AI6102: Machine Learning Methodologies & Applications

L4: Linear Models: Classification

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Outline

- Linear regression revisit
- Linear models for classification
  - Logistic Regression
  - Support Vector Machines (basic idea, details will be taught in next lecture)

Linear Regression Revisit

$$\widehat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{N} \ell(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i) + \lambda\Omega(\boldsymbol{\theta})$$

- $f(\boldsymbol{x}_i; \boldsymbol{\theta})$ is defined as

$$f(\boldsymbol{x}; \boldsymbol{\theta}) = \boldsymbol{w} \cdot \boldsymbol{x} + b$$

OR $f(\boldsymbol{x}; \boldsymbol{\theta}) = \boldsymbol{w} \cdot \boldsymbol{x}$ by introducing additional w_0 and x_0 to absorb b in $\boldsymbol{w}$

- The loss function $\ell(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)$ is defined as the squared difference between $f(\boldsymbol{x}_i; \boldsymbol{\theta})$ and y_i
- The regularization term is defined as the L2 norm

Linear Regression Revisit (cont.)

- With a set of N labeled data $\{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_N, y_N)\}$, the optimization problem is specified as

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w} \cdot \boldsymbol{x}_i - y_i)^2 + \frac{\lambda}{2} \|\boldsymbol{w}\|_2^2$$

- We have derived that there is a closed-form solution for regularized linear regression:

$$\boldsymbol{w} = (\mathbf{X}\mathbf{X}^T + \lambda \mathbf{I})^{-1} \mathbf{X} \boldsymbol{y}$$

Linear Models for Classification

$$\widehat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{N} \ell(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i) + \lambda\Omega(\boldsymbol{\theta})$$

- In general, for classification, $f(\boldsymbol{x}_i; \boldsymbol{w})$ is defined as

$$f(\boldsymbol{x}; \boldsymbol{\theta}) = h(\boldsymbol{w} \cdot \boldsymbol{x} + b)$$

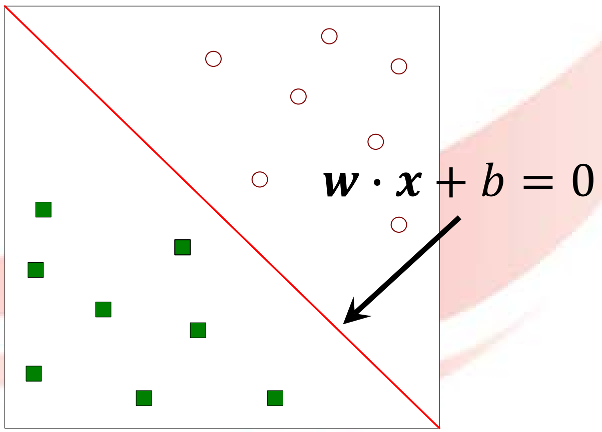
  where $h(z)$ is a function to map continuous values to discrete values (denoting different categories)
- For binary classification,

$$h(z) = \begin{cases} +1 & \text{if } z \geq 0 \\ -1 & \text{if } z < 0 \end{cases}$$

Hyperplane

- In linear algebra, from the geometry point of view,
$$\boldsymbol{w} \cdot \boldsymbol{x} + b = 0, \text{where } \boldsymbol{w}, \boldsymbol{x} \in \mathbb{R}^m$$
defines a hyperplane in the m-dimensional space, and separate the m-dimensional space into two regions
- For a data instance $\boldsymbol{x}_i$
  - If $\boldsymbol{w} \cdot \boldsymbol{x}_i + b = 0$, then $\boldsymbol{x}_i$ is on the hyperplane
  - If $\boldsymbol{w} \cdot \boldsymbol{x}_i + b > 0$, then $\boldsymbol{x}_i$ is on one side of the hyperplane
  - If $\boldsymbol{w} \cdot \boldsymbol{x}_i + b < 0$, then $\boldsymbol{x}_i$ is on the other side of the hyperplane

In the 3-dimensional space, hyperplanes are 2-dimensional planes, while in the 2-dimensional space, hyperplanes are lines



A Compact Form of Hyperplane

- Recall from Lecture 3

$$\boldsymbol{w} \cdot \boldsymbol{x} + b = 0, \text{where } \boldsymbol{w}, \boldsymbol{x} \in \mathbb{R}^m$$

$$\Downarrow$$

$$\sum_{i=1}^{m} w_i x_i + b = 0$$

$$\boldsymbol{x} = \begin{bmatrix} x_0 = 1 \\ x_1 \\ x_2 \\ \dots \\ x_m \end{bmatrix} \qquad \boldsymbol{w} = \begin{bmatrix} w_0 = b \\ w_1 \\ w_2 \\ \dots \\ w_m \end{bmatrix}$$

$$\boldsymbol{w} \cdot \boldsymbol{x} = 0, \text{where } \boldsymbol{w}, \boldsymbol{x} \in \mathbb{R}^{m+1}$$

$$\Downarrow$$

$$\sum_{i=0}^{m} w_i x_i = 0 \Rightarrow \sum_{i=1}^{m} w_i x_i + \overset{b}{\boxed{w_0 x_0}} = 0$$

Hyperplane as A Classifier

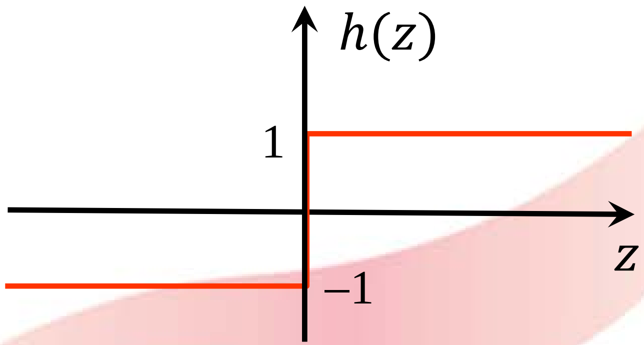
- Consider binary classification
- We can learn a hyperplane $\boldsymbol{w} \cdot \boldsymbol{x} = 0$ in terms of $\boldsymbol{w}$ to separate data instances of two different classes
- With the learned hyperplane, we can design a function $h(z)$ to generate classification result

$$\hat{y} = f(\boldsymbol{x}; \boldsymbol{\theta}) = h(\boldsymbol{w} \cdot \boldsymbol{x})$$

$z = \boldsymbol{w} \cdot \boldsymbol{x}$

$$h(z) = \begin{cases} +1 & \text{if } z \geq 0 \\ -1 & \text{if } z < 0 \end{cases}$$

This is also known as a sign or threshold function



Hyperplane as A Classifier (cont.)

