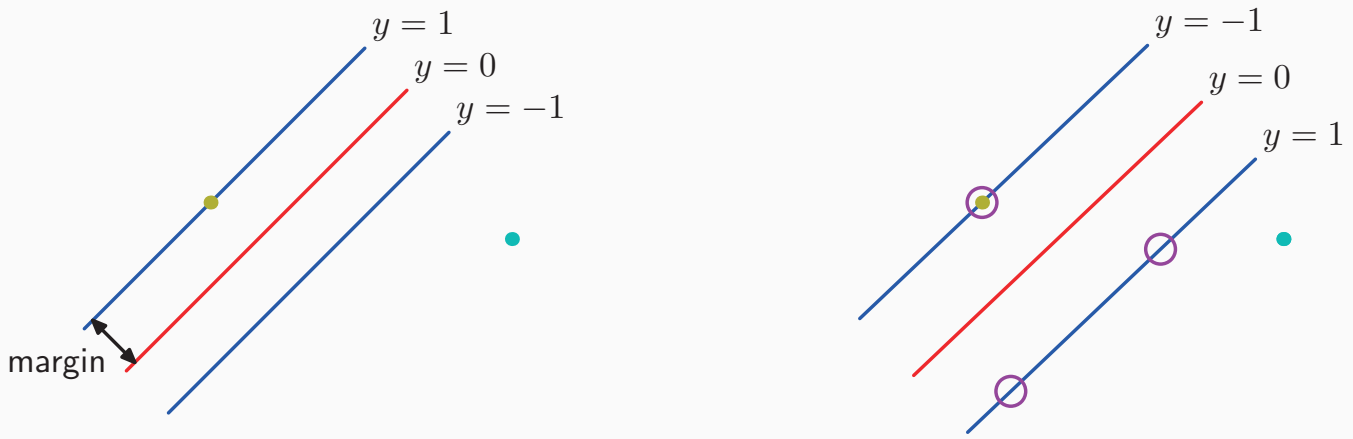
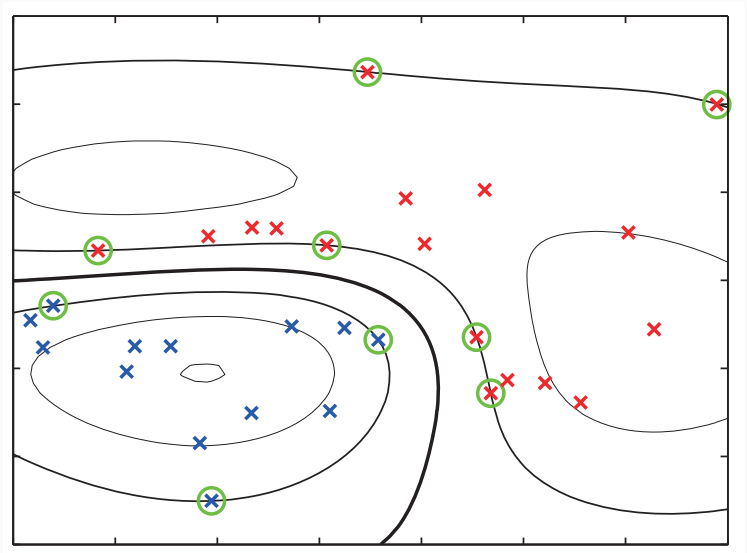


Figure 7.1 The margin is defined as the perpendicular distance between the decision boundary and the closest of the data points, as shown on the left figure. Maximizing the margin leads to a particular choice of decision boundary, as shown on the right. The location of this boundary is determined by a subset of the data points, known as support vectors, which are indicated by the circles.

KKT condition: complementary slackness

Figure 7.2 Example of synthetic data from two classes in two dimensions showing contours of constant $y(\mathbf{x})$ obtained from a support vector machine having a Gaussian kernel function. Also shown are the decision boundary, the margin boundaries, and the support vectors.



