

Lecture 12: Classification with Support Vector Machines

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Mathematics for Machine Learning

<https://yung-web.github.io/home/courses/mathml.html>

KAIST EE

April 7, 2021

April 7, 2021 1 / 28

Warm-Up

Please watch this tutorial video by Luis Serrano on Support Vector Machine.

https://youtu.be/Lpr__X8zuE8

April 7, 2021 2 / 28

- (1) Story and Separating Hyperplanes
- (2) Primal SVM: Hard SVM
- (3) Primal SVM: Soft SVM
- (4) Dual SVM
- (5) Kernels
- (6) Numerical Solution

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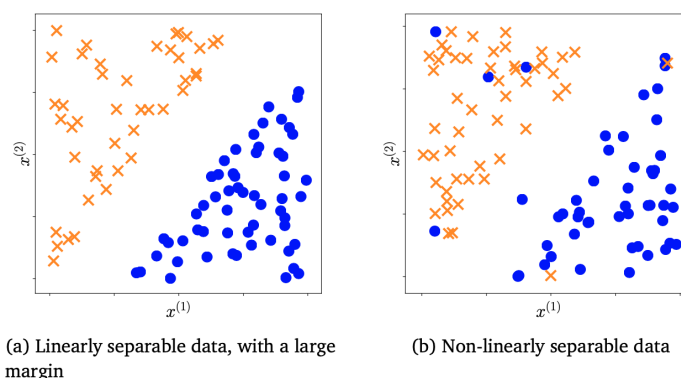
- (Binary) classification vs. regression
- A Classification predictor $f : \mathbb{R}^D \mapsto \{+1, -1\}$, where D is the dimension of features.
- Supervised learning as in the regression with a given dataset $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$, where our task is to learn the model parameters which produces the smallest classification errors.
- SVM
 - Geometric way of thinking about supervised learning
 - Relying on empirical risk minimization
 - Binary classification = Drawing a separating hyperplane
 - Various interpretation from various perspectives: geometric view, loss function view, the view from convex hulls of data points

L12(1)

April 7, 2021

5 / 28

Hard SVM vs. Soft SVM



- Hard SVM: Linearly separable, and thus, allow no classification error
- Soft SVM: Non-linearly separable, thus, allow some classification error

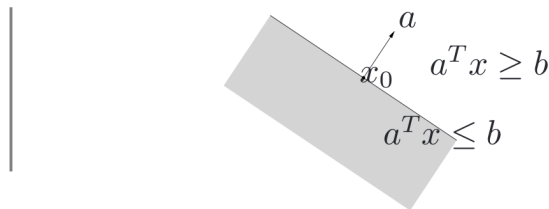
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April 7, 2021

6 / 28

- **Hyperplane** in \mathbb{R}^D is a set: $\{x \mid a^T x = b\}$ where $a \in \mathbb{R}^n, a \neq 0, b \in \mathbb{R}$ L7(3)
In other words, $\{x \mid a^T(x - x_0) = 0\}$, where x_0 is any point in the hyperplane, i.e., $a^T x_0 = b$.

- Divides \mathbb{R}^D into two **halfspaces**:
 $\{x \mid a^T x \leq b\}$ and $\{x \mid a^T x > b\}$



- In our problem, we consider the hyperplane $w^T x + b = 0$, where w and b are the parameters of the model.
- Classification logic

$$\begin{cases} w^T x_n + b \geq 0 & \text{when } y_n = +1 \\ w^T x_n + b < 0 & \text{when } y_n = -1 \end{cases} \implies y_n(w^T x_n + b) \geq 0$$

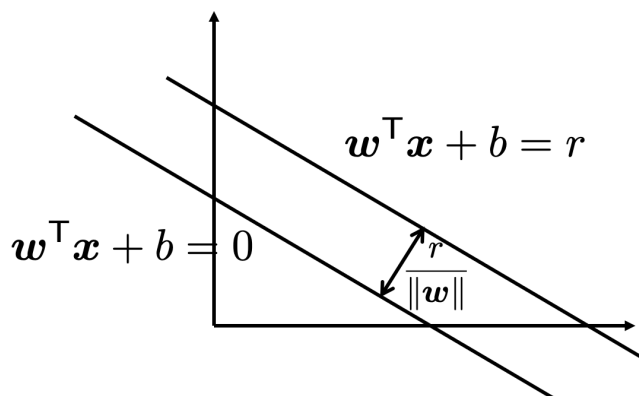
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April 7, 2021

7 / 28

Distance between Two Hyperplanes

- Consider two hyperplanes $w^T x - b = 0$ and $w^T x - b = r$, where assume $r > 0$.
- **Question.** What is the distance¹ between two hyperplanes? Answer: $\frac{r}{\|w\|}$



¹Shortest distance between two hyperplanes.

