CS 6316 Machine Learning

Support Vector Machines and Kernel Methods

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About Online Lectures

Course Information Update

- Record the lectures and upload the videos on Collab
- By default, turn off the video and mute yourself
- If you have a question
  - Unmuate yourself and chime in anytime
  - Use the raise hand feature
  - Send me a private message

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- Slack: as a stable communication channel to
  - send out instant messages if my network connection is unreliable
  - online discussion

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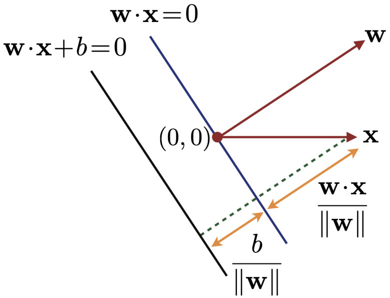
- Office hour
  - Wednesday 11 AM: I will be on Zoom
  - You can also send me an email or Slack message anytime

Separable Cases

Geometric Margin

The geometric margin of a linear binary classifier $h(\boldsymbol{x}) = \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b$ at a point $\boldsymbol{x}$ is its distance to the hyper-plane $\langle \boldsymbol{w}, \boldsymbol{x} \rangle = 0$

$$\rho_h(\boldsymbol{x}) = \frac{|\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b|}{\|\boldsymbol{w}\|_2} \tag{1}$$



Geometric Margin (II)

The geometric margin of $h(\boldsymbol{x})$ for a set of examples $T = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m\}$ is the minimal distance over these examples

$$\rho_h(T) = \min_{\boldsymbol{x}' \in T} \rho_h(\boldsymbol{x}') \tag{2}$$

[Mohri et al., 2018, Page 80]

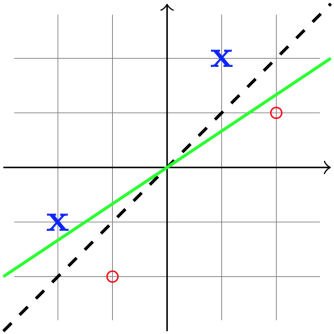
Half-Space Hypothesis Space

- Training set $S = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m)\}$ with $\boldsymbol{x}_i \in \mathbb{R}^d$ and $y_i \in \{+1, -1\}$
- If the training set is linearly separable

$$y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) > 0 \quad \forall i \in [m] \tag{3}$$

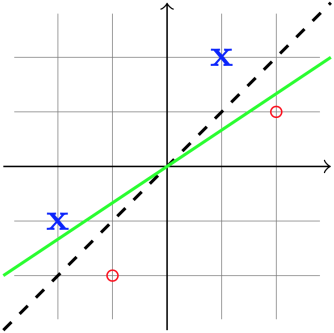
- Linearly separable cases
  - Existence of equation 3
  - All halfspace predictors that satisfy the condition in equation 3 are ERM hypotheses

Which Hypothesis is Better?



[Shalev-Shwartz and Ben-David, 2014, Page 203]

Which Hypothesis is Better?



- Intuitively, a hypothesis with larger *margin* is better, because it is more robust to noise
- Final definition of margin will be provided later

[Shalev-Shwartz and Ben-David, 2014, Page 203]

Hard SVM/Separable Cases

The mathematical formulation of the previous idea

$$\rho = \max_{(\boldsymbol{w},b)} \min_{i\in[m]} \frac{|\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b|}{\|\boldsymbol{w}\|_2} \tag{4}$$

$$\text{s.t. } y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) > 0 \quad \forall i \tag{5}$$

- $y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) > 0 \ \forall i$: guarantee $(\boldsymbol{w}, b)$ is an ERM hypothesis

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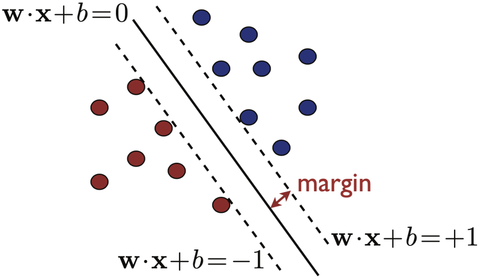
- $y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i\rangle + b) > 0\ \forall i$: guarantee $(\boldsymbol{w}, b)$ is an ERM hypothesis
- $\min_{i\in[m]}$: calculate the margin between a hyper-plane and a set of examples
- $\max_{(\boldsymbol{w},b)}$: maximize the margin