Soft margin SVM: Theory

Slack variables

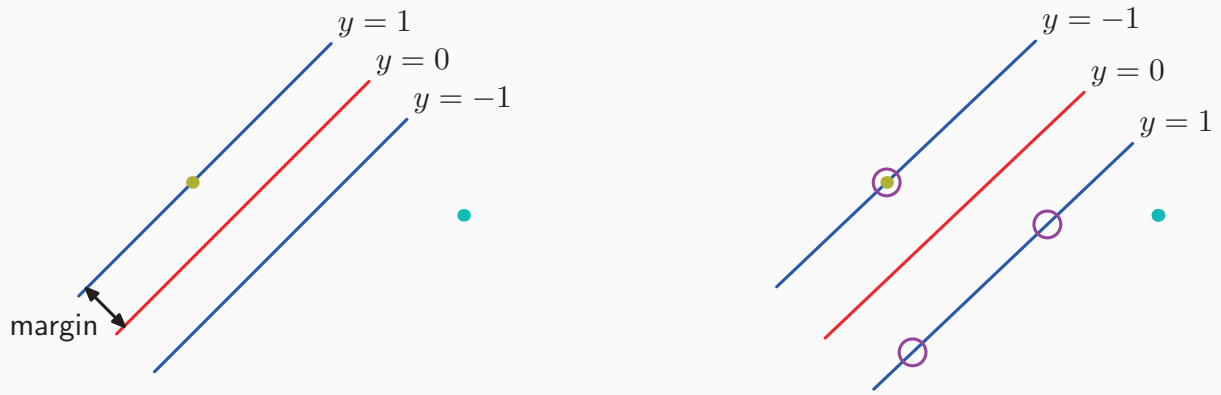
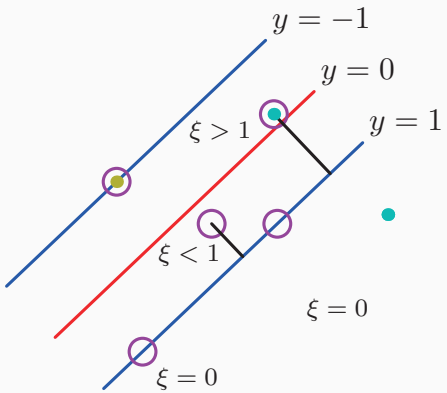


Figure 7.1 The margin is defined as the perpendicular distance between the decision boundary and the closest of the data points, as shown on the left figure. Maximizing the margin leads to a particular choice of decision boundary, as shown on the right. The location of this boundary is determined by a subset of the data points, known as support vectors, which are indicated by the circles.

Figure 7.3 Illustration of the slack variables $\xi_n \geqslant 0$. Data points with circles around them are support vectors.



Slack variables

So far, we have assumed that the training data points are linearly separable in the feature space $\phi(x)$. The resulting support vector machine will give exact separation of the training data in the original input space x, although the corresponding decision boundary will be nonlinear. In practice, however, the class-conditional distributions may overlap, in which case exact separation of the training data can lead to poor generalization.

We therefore need a way to modify the support vector machine so as to allow some of the training points to be misclassified.

Slack variables

We introduce *slack variables*, $\xi_n \geq 0$ where $n = 1, 2, ..., N$, with one slack variable for each training data point. These are defined by $\xi_n = 0$ for data points that are on or inside the correct margin boundary and $\xi_n = |t_n - y(\mathbf{x}_n)|$ for other points.

Thus a data point that is on the decision boundary $y(\mathbf{x}_n) = 0$ will have $\xi_n = 1$, and points with $\xi_n > 1$ will be misclassified.

The exact classification constraints are then replaced with

$$t_n y(\mathbf{x}_n) \geq 1 - \xi_n, \qquad n = 1, ..., N \tag{19}$$

in which the slack variables are constrained to satisfy $\xi_n \geq 0$.

Slack variables

Points for which $0 < \xi_n \leq 1$ lie inside the margin, but on the correct side of the decision boundary, and those data points for which $\xi_n > 1$ lie on the wrong side of the decision boundary and are misclassified. This is sometimes described as relaxing the hard margin constraint to give a *soft margin* and allows some of the training set data points to be misclassified.

Soft margin SVM

Our goal is to maximize the margin while softly penalizing points that lie on the wrong side of the margin boundary. We therefore

$$\text{minimize} \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n \tag{20}$$

$$\text{subject to} \quad t_n(\mathbf{w}^T\phi(\mathbf{x}_n) + b) \geq 1 - \xi_n \tag{21}$$

$$\xi_n \geq 0. \tag{22}$$

The parameter C is analogous to a regularization coefficient because it controls the trade-off between minimizing training errors and controlling model complexity.