L12(1)

April 7, 2021

8 / 28

- (1) Story and Separating Hyperplanes
- (2) Primal SVM: Hard SVM
- (3) Primal SVM: Soft SVM
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Hard Support Vector Machine

- Assume that the data points are linearly separable.
- Goal: Find the hyperplane that maximizes the margin between the positive and the negative samples
- Given the training dataset $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$ and a hyperplane $\mathbf{w}^T \mathbf{x} + b = 0$, what is the constraint that all data points are $\frac{r}{\|\mathbf{w}\|}$ -away from the hyperplane?

$$y_n(\mathbf{w}^T \mathbf{x}_n + b) \geq \frac{r}{\|\mathbf{w}\|}$$

- Note that r and $\|\mathbf{w}\|$ are scaled together, so if we fix $\|\mathbf{w}\| = 1$, then

$$y_n(\mathbf{w}^T \mathbf{x}_n + b) \geq r$$

- Maximize the margin, such that all the training data points are well-classified into their classes (+ or -)

$$\begin{aligned} & \max_{\mathbf{w}, b, r} \quad r \\ & \text{subject to} \quad y_n(\mathbf{w}^T \mathbf{x}_n + b) \geq r, \text{ for all } n = 1, \dots, N, \quad \|\mathbf{w}\| = 1, \quad r > 0 \end{aligned}$$

L12(2)

April 7, 2021 11 / 28

Formulation 2 (1)

$$\begin{aligned} & \max_{\mathbf{w}, b, r} \quad r \\ & \text{subject to} \quad y_n(\mathbf{w}^T \mathbf{x}_n + b) \geq r, \text{ for all } n = 1, \dots, N, \quad \|\mathbf{w}\| = 1, \quad r > 0 \end{aligned}$$

- Since $\|\mathbf{w}\| = 1$, reformulate \mathbf{w} by \mathbf{w}' as: $y_n\left(\frac{\mathbf{w}'^T}{\|\mathbf{w}'\|} \mathbf{x}_n + b\right) \geq r$
- Change the objective from r to r^2 .
- Define \mathbf{w}'' and b'' by rescaling the constraint:

$$y_n\left(\frac{\mathbf{w}'^T}{\|\mathbf{w}'\|} \mathbf{x}_n + b\right) \geq r \iff y_n(\mathbf{w}''^T \mathbf{x}_n + b'') \geq 1, \quad \mathbf{w}'' = \frac{\mathbf{w}'}{\|\mathbf{w}'\| r} \text{ and } b'' = \frac{b}{r}$$

L12(2)

April 7, 2021 12 / 28

- Note that $\|\mathbf{w}''\| = \frac{1}{r}$
- Thus, we have the following reformulated problem:

$$\begin{aligned} \max_{\mathbf{w}'', b''} \quad & \frac{1}{\|\mathbf{w}''\|^2} \\ \text{subject to} \quad & y_n(\mathbf{w}''^T \mathbf{x}_n + b'') \geq 1, \text{ for all } n = 1, \dots, N, \end{aligned}$$

=

$$\begin{aligned} \min_{\mathbf{w}, b} \quad & \frac{1}{2} \|\mathbf{w}\|^2 \\ \text{subject to} \quad & y_n(\mathbf{w}^T \mathbf{x}_n + b) \geq 1, \text{ for all } n = 1, \dots, N, \end{aligned}$$

L12(2)

April 7, 2021 13 / 28

Understanding Formulation 2 Intuitively

- Given the training dataset $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$ and a hyperplane $\mathbf{w}^T \mathbf{x} + b = 0$, what is the constraint that all data points are $\frac{r}{\|\mathbf{w}\|}$ -away from the hyperplane?

$$y_n(\mathbf{w}^T \mathbf{x}_n + b) \geq \frac{r}{\|\mathbf{w}\|}$$

- **Formulation 1.** Note that r and $\|\mathbf{w}\|$ are scaled together, so if we fix $\|\mathbf{w}\| = 1$, then

$$y_n(\mathbf{w}^T \mathbf{x}_n + b) \geq r.$$

And, maximize r .