- The sign function is NOT differentiable <u>everywhere</u>
- Need to look for a more smooth function

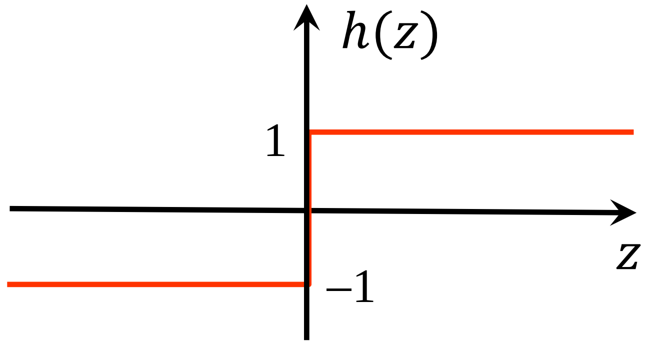
$$f(\boldsymbol{x}; \boldsymbol{\theta}) = h(\boldsymbol{w} \cdot \boldsymbol{x})$$

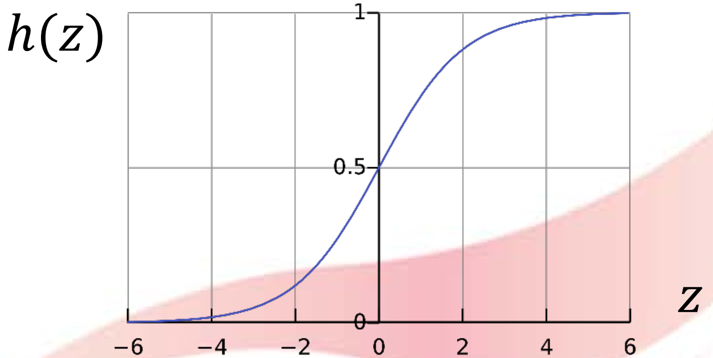
sigmoid function

$$h(z) = \begin{cases} +1 & \text{if } z \geq 0 \\ -1 & \text{if } z < 0 \end{cases}$$

$$h(z) = \frac{1}{1 + e^{-z}} = \frac{1}{1 + \exp(-z)}$$

$$z = \boldsymbol{w} \cdot \boldsymbol{x}$$

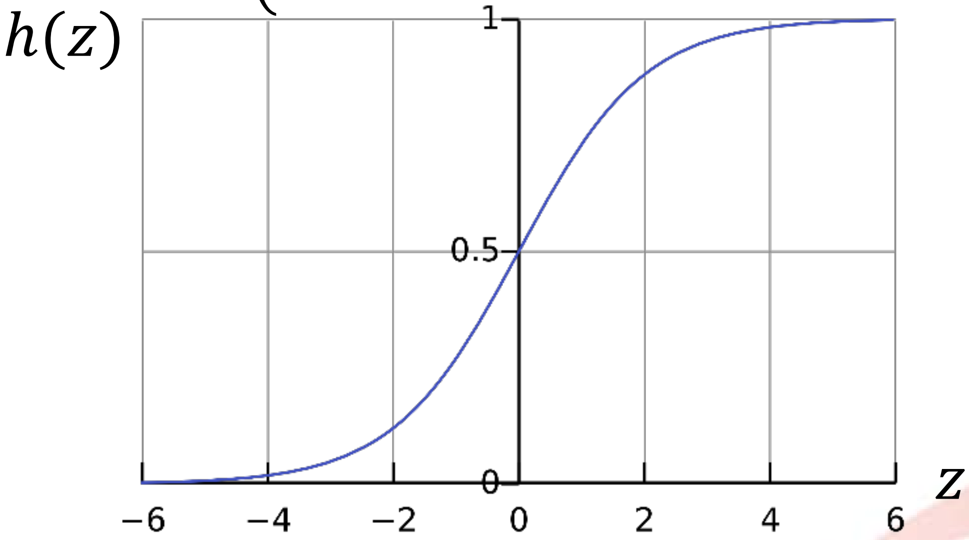




Hyperplane as A Classifier (cont.)

$$h(z) = \frac{1}{1+\exp(-z)} \qquad z = \boldsymbol{w} \cdot \boldsymbol{x}$$

$$\begin{cases} +1 & \text{if } h(z) \geq 0.5 \ (z \geq 0) \\ -1 & \text{if } h(z) < 0.5 \ (z < 0) \end{cases}$$



$$\{-1, +1\} \rightarrow \{0,1\}$$

$$\begin{cases} 1 & \text{if } h(z) \geq 0.5 \ (z \geq 0) \\ 0 & \text{if } h(z) < 0.5 \ (z < 0) \end{cases}$$

More convenient to design a loss function

Loss Function

- With the sigmoid function, the predicted values are in [0,1], the ground-truth values are in {0,1}, can we use the square loss as in linear regression?
- Given N training data instances $\{\boldsymbol{x}_i, y_i\}, i = 1, \dots, N$, where $\boldsymbol{x}_i$ is $(m+1)$-dimensional ($x_{0i} = 1$), and y_i is either 0 or 1