FYI, hard margin SVM

$$\text{minimize} \quad \frac{1}{2}\|\mathbf{w}\|^2 \tag{23}$$

$$\text{subject to} \quad t_n(\mathbf{w}^T\phi(\mathbf{x}_n) + b) \geq 1 \tag{24}$$

Soft margin SVM: Lagrangian dual problem

The corresponding Lagrangian is given by

$$L(\mathbf{w}, b, \mathbf{a}, \mu_n) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n - \sum_{n=1}^{N} a_n\{t_n y(\mathbf{x}_n) - 1 + \xi_n\} - \sum_{n=1}^{N}\mu_n\xi_n \tag{25}$$

where $\{a_n \geq 0\}$ and $\{\mu_n \geq 0\}$ are Lagrangian multipliers. The corresponding set of KKT conditions are given by

$$a_n \geq 0 \tag{26}$$

$$t_n y(\mathbf{x}_n) - 1 + \xi_n \geq 0 \tag{27}$$

$$a_n(t_n y(\mathbf{x}_n) - 1 + \xi_n) = 0 \tag{28}$$

$$\mu_n \geq 0 \tag{29}$$

$$\xi_n \geq 0 \tag{30}$$

$$\mu_n\xi_n = 0 \tag{31}$$

where $n = 1, 2, ..., N$.

Soft margin SVM: Lagrangian dual problem

We now optimize out $\mathbf{w}$, b, and $\{\xi_n\}$ making use of the definition of $y(x)$ to give

$$\frac{\partial L}{\partial \mathbf{w}} = 0 \quad \Longrightarrow \quad \mathbf{w} = \sum_{n=1}^{N} a_n t_n \phi(\mathbf{x}_n) \tag{32}$$

$$\frac{\partial L}{\partial b} = 0 \quad \Longrightarrow \quad \sum_{n=1}^{N} a_n t_n = 0 \tag{33}$$

$$\frac{\partial L}{\partial \xi_n} = 0 \quad \Longrightarrow \quad a_n = C - \mu_n \tag{34}$$

We obtain the dual Lagrangian in the form

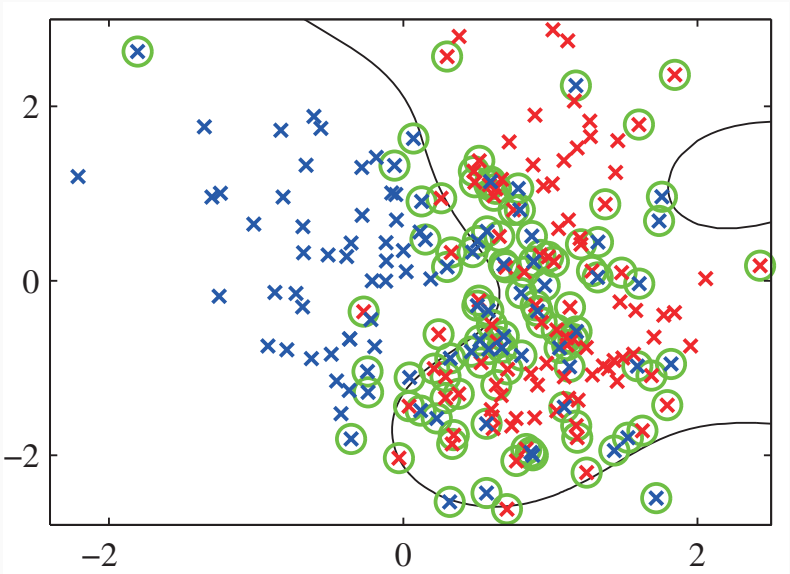
$$\text{maximize} \quad \tilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m) \tag{35}$$

$$\text{subject to} \quad 0 \geq a_n \geq C \tag{36}$$

$$\sum_{n=1}^{N} a_n t_n = 0 \tag{37}$$

Soft margin SVM

Figure 7.4 Illustration of the ν-SVM applied to a nonseparable data set in two dimensions. The support vectors are indicated by circles.