- **Formulation 2.** If we fix $r = 1$, then

$$y_n(\mathbf{w}^T \mathbf{x}_n + b) \geq 1.$$

And, minimize $\|\mathbf{w}\|$

L12(2)

April 7, 2021 14 / 28

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L12(3)

April 7, 2021

15 / 28

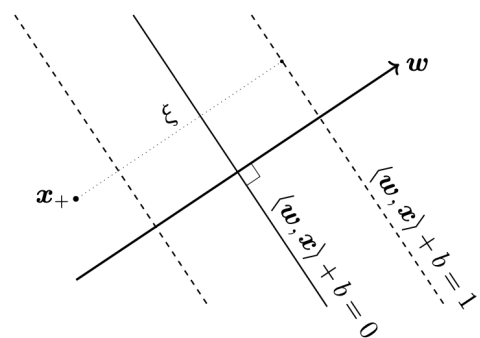
Soft SVM: Geometric View

- Now we allow some classification errors, because it's not linearly separable.
- Introduce a slack variable that quantifies how much errors will be allowed in my optimization problem

- $\xi = (\xi_n : n = 1, \dots, N)$
- ξ_n : slack for the n -th sample (\mathbf{x}_n, y_n)

$$\begin{aligned} \min_{\mathbf{w}, b} \quad & \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{n=1}^N \xi_n \\ \text{subject to} \quad & y_n(\mathbf{w}^T \mathbf{x}_n + b) \geq 1 - \xi_n, \\ & \xi_n \geq 0, \quad \text{for all } n \end{aligned}$$

- C : Trade-off between width and slack



L12(3)

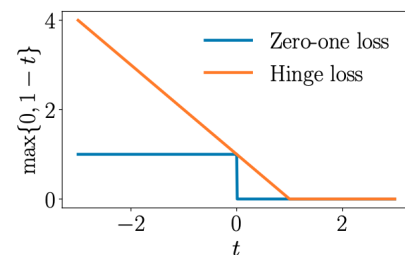
April 7, 2021

16 / 28

- From the perspective of empirical risk minimization
- Loss function design
 - **zero-one loss** $1(f(x_n) \neq y_n)$: # of mismatches between the prediction and the label
 \implies combinatorial optimization (typically NP-hard)
 - **hinge loss**

$$\ell(t) = \max(0, 1 - t), \text{ where } t = yf(\mathbf{x}) = y(\mathbf{w}^T \mathbf{x} + b)$$

- ▶ If \mathbf{x} is really at the correct side, $t \geq 1$
 $\rightarrow \ell(t) = 0$
- ▶ If \mathbf{x} is at the correct side, but too close to the boundary, $0 < t < 1$
 $\rightarrow 0 < \ell(t) = 1 - t < 1$
- ▶ If \mathbf{x} is at the wrong side, $t < 0$
 $\rightarrow 1 < \ell(t) = 1 - t$



L12(3)

April 7, 2021 17 / 28

$$\min_{\mathbf{w}, b} (\text{regularizer} + \text{loss}) = \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{n=1}^N \max\{0, 1 - y(\mathbf{w}^T \mathbf{x} + b)\}$$

- $\frac{1}{2} \|\mathbf{w}\|^2$: L2-regularizer (margin maximization = regularization)
- C : regularization parameter, which moves from the regularization term to the loss term
- Why this loss function view = geometric view?

$$\min_t \max(0, 1 - t) \iff \min_{\xi, t} \xi, \text{ subject to } \xi \geq 0, \xi \geq 1 - t$$

L12(3)

April 7, 2021 18 / 28

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- (4) **Dual SVM**
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L12(4)

April 7, 2021 19 / 28

Dual SVM: Idea

$$\min_{\mathbf{w}, b} \quad \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{n=1}^N \xi_n$$

subject to $y_n(\mathbf{w}^T \mathbf{x}_n + b) \geq 1 - \xi_n, \xi_n \geq 0, \text{ for all } n$

- The above primal problem is a convex optimization problem.
- Let's apply Lagrange multipliers, find another formulation, and see what other nice properties are shown **L7(2), L7(4)**
- Convert the problem into " \leq " constraints, so as to apply **min-min-max** rule

$$\min_{\mathbf{w}, b} \quad \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{n=1}^N \xi_n, \text{ s.t. } -y_n(\mathbf{w}^T \mathbf{x}_n + b) \leq -1 + \xi_n, -\xi_n \leq 0, \text{ for all } n$$

L12(4)

April 7, 2021 20 / 28

$$\min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{n=1}^N \xi_n, \text{ s.t. } -y_n(\mathbf{w}^T \mathbf{x}_n + b) \leq -1 + \xi_n, \quad -\xi_n \leq 0, \quad \text{for all } n$$

- Lagrangian with multipliers $\alpha_n \geq 0$ and $\gamma_n \geq 0$

$$\mathcal{L}(\mathbf{w}, b, \xi, \alpha, \gamma) = \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{n=1}^N \xi_n - \sum_{n=1}^N \alpha_n [y_n(\mathbf{w}^T \mathbf{x}_n + b) - 1 + \xi_n] - \sum_{n=1}^N \gamma_n \xi_n$$