Illustration

Original form

$$\rho = \max_{(w,b)} \min_{i \in [m]} \frac{|\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b|}{\|\boldsymbol{w}\|_2} \tag{6}$$

$$\text{s.t. } y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) > 0 \quad \forall i \tag{7}$$



Alternative Forms

- Original form

$$\rho = \max_{(w,b)} \min_{i\in[m]} \frac{|\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b|}{\|\boldsymbol{w}\|_2} \tag{8}$$

$$\text{s.t. } y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) > 0 \quad \forall i \tag{9}$$

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- Alternative form 1

$$\rho = \max_{(\boldsymbol{w},b)} \min_{i\in[m]} \frac{y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i\rangle + b)}{\|\boldsymbol{w}\|_2} \tag{10}$$

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- Alternative form 2

$$\rho = \max_{(\boldsymbol{w},b):\ \min_{i\in[m]} y_i(\langle \boldsymbol{w},\boldsymbol{x}_i\rangle + b = 1} \frac{1}{\|\boldsymbol{w}\|_2} \tag{11}$$

$$= \max_{(\boldsymbol{w},b):\ y_i(\langle \boldsymbol{w},\boldsymbol{x}_i\rangle + b \geq 1} \frac{1}{\|\boldsymbol{w}\|_2} \tag{12}$$

Alternative Forms (II)

- Alternative form 2

$$\rho = \max_{(\boldsymbol{w},b):\ y_i(\langle \boldsymbol{w},\boldsymbol{x}_i\rangle + b \geq 1} \frac{1}{\|\boldsymbol{w}\|_2} \tag{13}$$

- Alternative form 3: Quadratic programming (QP)

$$\begin{aligned} \min_{(\boldsymbol{w},b)} \quad & \frac{1}{2}\|\boldsymbol{w}\|_2^2 \\ \text{s.t.} \quad & y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) \geq 1, \quad \forall i \in [m] \end{aligned} \tag{14}$$

which is a constrained optimization problem that can be solved by standard QP packages

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- *Exercise*: Solve a SVM problem with quadratic programming

Unconstrained Optimization Problem

The quadratic programming problem with constraints can be converted to an unconstrained optimization problem with the Lagrangian method

$$L(\boldsymbol{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\boldsymbol{w}\|_2^2 - \sum_{i=1}^{m} \alpha_i (y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) - 1) \qquad (15)$$

where

- $\boldsymbol{\alpha} = \{\alpha_1, \ldots, \alpha_m\}$ is the Lagrange multiplier, and
- $\alpha_i \geq 0$ is associated with the i-th training example

Constrained Optimization Problems

Constrained Optimization Problems: Definition

- $\mathcal{X} \subseteq \mathbb{R}^d$ and
- $f, g_i : \mathcal{X} \to \mathbb{R}, \forall i \in [m]$

Then, a constrained optimization problem is defined in the form of

$$\min_{x \in \mathcal{X}} \quad f(\boldsymbol{x}) \tag{16}$$

$$\text{s.t.} \quad g_i(\boldsymbol{x}) \leq 0, \forall i \in [m] \tag{17}$$

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Comments

- In general definition, $\boldsymbol{x}$ is the target variable for optimization
- Special cases of $g_i(\boldsymbol{x})$: (1) $g_i(\boldsymbol{x}) = 0$, (2) $g_i(\boldsymbol{x}) \geq 0$, and (3) $g_i(\boldsymbol{x}) \leq b$

Lagrangian

The Lagrangian associated to the general constrained optimization problem defined in equation 16 – 17 is the function defined over $\mathcal{X} \times \mathbb{R}_+^m$ as

$$L(\boldsymbol{x}, \boldsymbol{\alpha}) = f(\boldsymbol{x}) + \sum_{i=1}^{m} \alpha_i g_i(\boldsymbol{x}) \tag{18}$$

where

- $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_m) \in \mathbb{R}_+^m$
- $\alpha_i \geq 0$ for any $i \in [m]$