Kernel Method

Kernel method

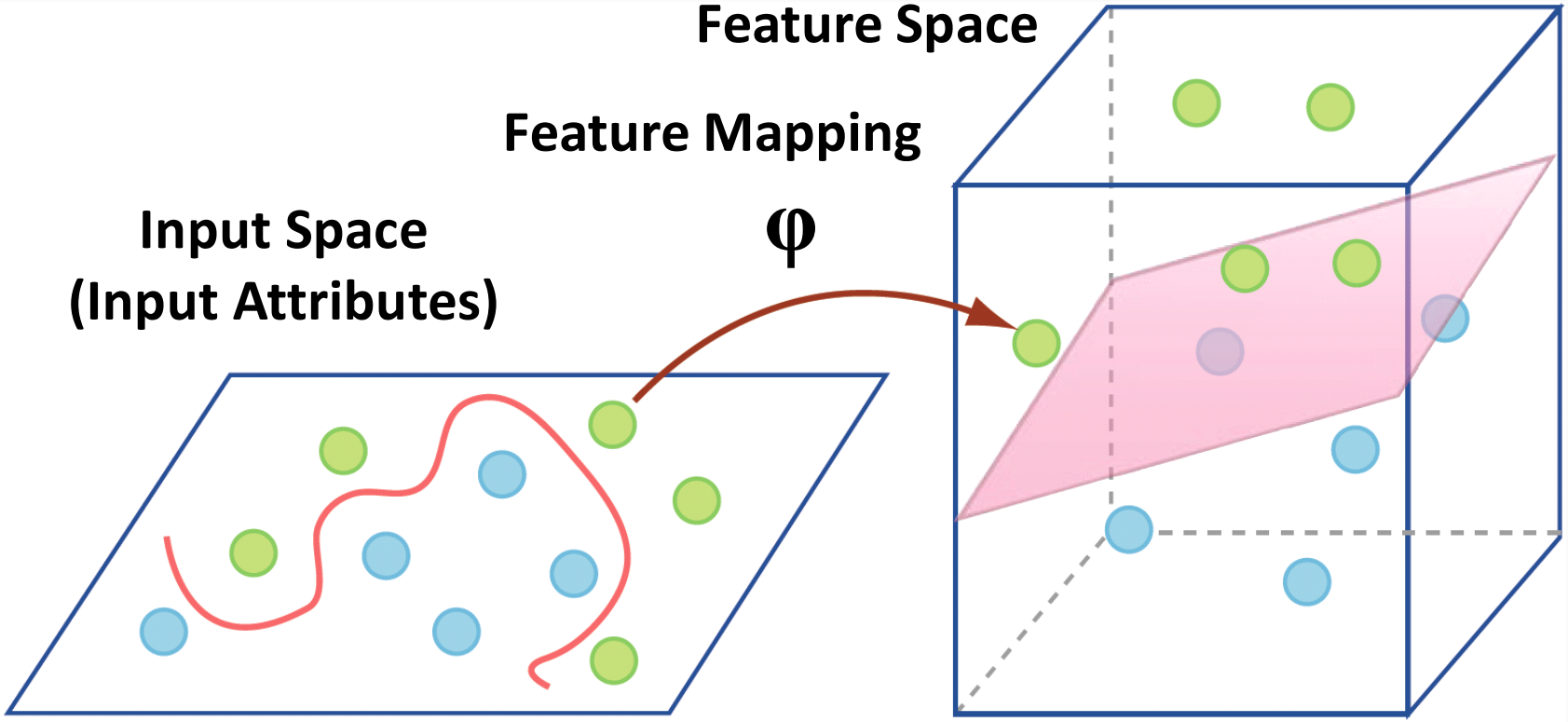


Image by MIT OpenCourseWare

Kernel method

Kernel function: Kernel function이란 어떤 feature space에서 feature의 inner product와 동등한 함수를 말함. Feature mapping $\boldsymbol{\phi}(\mathbf{x})$에 대한 kernel function은 다음과 같이 정의할 수 있음.

$$k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^T \boldsymbol{\phi}(\mathbf{x}') \tag{38}$$

Similarity: Kernel function $k(\mathbf{x}, \mathbf{x}')$는 $\mathbf{x}$와 $\mathbf{x}'$ 간의 similarity로 볼 수 있음.