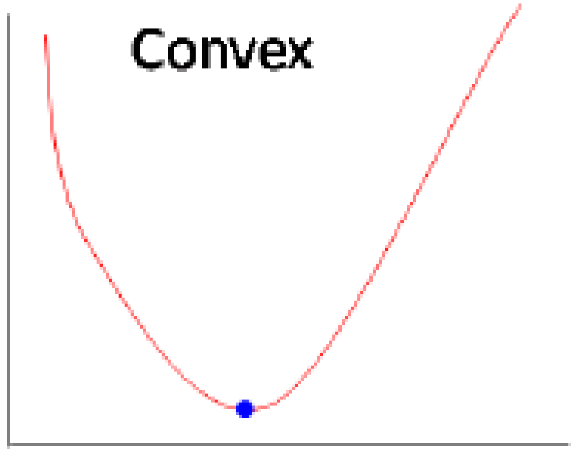
$$\sum_{i=1}^{N} \ell(h(\boldsymbol{x}_i; \boldsymbol{w}), y_i) = \sum_{i=1}^{N} (h(\boldsymbol{x}_i; \boldsymbol{w}) - y_i)^2$$

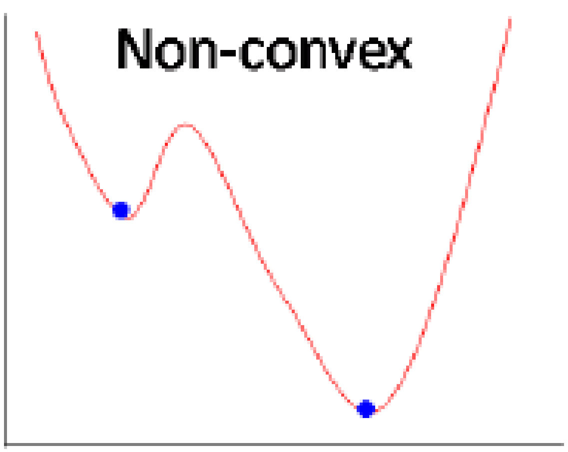
- However, $h(\boldsymbol{x}_i; \boldsymbol{w}) = \frac{1}{1+\exp(-\boldsymbol{w}\cdot\mathbf{x}_i)}$ is nonlinear w.r.t. $\boldsymbol{w}$. It can be shown that the square loss is non-convex

Loss Function (cont.)

$$\arg\min_{\boldsymbol{w}} \sum_{i=1}^{N} \left(\frac{1}{1+\exp(-\boldsymbol{w}\cdot\mathbf{x}_i)} - y_i \right)^2$$

- What is the problem if the objective is not convex?



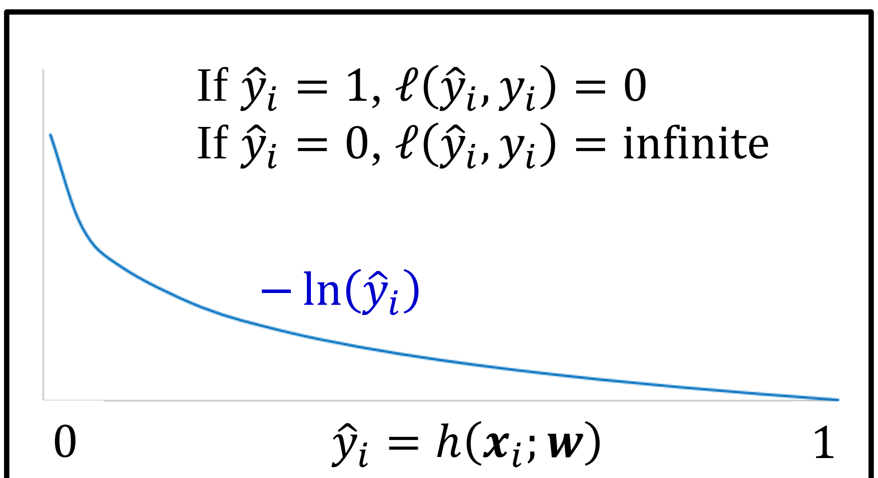


Logistic Regression Loss

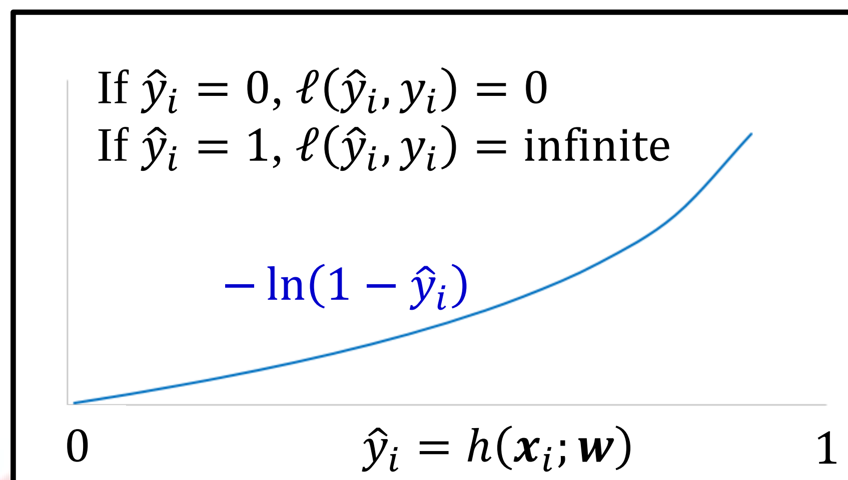
- Define the loss function as

$$\ell(h(\boldsymbol{x}_i;\boldsymbol{w}),y_i) = \begin{cases} -\ln\big(h(\boldsymbol{x}_i;\boldsymbol{w})\big) & \text{if } y_i = 1 \\ -\ln\big(1-h(\boldsymbol{x}_i;\boldsymbol{w})\big) & \text{if } y_i = 0 \end{cases}$$