Karush-Kuhn-Tucker's Theorem

Assume that $f, g_i : \mathcal{X} \to \mathbb{R}, \forall i \in [m]$ are convex and differentiable and that the constraints are qualified. Then $\boldsymbol{x}'$ is a solution of the constrained problem if and only if there exist $\boldsymbol{\alpha}' \geq 0$ such that

$$\begin{aligned}
\nabla_{\boldsymbol{x}} L(\boldsymbol{x}', \boldsymbol{\alpha}') &= \nabla_{\boldsymbol{x}} f(\boldsymbol{x}') + \boldsymbol{\alpha}' \cdot \nabla_{\boldsymbol{x}} g(\boldsymbol{x}) = 0 \qquad (19)\\
\nabla_{\boldsymbol{\alpha}} L(\boldsymbol{x}, \boldsymbol{\alpha}) &= g(\boldsymbol{x}') \leq 0 \qquad (20)\\
\boldsymbol{\alpha}' \cdot g(\boldsymbol{x}') &= \sum_{i=1}^{m} \alpha'_i g_i(\boldsymbol{x}') = 0 \qquad (21)
\end{aligned}$$

Equations 19 – 21 are called KKT conditions

[Mohri et al., 2018, Thm B.30]

KKT in SVM

Apply the KKT conditions to the SVM problem

$$L(\boldsymbol{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\boldsymbol{w}\|_2^2 - \sum_{i=1}^{m} \alpha_i (y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) - 1) \tag{22}$$

We have

$$\nabla_{\boldsymbol{w}} L = \boldsymbol{w} - \sum_{i=1}^{m} \alpha_i y_i \boldsymbol{x}_i = 0 \quad \Rightarrow \quad \boldsymbol{w} = \sum_{i=1}^{m} \alpha_i y_i \boldsymbol{x}_i$$

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$$\nabla_b L = -\sum_{i=1}^{m} \alpha_i y_i = 0 \quad \Rightarrow \quad \sum_{i=1}^{m} \alpha_i y_i = 0$$

KKT in SVM

Apply the KKT conditions to the SVM problem

$$L(\boldsymbol{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\boldsymbol{w}\|_2^2 - \sum_{i=1}^{m} \alpha_i (y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) - 1) \qquad (22)$$

We have

$$\nabla_w L = \boldsymbol{w} - \sum_{i=1}^{m} \alpha_i y_i \boldsymbol{x}_i = 0 \quad \Rightarrow \quad \boldsymbol{w} = \sum_{i=1}^{m} \alpha_i y_i \boldsymbol{x}_i$$

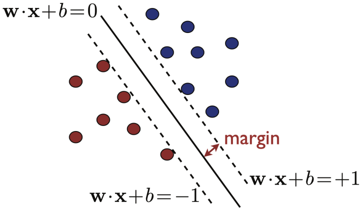
$$\nabla_b L = -\sum_{i=1}^{m} \alpha_i y_i = 0 \quad \Rightarrow \quad \sum_{i=1}^{m} \alpha_i y_i = 0$$

$$\forall i, \alpha_i (y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) - 1) = 0 \quad \Rightarrow \quad \alpha_i = 0 \text{ or } y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) = 1$$

Support Vectors

Consider the implication of the last equation in the previous page, $\forall i$

- $\alpha_i > 0$ and $y_i(\langle w, x_i \rangle + b) = 1$ or



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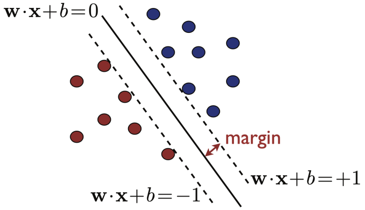
- $\alpha_i > 0$ and $y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) = 1$ or
- $\alpha_i = 0$ and $y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) \geq 1$



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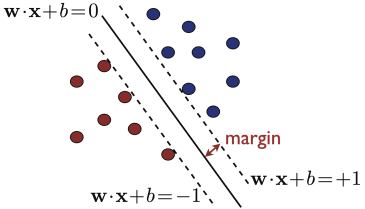


$$\boldsymbol{w} = \sum_{i=1}^{m} \alpha_i y_i \boldsymbol{x}_i \tag{23}$$

- Examples with $\alpha_i > 0$ are called **support vectors**
- In $\mathbb{R}^d$, $d+1$ examples are sufficient to define a hyper-plane

Non-separable Cases

Non-separable Cases

Recall the separable case:

$$\begin{aligned} &\min_{(\boldsymbol{w},b)} \frac{1}{2}\|\boldsymbol{w}\|_2^2 \\ &\text{s.t. } y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i\rangle + b) \geq 1, \quad \forall i \in [m] \end{aligned} \tag{24}$$