또한 일반적으로 feature mapping을 통한 $\boldsymbol{\phi}(\mathbf{x})^T \boldsymbol{\phi}(\mathbf{x}')$에 비해 $k(\mathbf{x}, \mathbf{x}')$의 계산이 훨씬 간단함. 예를 들어

$$k(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^T \mathbf{x}')^2 \tag{39}$$

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} 1 & x_1^2 & \sqrt{2}x_1 x_2 & x_2^2 & \sqrt{2}x_1 & \sqrt{2}x_2 \end{bmatrix} \tag{40}$$

Construction of kernel

임의의 kernel function 대해서 $k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^T \boldsymbol{\phi}(\mathbf{x}')$가 성립하는 feature mapping이 존재하는지 검사하는 것은 매우 까다로움.

Mercer's theorem

Every positive semi-definite symmetric function is a kernel.

다음과 같이 정의되는 Gram matrix K가 positive semi-definite symmetric matrix면 function k는 kernel function임.

$$\mathbf{K} = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & k(\mathbf{x}_1, \mathbf{x}_2) & \cdots & k(\mathbf{x}_1, \mathbf{x}_N) \\ k(\mathbf{x}_2, \mathbf{x}_1) & k(\mathbf{x}_2, \mathbf{x}_2) & \cdots & k(\mathbf{x}_2, \mathbf{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ k(\mathbf{x}_N, \mathbf{x}_1) & k(\mathbf{x}_N, \mathbf{x}_2) & \cdots & k(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix} \tag{41}$$

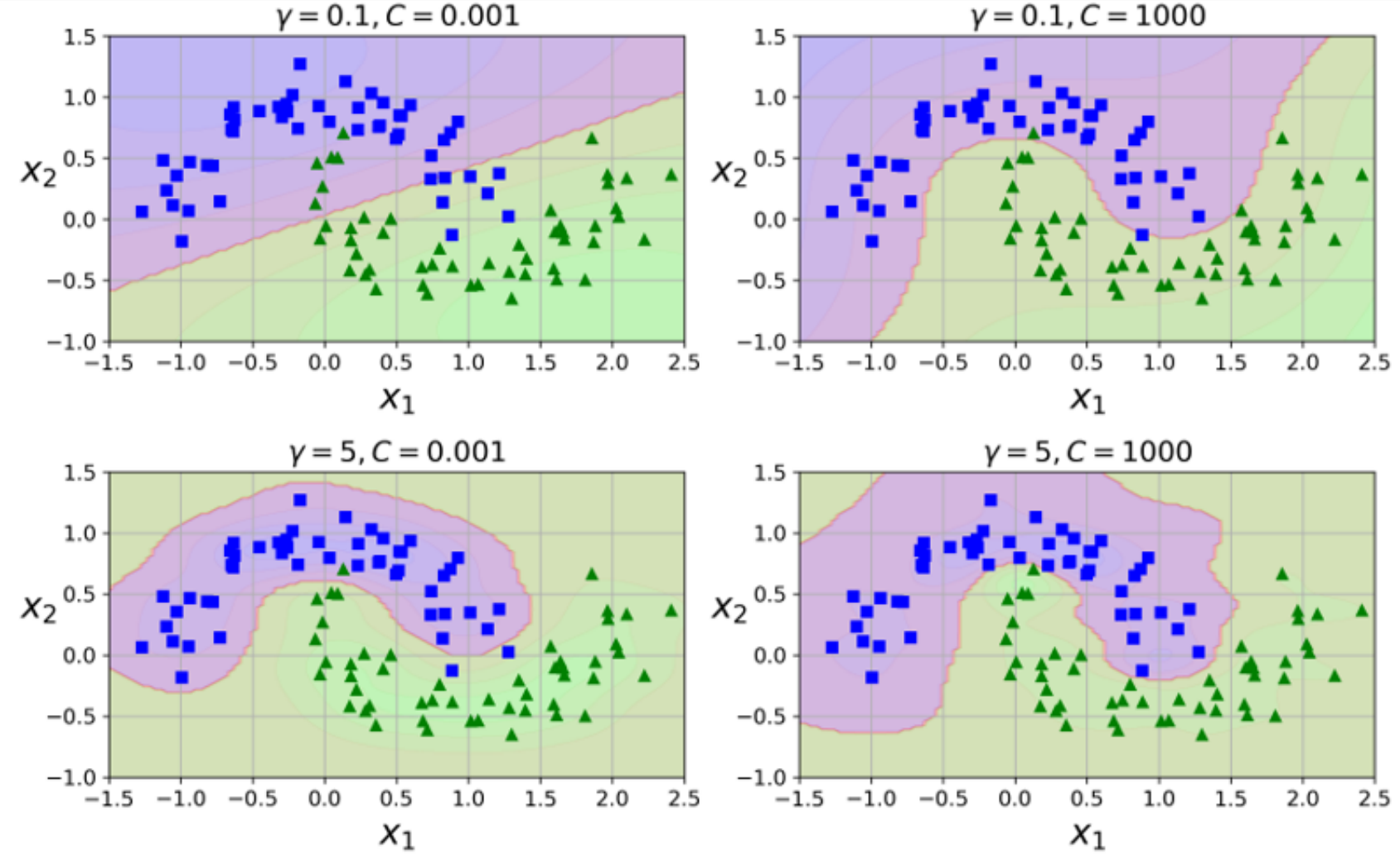
Gaussian radial basis function (RBF) kernel