- Dual function: $\mathcal{D}(\alpha, \gamma) = \inf_{\mathbf{w}, b, \xi} \mathcal{L}(\mathbf{w}, b, \xi, \alpha, \gamma)$ for which the followings should be met:

$$(D1) \frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \mathbf{w}^T - \sum_{n=1}^N \alpha_n y_n \mathbf{x}_n^T = 0, \quad (D2) \frac{\partial \mathcal{L}}{\partial b} = \sum_{n=1}^N \alpha_n y_n = 0, \quad (D3) \frac{\partial \mathcal{L}}{\partial \xi_n} = C - \alpha_n - \gamma_n = 0$$

L12(4)

April 7, 2021 21 / 28

- Dual function $\mathcal{D}(\alpha, \gamma) = \inf_{\mathbf{w}, b, \xi} \mathcal{L}(\mathbf{w}, b, \xi, \alpha, \gamma)$ with (D1) is given by:

$$\begin{aligned} \mathcal{D}(\alpha, \gamma) = & \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \alpha_i \alpha_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle - \sum_{i=1}^N y_i \alpha_i \left\langle \sum_{j=1}^N y_j \alpha_j \mathbf{x}_j, \mathbf{x}_i \right\rangle - b \sum_{i=1}^N y_i \alpha_i \\ & + \sum_{i=1}^N \alpha_i + \sum_{i=1}^N (C - \alpha_i - \gamma_i) \xi_i \end{aligned}$$

- From (D2) and (D3), the above is simplified into:

$$\mathcal{D}(\alpha, \gamma) = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \alpha_i \alpha_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle + \sum_{i=1}^N \alpha_i$$

- $\alpha_i, \gamma_i \geq 0$ and $C - \alpha_i - \gamma_i = 0 \implies 0 \leq \alpha_i \leq C$

L12(4)

April 7, 2021 22 / 28

- (Lagrangian) Dual Problem: **maximize** $\mathcal{D}(\alpha, \gamma)$

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N y_i y_j \alpha_i \alpha_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle + \sum_{i=1}^N \alpha_i \\ \text{subject to} \quad & \sum_{i=1}^N y_i \alpha_i = 0, \quad 0 \leq \alpha_i \leq C, \quad \forall i = 1, \dots, N \end{aligned}$$

- Primal SVM: the number of parameters scales as **the number of features** (D)
- Dual SVM
 - the number of parameters scales as **the number of training data** (N)
 - only depends on the inner products of individual training data points $\langle \mathbf{x}_i, \mathbf{x}_j \rangle \rightarrow$ allow the application of **kernel**

L12(4)

April 7, 2021 23 / 28

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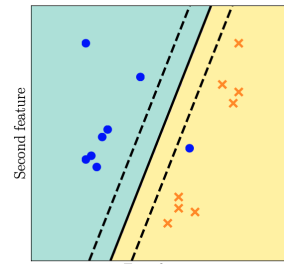
L12(5)

April 7, 2021 24 / 28

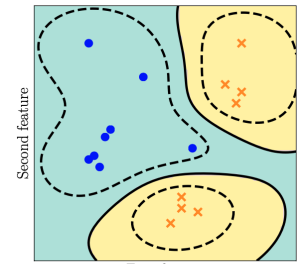
- Modularity: Using the feature transformation $\phi(\mathbf{x})$, dual SVMs can be modularized

$$\langle \mathbf{x}_i, \mathbf{x}_j \rangle \implies \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$$

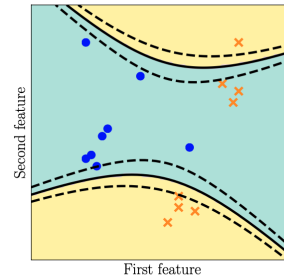
- Similarity function $k : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$, $k(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$
- Kernel matrix, Gram matrix: must be symmetric and positive semidefinite
- Examples: polynomial kernel, Gaussian radial basis function, rational quadratic kernel



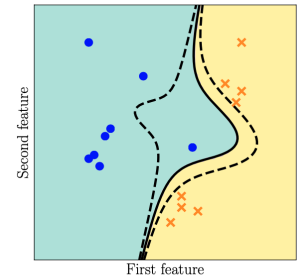
(a) SVM with linear kernel



(b) SVM with RBF kernel



(c) SVM with polynomial (degree 2) kernel



(d) SVM with polynomial (degree 3) kernel

L12(5)

April 7, 2021 25 / 28

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L12(5)

April 7, 2021 26 / 28

Questions?

L12(5)

April 7, 2021 27 / 28

Review Questions

1)

L12(5)

April 7, 2021 28 / 28