Non-separable Cases

Recall the separable case:

$$\begin{aligned} \min_{(w,b)} \ & \frac{1}{2}\|\boldsymbol{w}\|_2^2 \\ \text{s.t. } & y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) \geq 1, \quad \forall i \in [m] \end{aligned} \tag{24}$$

For non-separable cases, there always exists an $\boldsymbol{x}_i$, such that

$$y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) \ngeq 1 \tag{25}$$

or, we can formulate it as

$$y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) \geq 1 - \xi_i \tag{26}$$

with $\xi_i \geq 0$

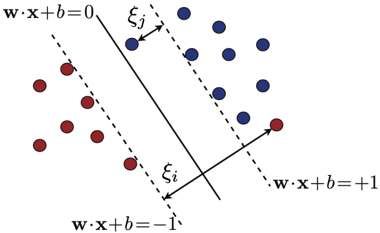
Geometric Meaning of ξ_i

Consider the relaxed constraint

$$y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) \geq 1 - \xi_i \tag{27}$$

and three cases of ξ_i

- $\xi_i = 0$
- $0 < \xi_i < 1$
- $\xi_i \geq 1$



Non-separable Cases (II)

In general, the SVM problem of non-separable cases can be formulated as

$$\begin{aligned}
\min_{(\boldsymbol{w},b)} \ & \frac{1}{2}\|\boldsymbol{w}\|_2^2 + C\sum_{i=1}^{m}\xi_i^p \\
\text{s.t. } & y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i\rangle + b) \geq 1 - \xi_i, \quad \forall i \in [m] \\
& \xi_i \geq 0
\end{aligned} \tag{28}$$

where $C \geq 0$, $p \geq 1$, and $\{\xi_i\}_{i=1}^m \geq 0$ are known as **slack variables** and are commonly used in optimization to define relaxed versions of constraints.

Lagrangian

Follows the same procedure as the separable cases, the Lagrangian is defined as

$$
\begin{aligned}
L(\boldsymbol{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) =& \frac{1}{2}\|\boldsymbol{w}\|_2^2 + C\sum_{i=1}^{m}\xi_i \\
&- \sum_{i=1}^{m}\alpha_i(y_i(\boldsymbol{w}^\top \boldsymbol{x}_i + b) - 1 + \xi_i) \\
&- \sum_{i=1}^{m}\beta_i\xi_i
\end{aligned}
\tag{29}
$$

with $\alpha_i, \beta_i \geq 0$

Lagrangian

Follows the same procedure as the separable cases, the Lagrangian is defined as

$$\begin{aligned} L(\boldsymbol{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = & \frac{1}{2}\|\boldsymbol{w}\|_2^2 + C\sum_{i=1}^{m}\xi_i \\ & - \sum_{i=1}^{m}\alpha_i(y_i(\boldsymbol{w}^\top \boldsymbol{x}_i + b) - 1 + \xi_i) \\ & - \sum_{i=1}^{m}\beta_i\xi_i \end{aligned} \tag{29}$$

with $\alpha_i, \beta_i \geq 0$

Exercise: show the KKT conditions of equation 29

Support Vectors

The first two equations in the KKT conditions are similar to the separable cases, and the rest are

$$
\begin{aligned}
\alpha_i + \beta_i \quad &= \quad C && (30)\\
\alpha_i = 0 \quad \text{or} \quad & y_i(\boldsymbol{w}^\top \boldsymbol{x}_i + b) = 1 - \xi_i && (31)\\
\beta_i = 0 \quad \text{or} \quad & \xi_i = 0 && (32)
\end{aligned}
$$

Depending the value of ξ_i, there are two types of support vectors

- $\xi_i = 0$: $\beta_i \geq 0$ and $0 < \alpha_i \leq C$
  - $\boldsymbol{x}_i$ may lie on the marginal hyper-planes (as in the separable case)

Support Vectors

The first two equations in the KKT conditions are similar to the separable cases, and the rest are

$$\alpha_i + \beta_i = C \quad (30)$$

$$\alpha_i = 0 \quad \text{or} \quad y_i(\boldsymbol{w}^\top \boldsymbol{x}_i + b) = 1 - \xi_i \quad (31)$$

$$\beta_i = 0 \quad \text{or} \quad \xi_i = 0 \quad (32)$$

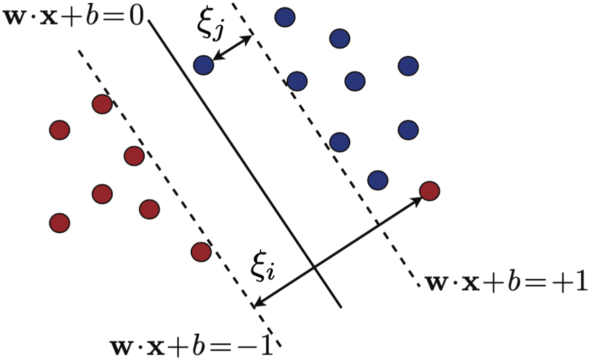
Depending the value of ξ_i, there are two types of support vectors