$y_i = 1$



$y_i = 0$



Logistic Regression Loss (cont.)

$$\ell(h(\boldsymbol{x}_i;\boldsymbol{w}), y_i) = \begin{cases} -\ln\big(h(\boldsymbol{x}_i;\boldsymbol{w})\big) & \text{if } y_i = 1 \\ -\ln\big(1 - h(\boldsymbol{x}_i;\boldsymbol{w})\big) & \text{if } y_i = 0 \end{cases}$$

- The above loss can be simplified as

$$\ell(h(\boldsymbol{x}_i;\boldsymbol{w}), y_i) = -y_i \ln\big(h(\boldsymbol{x}_i;\boldsymbol{w})\big) - (1 - y_i)\ln\big(1 - h(\boldsymbol{x}_i;\boldsymbol{w})\big)$$

- If $y_i = 1$, then $\ell(h(\boldsymbol{x}_i;\boldsymbol{w}), y_i) = -\ln\big(h(\boldsymbol{x}_i;\boldsymbol{w})\big) - 0$
- If $y_i = 0$, then $\ell(h(\boldsymbol{x}_i;\boldsymbol{w}), y_i) = 0 - \ln\big(1 - h(\boldsymbol{x}_i;\boldsymbol{w})\big)$

Logistic Regression Objective

$$\arg\min_{\boldsymbol{w}} \sum_{i=1}^{N} \left[-y_i \ln\big(h(\boldsymbol{x}_i; \boldsymbol{w})\big) - (1 - y_i) \ln\big(1 - h(\boldsymbol{x}_i; \boldsymbol{w})\big) \right]$$

$$\Downarrow$$

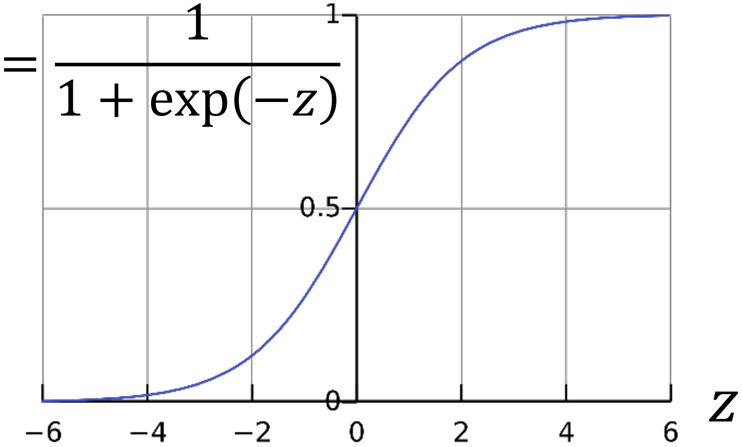
$$\arg\min_{\boldsymbol{w}} - \sum_{i=1}^{N} \left[y_i \ln\big(h(\boldsymbol{x}_i; \boldsymbol{w})\big) + (1 - y_i) \ln\big(1 - h(\boldsymbol{x}_i; \boldsymbol{w})\big) \right]$$

$$\text{where } h(\boldsymbol{x}_i; \boldsymbol{w}) = \frac{1}{1 + \exp(-\boldsymbol{w} \cdot \mathbf{x}_i)}$$

The objective is convex w.r.t. $\boldsymbol{w}$, and differentiable

Probabilistic Point of View

$z = \boldsymbol{w}^T \boldsymbol{x}$ $\qquad y = \dfrac{1}{1 + \exp(-z)}$



- Assume the conditional probability of class 1 is modeled as

$$P(y = 1|\boldsymbol{x}) = h(\boldsymbol{x}; \boldsymbol{w}) = \frac{1}{1 + \exp(-\boldsymbol{w}^T \boldsymbol{x})}$$

- Thus, the conditional probability of class 0 is

$$P(y = 0|\boldsymbol{x}) = 1 - P(y = 1|\boldsymbol{x}) = 1 - h(\boldsymbol{x}; w) = \frac{\exp(-\boldsymbol{w}^T \boldsymbol{x})}{1 + \exp(-\boldsymbol{w}^T \boldsymbol{x})}$$

Probability Review

- Let A be a random variable (a feature / a label in machine learning)
- Marginal probability $0 \leq P(A = a) \leq 1$

  $$P(A = a)$$

  refers to the probability that variable $A = a$

  $$\sum_{a_i} P(A = a_i) = 1$$

- For example, in binary classification problem, a class label y has two possible values, 0 or 1 (-1 or $+1$)

  $$P(y = 0) + P(y = 1) = 1$$

Probability Review (cont.)

- Let A and B be a pair of random variables (features/labels in machine learning).
- Their joint probability
$$P(A = a, B = b)$$
refers to the probability that variable $A = a$, and at the same time variable $B = b$
- E.g., for pair of input data instance and output label $(\boldsymbol{x}_i, y_i)$, its joint probability is
$$P(\boldsymbol{x} = \boldsymbol{x}_i, y = y_i)$$
OR
$P(\boldsymbol{x}_i, y_i)$ for simplicity

Probability Review (cont.)