Gaussian RBF kernel

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right) = \exp(-\gamma\|\mathbf{x} - \mathbf{x}'\|^2) \tag{42}$$

- kernel value는 $\mathbf{x}'$가 landmark $\mathbf{x}$와 가까울수록 큰 값
- γ 값이 커지는 경우 landmark에서 멀어질수록 kernel 값이 급격하게 작아짐 = 영향력의 범위가 좁아짐

Hyperparameter of soft SVM-RBF



SVM: strength and limitations

장점

- 강력하고 우수한 이론을 바탕으로 함
- 많은 블랙박스 알고리즘과는 대조적으로 비교적 직관적인 해석과 이해가 가능
- 학습이 상대적으로 쉬움
- 신경망처럼 지역 최적값에 빠지는 일이 없음
- 학습 시간이 차원에 의존하지 않으며 kernel trick 덕분에 고정된 입력에만 의존
- 과적합이 잘 조절되는 경향
- 많은 분야에서 신경망 및 기타 알고리즘과 필적하는 성능
- 데이터가 작은 조건이나 고차원 공간에서도 잘 일반화

SVM: strength and limitations

단점

- 노이즈에 민감: 비교적 적은 수의 잘못된 label로 성능이 심각하게 악화
- 커널 함수의 선택/구축하는 방법에 대한 정리된 원칙이 없음
- hyperparameter C의 적정값을 정하기 위한 원칙이 없음
- 컴퓨터의 메모리와 계산 시간 측면에서 비용이 높은 편이며 multiclass에서 더욱더 심화됨

Appendix

Reference and further reading

- “Chap 7 | Sparse Kernel Machines” of C. Bishop, Pattern Recognition and Machine Learning
- “Chap 5 | Support Vector Machines” of A. Geron, Hands-On Machine Learning with Scikit-Learn, Keras & TensorFlow
- “Chap 4 | Convex Optimization Problems”, “Chap 5 | Duality” of S. Boyd, Convex Optimization
- “Lecture 6 | Support Vector Machines” of Kwang Il Kim, Machine Learning (2019)

HW #5

Due: 10월 20일 화요일, 23시 59분까지

- 컴퓨터로 작성(latex, word, ppt, 한글 등)해서 pdf로 업로드해주세요.
- 또는 손으로 작성한 파일을 스캔앱(Adobe scan, Office lens 등)을 써서 pdf로 업로드해주세요.

1. 행렬의 singular value decomposition (SVD)에 대해 공부해보고 다음에 대해 설명하세요.
   - 1.1 Linear transformation 관점에서 행렬 A를 $A = U\Sigma V^T$로 SVD 했을 때, 주어진 벡터 x를 어떤 단계를 거쳐 $y = Ax$로 변환하는지 (10점)
   - 1.2 $A = U\Sigma V^T$에서 각 행렬 U, V이 행렬의 column space 및 row space와 어떤 물리적인 관계를 갖는지 (5점)
   - 1.3 행렬의 singular value와 Σ 행렬의 관계 (5점)
   - 1.4 행렬의 positive definiteness와 singular value 사이의 관계 (10점)