- $\xi_i = 0$: $\beta_i \geq 0$ and $0 < \alpha_i \leq C$
  - $\boldsymbol{x}_i$ may lie on the marginal hyper-planes (as in the separable case)
- $\xi_i > 0$: $\beta_i = 0$ and $\alpha_i = C$
  - $\boldsymbol{x}_i$ is an outlier

Support Vectors (II)

Two types of support vectors

- $\alpha_i = C$: $\boldsymbol{x}_i$ is an outlier
- $0 < \alpha_i < C$: $\boldsymbol{x}_i$ lies on the marginal hyper-planes



Dual Optimization Problem

Lagrangian

Combine the Lagrangian

$$
\begin{aligned}
L &= \frac{1}{2}\|\boldsymbol{w}\|_2^2 - \sum_{i=1}^{m} \alpha_i [y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) - 1] \\
&= \frac{1}{2}\|\boldsymbol{w}\|_2^2 - \sum_{i=1}^{m} \alpha_i y_i \langle \boldsymbol{w}, \boldsymbol{x}_i \rangle - b \sum_{i=1}^{m} \alpha_i y_i + \sum_{i=1}^{m} \alpha_i
\end{aligned}
$$

Lagrangian

Combine the Lagrangian

$$
\begin{aligned}
L &= \frac{1}{2}\|\boldsymbol{w}\|_2^2 - \sum_{i=1}^{m} \alpha_i [y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) - 1] \\
&= \frac{1}{2}\|\boldsymbol{w}\|_2^2 - \sum_{i=1}^{m} \alpha_i y_i \langle \boldsymbol{w}, \boldsymbol{x}_i \rangle - b \sum_{i=1}^{m} \alpha_i y_i + \sum_{i=1}^{m} \alpha_i
\end{aligned}
$$

with some of the KKT conditions

$$
\boldsymbol{w} = \sum_{i=1}^{m} \alpha_i y_i \boldsymbol{x}_i \tag{33}
$$

$$
\sum_{i=1}^{m} \alpha_i y_i = 0, \tag{34}
$$

we have ...

Dual Problem

$$
\begin{aligned}
L =& \frac{1}{2} \| \sum_{i=1}^{m} \alpha_i y_i \boldsymbol{x}_i \|_2^2 - \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle \\
& - b \underbrace{\sum_{i=1}^{m} \alpha_i y_i}_{=0} + \sum_{i=1}^{m} \alpha_i
\end{aligned} \tag{35}
$$

Dual Problem

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\begin{aligned}
L =& \frac{1}{2} \| \sum_{i=1}^{m} \alpha_i y_i \boldsymbol{x}_i \|_2^2 - \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle \\
& \underbrace{- b \sum_{i=1}^{m} \alpha_i y_i}_{=0} + \sum_{i=1}^{m} \alpha_i
\end{aligned}
\tag{35}
$$

Given $\| \sum_{i=1}^{m} \alpha_i y_i \boldsymbol{x}_i \|_2^2 = \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle$, we have

$$
L = -\frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle + \sum_{i=1}^{m} \alpha_i \tag{36}
$$

Dual Problem (II)

The dual optimization problem for SVMs of the separable cases is

$$\max_{\boldsymbol{\alpha}} \quad \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle \tag{37}$$

$$\text{s.t.} \quad \alpha_i \geq 0 \tag{38}$$

$$\sum_{i=1}^{m} \alpha_i y_i = 0 \ \forall i \in [m] \tag{39}$$

Dual Problem (II)

The dual optimization problem for SVMs of the separable cases is

$$\max_{\boldsymbol{\alpha}} \quad \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle \tag{37}$$

$$\text{s.t.} \quad \alpha_i \geq 0 \tag{38}$$

$$\sum_{i=1}^{m} \alpha_i y_i = 0 \ \forall i \in [m] \tag{39}$$

- Lagrange multiplier $\boldsymbol{\alpha}$ is also called dual variable
- This is an optimization problem only about $\boldsymbol{\alpha}$