- Conditional probability

$$P(B = b|A = a)$$

refers to the probability that variable B will take on the value b, given that the variable A is observed to have the value a

$$\sum_{b_i} P(B = b_i|A = a) = 1$$

- For example, in binary classification, given a data instance $\boldsymbol{x}_i$

$$P(y_i = 1|\boldsymbol{x}_i) + P(y_i = 0|\boldsymbol{x}_i) = 1$$

Parametric Form

$$P(y=1|\boldsymbol{x}) = h(\boldsymbol{x};\boldsymbol{w}) = \frac{1}{1+\exp(-\boldsymbol{w}^T\boldsymbol{x})}$$

$$P(y=0|\boldsymbol{x}) = 1 - h(\boldsymbol{x};w) = \frac{\exp(-\boldsymbol{w}^T\boldsymbol{x})}{1+\exp(-\boldsymbol{w}^T\boldsymbol{x})}$$

- We can define more compact form as

$$P(y|\boldsymbol{x};\boldsymbol{w}) = h(\boldsymbol{x};\boldsymbol{w})^y(1-h(\boldsymbol{x};\boldsymbol{w}))^{1-y}$$

- If $y=1$, then $P(y|\boldsymbol{x};\boldsymbol{w}) = h(\boldsymbol{x};\boldsymbol{w})^1(1-h(\boldsymbol{x};\boldsymbol{w}))^0$
- If $y=0$, then $P(y|\boldsymbol{x};\boldsymbol{w}) = h(\boldsymbol{x};\boldsymbol{w})^0(1-h(\boldsymbol{x};\boldsymbol{w}))^1$
- To find $\boldsymbol{w}$ that makes sampling y_i conditioned on $\boldsymbol{x}_i$ from $P(y|\boldsymbol{x};\boldsymbol{w})$ as likely as possible
  - Maximum likelihood estimation

Maximum Likelihood Estimation

- For each training pair $\{\boldsymbol{x}_i, y_i\}$, the likelihood of parameter $\boldsymbol{w}$ of the conditional probability $P(y|\boldsymbol{x};\boldsymbol{w})$ is

$$l(\boldsymbol{w}|\{\boldsymbol{x}_i, y_i\}) \triangleq P(y_i|\boldsymbol{x}_i;\boldsymbol{w}) = h(\boldsymbol{x}_i;\boldsymbol{w})^{y_i}(1 - h(\boldsymbol{x}_i;\boldsymbol{w}))^{1-y_i}$$

  - Ideally, for each training pair $\{\boldsymbol{x}_i, y_i\}$, $l(\boldsymbol{w}|\{\boldsymbol{x}_i, y_i\}) = P(y_i|\boldsymbol{x}_i;\boldsymbol{w}) = 1$
- Maximum likelihood estimation (MLE) aims to find a solution of $\boldsymbol{w}$ such that $P(y_i|\boldsymbol{x}_i;\boldsymbol{w})$ is maximized

$$\hat{\boldsymbol{w}} = \arg\max_{\boldsymbol{w}} l(\boldsymbol{w}|\{\boldsymbol{x}_i, y_i\}) = \arg\max_{\boldsymbol{w}} P(y_i|\boldsymbol{x}_i;\boldsymbol{w})$$

  - The parametric form of the conditional probability fits the pair of input data instance and corresponding output well

MLE (cont.)

- Given a set of N training input-output pairs $\{\boldsymbol{x}_i, y_i\}, i = 1, \dots, N$, which are i.i.d., the likelihood is defined as the product of the likelihoods of each individual data pairs

$$\mathcal{L}(\boldsymbol{w}) = \prod_{i=1}^{N} l(\boldsymbol{w}|\{\boldsymbol{x}_i, y_i\}) = \prod_{i=1}^{N} P(y_i|\boldsymbol{x}_i; \boldsymbol{w})$$

- The goal of MLE is to find a solution of $\boldsymbol{w}$ such that $\mathcal{L}(\boldsymbol{w})$ is maximized, ideally for all $\{\boldsymbol{x}_i, y_i\}, i = 1, \dots, N$, $P(y_i|\boldsymbol{x}_i; \boldsymbol{w}) = 1$, and thus $\mathcal{L}(\boldsymbol{w}) = 1$

$$\widehat{\boldsymbol{w}} = \arg\max_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) = \arg\max_{\boldsymbol{w}} \prod_{i=1}^{N} P(y_i|\boldsymbol{x}_i; \boldsymbol{w})$$

MLE (cont.)

$\ln(ab) = \ln a + \ln b$

$$\hat{\boldsymbol{w}} = \arg\max_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) = \arg\max_{\boldsymbol{w}} \boxed{\prod_{i=1}^{N} P(y_i|\boldsymbol{x}_i;\boldsymbol{w})}$$

- In practice, we maximize $\ln\mathcal{L}(\boldsymbol{w})$ instead. Why?
  1. The $\ln(\cdot)$ function converts the product into a sum

$$\ln\mathcal{L}(\boldsymbol{w}) = \ln\left(\prod_{i=1}^{N} P(y_i|\boldsymbol{x}_i;\boldsymbol{w})\right) = \boxed{\sum_{i=1}^{N} \ln P(y_i|\boldsymbol{x}_i;\boldsymbol{w})}$$

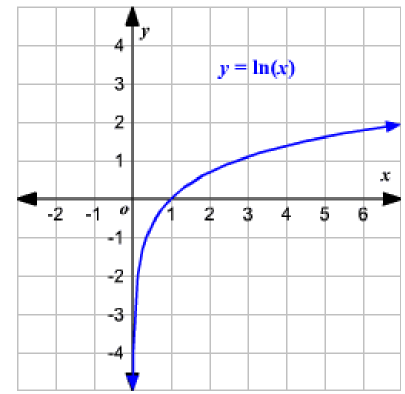
  2. The $\ln(\cdot)$ function is a strictly increasing function, the solution of $\boldsymbol{w}$ remains the same