Dual Problem (II)

The dual optimization problem for SVMs of the separable cases is

$$\max_{\boldsymbol{\alpha}} \quad \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle \tag{37}$$

$$\text{s.t.} \quad \alpha_i \geq 0 \tag{38}$$

$$\sum_{i=1}^{m} \alpha_i y_i = 0 \ \forall i \in [m] \tag{39}$$

- Lagrange multiplier $\boldsymbol{\alpha}$ is also called dual variable
- This is an optimization problem only about $\boldsymbol{\alpha}$
- The dual problem is defined on the inner product $\langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle$

Primal and Dual Problem

- Primal problem

$$\begin{aligned} \min_{(\boldsymbol{w},b)} \quad & \frac{1}{2}\|\boldsymbol{w}\|_2^2 \\ \text{s.t.} \quad & y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) \geq 1, \quad \forall i \in [m] \end{aligned} \tag{40}$$

- Dual problem

$$\begin{aligned} \max_{\boldsymbol{\alpha}} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle \\ \text{s.t.} \sum_{i=1}^{m} \alpha_i y_i = 0 \text{ and } \alpha_i \geq 0 \; \forall i \in [m] \end{aligned} \tag{41}$$

- These two problems are equivalent

[Boyd and Vandenberghe, 2004, Chapter 5]

SVM Hypothesis, revisited

Once we solve the dual problem with $\boldsymbol{\alpha}$, we have the solution of $\boldsymbol{w}$ as

$$\boldsymbol{w} = \sum_{i=1}^{m} \alpha_i y_i \boldsymbol{x}_i \tag{42}$$

and the hypothesis $h(\boldsymbol{x})$ as

$$h(\boldsymbol{x}) = \text{sign}(\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b) \tag{43}$$

(45)

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Exercise: Prove $b = y_i - \sum_{i=1}^{m} \alpha_i y_i \langle \boldsymbol{x}_i, \boldsymbol{x} \rangle$ for any $\boldsymbol{x}_i$ with $\alpha_i > 0$

Kernel Methods

Properties of Inner Product

In the solution of SVMs

$$
\begin{aligned}
h(\boldsymbol{x}) &= \operatorname{sign}\Big(\sum_{i=1}^{m} \alpha_i y_i \langle \boldsymbol{x}_i, \boldsymbol{x} \rangle + b\Big) \\
b &= y_i - \sum_{i=1}^{m} \alpha_i y_i \langle \boldsymbol{x}_i, \boldsymbol{x} \rangle
\end{aligned}
\tag{46}
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$$

Extend the capacity of SVMs by replacing the inner product $\langle \boldsymbol{x}_i, \boldsymbol{x} \rangle$ with a kernel function

$$
K(\boldsymbol{x}_i, \boldsymbol{x}) = \langle \Phi(\boldsymbol{x}_i), \Phi(\boldsymbol{x}) \rangle \tag{47}
$$

where $\Phi(\cdot)$ is a nonlinear mapping function.

Examples: Polynomial Kernels

For any constant $c > 0$, a **polynomial kernel** of degree $d \in \mathbb{N}$ is the kernel K defined over $\mathbb{R}^n$ by

$$K(\boldsymbol{x}, \boldsymbol{x}') = (\langle \boldsymbol{x}, \boldsymbol{x}' \rangle + c)^d, \forall \boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^n \tag{48}$$

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Special cases

- $d = 1$: $K(\boldsymbol{x}, \boldsymbol{x}') = \langle \boldsymbol{x}, \boldsymbol{x}' \rangle + c$
- $d = 2$: $K(\boldsymbol{x}, \boldsymbol{x}') = (\langle \boldsymbol{x}, \boldsymbol{x}' \rangle + c)^2$

Examples: Polynomial Kernels (II)

For the special case with $d = 2$, assume $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^2$

$$
\begin{aligned}
K(\boldsymbol{x}, \boldsymbol{x}') &= (\langle \boldsymbol{x}, \boldsymbol{x}' \rangle + c)^2 && (49) \\
&= (x_1 x_1' + x_2 x_2' + c)^2 && (50) \\
&= x_1^2 x_1'^2 + x_1 x_2 x_1' x_2' + c x_1 x_1' + x_1 x_2 x_1' x_2' \\
&\quad + x_2^2 x_2'^2 + c x_2 x_2' + c x_1 x_1' + c x_2 x_2' + c^2 && (51)
\end{aligned}
$$

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&= [x_1^2, x_2^2, \sqrt{2} x_1 x_2, \sqrt{2c} x_1, \sqrt{2c} x_2, c] \begin{bmatrix} x_1'^2 \\ x_2'^2 \\ \sqrt{2} x'_1 x'_2 \\ \sqrt{2c} x'_1 \\ \sqrt{2c} x'_2 \\ c \end{bmatrix}
\end{aligned}
$$

Examples: Polynomial Kernels (III)

Let $K(\boldsymbol{x}, \boldsymbol{x}') = \langle \Phi(\boldsymbol{x}), \Phi(\boldsymbol{x}') \rangle$, then

$$\Phi(\boldsymbol{x}) = [x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2c}x_1, \sqrt{2c}x_2, c] \tag{54}$$

which maps a 2-D data point $\boldsymbol{x}$ into a 6-D space as $\Phi(\boldsymbol{x})$

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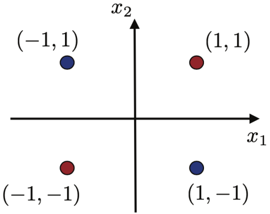
Recall the XOR problem



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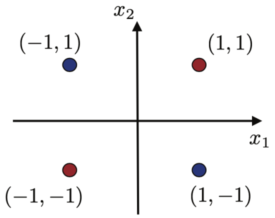
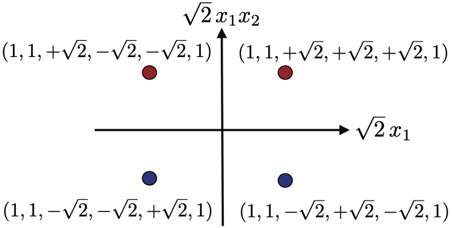
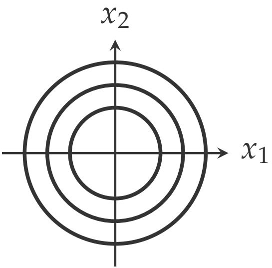




Gaussian Kernels

For any constant $\sigma > 0$, a **Gaussian kernel** or **radial basis function** (RBF) is the kernel K defined over $\mathbb{R}^d$ by

$$K(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(-\frac{\|\boldsymbol{x}' - \boldsymbol{x}\|_2^2}{2\sigma^2}\right) \tag{55}$$



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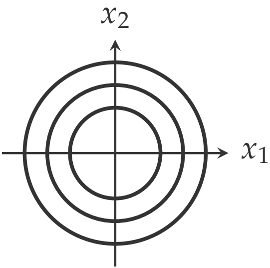

Question: What $\Phi(\boldsymbol{x})$ looks like in this case?

SVMs with Kernel Functions

- Problem definition

$$\max_{\boldsymbol{\alpha}} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j K(x_i, x_j)$$
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- Solution: separable case

$$h(\boldsymbol{x}) = \operatorname{sign}\left(\sum_{i=1}^{m} \alpha_i y_i K(\boldsymbol{x}_i, \boldsymbol{x}) + b\right) \tag{57}$$

with $b = y_i - \sum_{j=1}^{m} \alpha_j y_j K(\boldsymbol{x}_j, \boldsymbol{x}_i)$ for any $\boldsymbol{x}_i$ with $\alpha_i > 0$

The Choice of Kernels

- The choice of $K(\boldsymbol{x}, \boldsymbol{x}')$ can be arbitrary, as long as the existence of $\Phi(\cdot)$ is guaranteed
  - For many cases, $\Phi(\cdot)$ cannot be found explicitly

[Mohri et al., 2018, Section 6.1 - 6.2]

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- Alternatively, we only need to make sure $K(\boldsymbol{x}, \boldsymbol{x}')$ is *positive definite symmetric* (PDS)
  - A kernel K is PDS if for any $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m\}$ the matrix $\mathbf{K}$ is symmetric positive semi-definite

$$\mathbf{K} = [K(\boldsymbol{x}_i, \boldsymbol{x}_j)]_{i,j} \in \mathbb{R}^{m \times m} \tag{58}$$

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- A symmetric positive semi-definite matrix is defined as

$$\boldsymbol{c}^\top \mathbf{K} \boldsymbol{c} \geq 0 \tag{59}$$

[Mohri et al., 2018, Section 6.1 - 6.2]

Reference

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