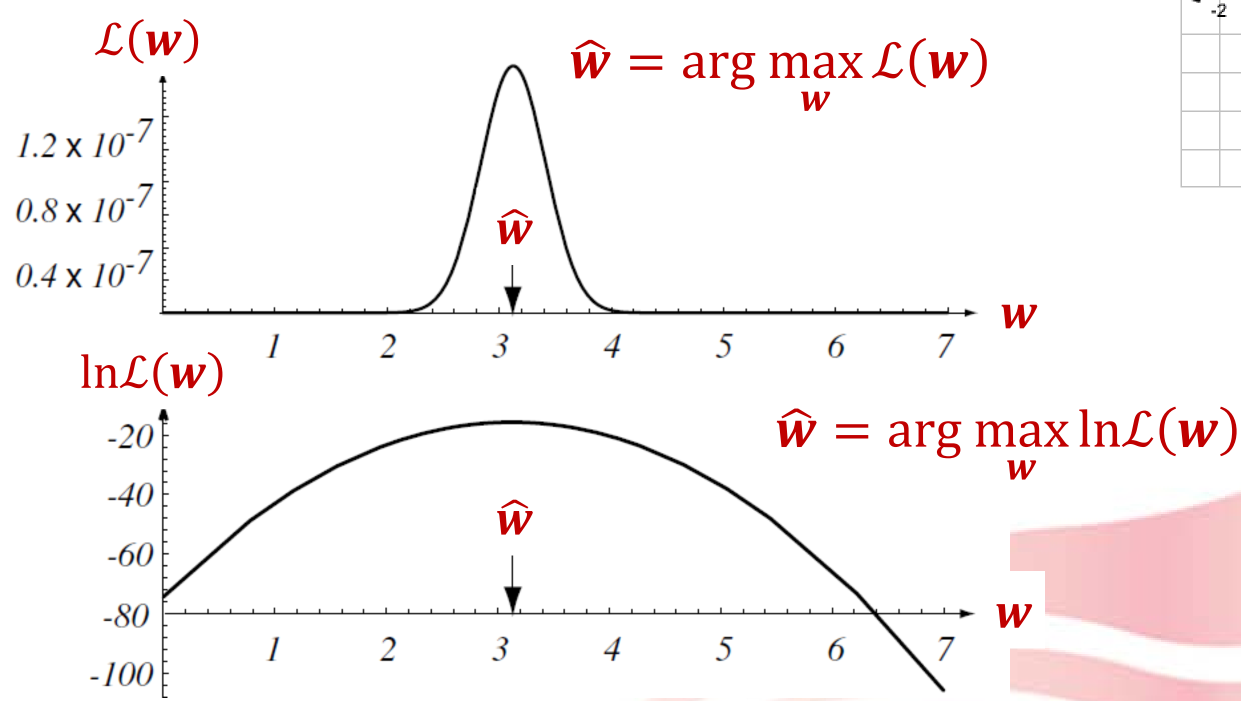
$$\hat{\boldsymbol{w}} = \arg\max_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) \Leftrightarrow \hat{\boldsymbol{w}} = \arg\max_{\boldsymbol{w}} \ln\mathcal{L}(\boldsymbol{w})$$

Maximum Log-Likelihood

- How to understand "the $\ln(\cdot)$ function is a strictly increasing function, the solution of $\boldsymbol{w}$ remains the same"

$$\widehat{\boldsymbol{w}} = \arg\max_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) \Leftrightarrow \widehat{\boldsymbol{w}} = \arg\max_{\boldsymbol{w}} \ln\mathcal{L}(\boldsymbol{w})$$





Maximum Log-Likelihood (cont.)

$$\hat{\boldsymbol{w}} = \arg\max_{\boldsymbol{w}} \ln \mathcal{L}(\boldsymbol{w}) = \arg\max_{\boldsymbol{w}} \sum_{i=1}^{N} \ln P(y_i|\boldsymbol{x}_i;\boldsymbol{w})$$

Recall that $P(y_i|\boldsymbol{x}_i;\boldsymbol{w}) = h(\boldsymbol{x}_i;\boldsymbol{w})^{y_i}(1 - h(\boldsymbol{x}_i;\boldsymbol{w}))^{1-y_i}$

$$\hat{\boldsymbol{w}} = \arg\max_{\boldsymbol{w}} \sum_{i=1}^{N} \ln(h(\boldsymbol{x}_i;\boldsymbol{w})^{y_i}(1 - h(\boldsymbol{x}_i;\boldsymbol{w}))^{1-y_i})$$

$$\ln\left(a^c b^d\right) = \ln a^c + \ln b^d = c \ln a + d \ln b$$

$$\hat{\boldsymbol{w}} = \arg\max_{\boldsymbol{w}} \sum_{i=1}^{N} \left[y_i \ln\left(h(\boldsymbol{x}_i;\boldsymbol{w})\right) + (1 - y_i) \ln\left(1 - h(\boldsymbol{x}_i;\boldsymbol{w})\right)\right]$$

Maximum Log-Likelihood (cont.)

$$\hat{\boldsymbol{w}} = \arg\max_{\boldsymbol{w}} \sum_{i=1}^{N} \left[y_i \ln\left(h(\boldsymbol{x}_i; \boldsymbol{w})\right) + (1 - y_i) \ln\left(1 - h(\boldsymbol{x}_i; \boldsymbol{w})\right) \right]$$

Equivalent!

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} - \sum_{i=1}^{N} \left[y_i \ln\left(h(\boldsymbol{x}_i; \boldsymbol{w})\right) + (1 - y_i) \ln\left(1 - h(\boldsymbol{x}_i; \boldsymbol{w})\right) \right]$$

The objective induced on Page 15 based on empirical risk minimization

Why Called Logistic Regression?

- In statistics, given a variable z that has two outcomes $\{0, 1\}$, denoted by $p = P(z = 1)$, then $1 - p = P(z = 0)$
- The odds of the probability p is defined as the ratio of p and $1 - p$

$$\text{odds} = \frac{P(z = 1)}{P(z = 0)} = \frac{p}{1 - p}$$

- The logit of the probability p is the logarithm of the odds:

$$\text{logit}(p) = \ln(\text{odds}) = \ln\left(\frac{p}{1 - p}\right)$$

- Recall that

$$P(y = 1|\boldsymbol{x}) = h(\boldsymbol{x}; \boldsymbol{w}) = \frac{1}{1 + \exp(-\boldsymbol{w}^T\boldsymbol{x})}$$

$$P(y = 0|\boldsymbol{x}) = 1 - h(\boldsymbol{x}; w) = \frac{\exp(-\boldsymbol{w}^T\boldsymbol{x})}{1 + \exp(-\boldsymbol{w}^T\boldsymbol{x})}$$

Logit + Regression

- Denote by

$$p = P(y = 1|\boldsymbol{x}) = \frac{1}{1 + \exp(-\boldsymbol{w}^T\boldsymbol{x})}$$

- The logit of p is

$$\underbrace{\boxed{\ln\left(\frac{p}{1-p}\right)}}_{\text{logit}} = \ln\left(\frac{\frac{1}{1+\exp(-\boldsymbol{w}^T\boldsymbol{x})}}{\frac{\exp(-\boldsymbol{w}^T\boldsymbol{x})}{1+\exp(-\boldsymbol{w}^T\boldsymbol{x})}}\right)$$

$$= \ln(\exp(-\boldsymbol{w}^T\boldsymbol{x}))^{-1}$$

logistic regression

$$\ln(\exp(a)^{-1}) = -1 \ln \exp(a) = -a$$

$$= -1 \times (-\boldsymbol{w}^T\boldsymbol{x})$$

$$= \boxed{\boldsymbol{w}^T\boldsymbol{x}} \quad \text{Linear regression}$$

Approaches to Solution

Objective $E(\boldsymbol{w})$

$$\widehat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} \boxed{-\sum_{i=1}^{N}\left[y_i \ln\big(h(\boldsymbol{x}_i;\boldsymbol{w})\big) + (1-y_i)\ln\big(1-h(\boldsymbol{x}_i;\boldsymbol{w})\big)\right]}$$

- The objective is convex, differentiable, without constraints
- Can we set derivatives equal to zero and solve the resultant equations to get a closed form solution?
- Optimization methods
  - Gradient descent – first order methods
  - Newton’s method – second order methods

Optimization

- Gradient descent

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \rho \frac{\partial E(\boldsymbol{w})}{\partial \boldsymbol{w}}$$

$$\frac{\partial E(\boldsymbol{w})}{\partial \boldsymbol{w}} = \frac{\partial\left(-\sum_{i=1}^{N}\left[y_i \ln\left(h(\boldsymbol{x}_i;\boldsymbol{w})\right) + (1-y_i)\ln\left(1-h(\boldsymbol{x}_i;\boldsymbol{w})\right)\right]\right)}{\partial \boldsymbol{w}}$$

$$= -\sum_{i=1}^{N} \frac{\partial\left[y_i \ln\left(h(\boldsymbol{x}_i;\boldsymbol{w})\right) + (1-y_i)\ln\left(1-h(\boldsymbol{x}_i;\boldsymbol{w})\right)\right]}{\partial \boldsymbol{w}}$$

$$= -\sum_{i=1}^{N} \left(\frac{\partial\left(y_i \ln\left(h(\boldsymbol{x}_i;\boldsymbol{w})\right)\right)}{\partial \boldsymbol{w}} + \frac{\partial\left((1-y_i)\ln\left(1-h(\boldsymbol{x}_i;\boldsymbol{w})\right)\right)}{\partial \boldsymbol{w}} \right)$$

Optimization (cont.)

$$\frac{\partial\left(y_i \ln\left(h(\boldsymbol{x}_i;\boldsymbol{w})\right)\right)}{\partial \boldsymbol{w}}$$

$$\frac{\partial \ln f(z)}{\partial z} = \frac{\partial \ln f(z)}{\partial f(z)} \frac{\partial f(z)}{\partial z} = \frac{1}{f(z)} \frac{\partial f(z)}{\partial z}$$

$$= y_i \frac{1}{h(\boldsymbol{x}_i;\boldsymbol{w})} \frac{\partial\left(h(\boldsymbol{x}_i;\boldsymbol{w})\right)}{\partial \boldsymbol{w}}$$

$$P(y=1|\boldsymbol{x}_i) = h(\boldsymbol{x}_i;\boldsymbol{w}) = \frac{1}{1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)}$$

$$= y_i \frac{1}{h(\boldsymbol{x}_i;\boldsymbol{w})} \frac{\partial\left((1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i))^{-1}\right)}{\partial \boldsymbol{w}}$$

$$\frac{\partial f(z)^k}{\partial z} = \frac{\partial f(z)^k}{\partial f(z)} \frac{\partial f(z)}{\partial z} = k f(z)^{k-1} \frac{\partial f(z)}{\partial z}$$

$$= y_i \frac{1}{h(\boldsymbol{x}_i;\boldsymbol{w})} (-1)(1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)\,)^{-2} \frac{\partial \exp(-\boldsymbol{w}^T\boldsymbol{x}_i)}{\partial \boldsymbol{w}}$$

Optimization (cont.)

$$y_i \frac{1}{h(\boldsymbol{x}_i;\boldsymbol{w})}(-1)\left(1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)\right)^{-2}\frac{\partial \exp(-\boldsymbol{w}^T\boldsymbol{x}_i)}{\partial \boldsymbol{w}}$$

$$\frac{\partial \exp\big(f(z)\big)}{\partial z} = \frac{\partial \exp(f(z))}{\partial f(z)}\frac{\partial f(z)}{\partial z} = \exp(f(z))\frac{\partial f(z)}{\partial z}$$

$$= y_i \frac{1}{h(\boldsymbol{x}_i;\boldsymbol{w})}(-1)\left(1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)\right)^{-2}\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)(-\boldsymbol{x}_i)$$

$$P(y=1|\boldsymbol{x}_i) = h(\boldsymbol{x}_i;\boldsymbol{w}) = \frac{1}{1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)}$$

$$= y_i(1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i))\frac{1}{(1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i))^2}\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)\boldsymbol{x}_i$$

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

Optimization (cont.)

$$\frac{\partial\left((1-y_i)\ln\left(1-h(\boldsymbol{x}_i;\boldsymbol{w})\right)\right)}{\partial \boldsymbol{w}}$$

$$=(1-y_i)\frac{1}{1-h(\boldsymbol{x}_i;\boldsymbol{w})}(-1)\frac{\partial\left(h(\boldsymbol{x}_i;\boldsymbol{w})\right)}{\partial \boldsymbol{w}}$$

$$P(y=1|\boldsymbol{x}_i)=h(\boldsymbol{x}_i;\boldsymbol{w})=\frac{1}{1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)}$$

$$=(y_i-1)\frac{1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)}{\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)}\frac{1}{(1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i))^2}\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)\boldsymbol{x}_i$$

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

Optimization (cont.)

$$\frac{\partial\Big((1-y_i)\ln\big(1-h(\boldsymbol{x}_i;\boldsymbol{w})\big)\Big)}{\partial\boldsymbol{w}} = (y_i-1)\frac{1}{1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)}\boldsymbol{x}_i$$

$$= (y_i-1)h(\boldsymbol{x}_i;\boldsymbol{w})\boldsymbol{x}_i$$

$$\frac{\partial\Big(y_i\ln\big(h(\boldsymbol{x}_i;\boldsymbol{w})\big)\Big)}{\partial\boldsymbol{w}} = y_i\frac{\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)}{1+\exp(-\boldsymbol{w}^T\boldsymbol{x}_i)}\boldsymbol{x}_i$$

$$= y_i\big(1-h(\boldsymbol{x}_i;\boldsymbol{w})\big)\boldsymbol{x}_i$$

$$\frac{\partial\Big((1-y_i)\ln\big(1-h(\boldsymbol{x}_i;\boldsymbol{w})\big)\Big)}{\partial\boldsymbol{w}} + \frac{\partial\Big(y_i\ln\big(h(\boldsymbol{x}_i;\boldsymbol{w})\big)\Big)}{\partial\boldsymbol{w}} = \big(y_i-h(\boldsymbol{x}_i;\boldsymbol{w})\big)\boldsymbol{x}_i$$

Optimization (cont.)

$$\frac{\partial E(\boldsymbol{w})}{\partial \boldsymbol{w}} = -\sum_{i=1}^{N}\left(\frac{\partial\Big(y_i \ln\big(h(\boldsymbol{x}_i;\boldsymbol{w})\big)\Big)}{\partial \boldsymbol{w}} + \frac{\partial\Big((1-y_i)\ln\big(1-h(\boldsymbol{x}_i;\boldsymbol{w})\big)\Big)}{\partial \boldsymbol{w}}\right)$$

$$= -\sum_{i=1}^{N}\big(y_i - h(\boldsymbol{x}_i;\boldsymbol{w})\big)\boldsymbol{x}_i$$

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \rho\frac{\partial E(\boldsymbol{w})}{\partial \boldsymbol{w}} = \boldsymbol{w}_t + \rho\sum_{i=1}^{N}\big(y_i - h(\boldsymbol{x}_i;\boldsymbol{w})\big)\boldsymbol{x}_i$$

Recall: Approaches to Solution

Objective $E(\boldsymbol{w})$

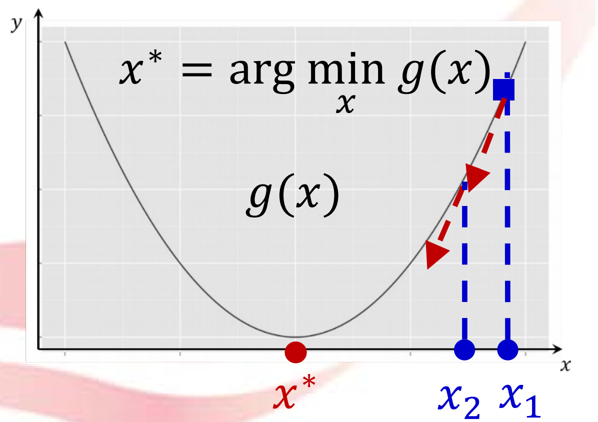
$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} \boxed{-\sum_{i=1}^{N}\left[y_i \ln\left(h(\boldsymbol{x}_i;\boldsymbol{w})\right) + (1-y_i)\ln\left(1-h(\boldsymbol{x}_i;\boldsymbol{w})\right)\right]}$$

- The objective is convex, differentiable, without constraints
- ~~Can we set derivatives equal to zero and solve the resultant equations to get a closed form solution?~~
- Optimization methods
  - Gradient descent – first order methods ✓
  - Newton's method – second order methods

Newton's Method in Optimization

- Consider one dimension case, and our goal is to find an optimal solution x^* that minimizes a convex objective $g(x)$
- Gradient descent methods only use the first derivative together with a learning rate (step size) to generate a series $\{x_t\}, t = 0,1, \ldots,$ iteratively, which converges to the optimal solution x^*
  – May take many steps to converge to the optimum
- Newton's method aims to exploit the second order derivative to "guess" a better x_t at each iteration t
  – Needs fewer steps to converge to the optimum
  – Assumption: $g(x)$ is at least twice differentiable, and $g''(x) \neq 0$

Out of scope



Regularized Logistic Regression

Objective $E(\boldsymbol{w})$

$$\min_{\boldsymbol{w}} \boxed{-\sum_{i=1}^{N}\left[y_i \ln\big(h(\boldsymbol{x}_i;\boldsymbol{w})\big) + (1-y_i)\ln\big(1-h(\boldsymbol{x}_i;\boldsymbol{w})\big)\right] + \frac{\lambda}{2}\|\boldsymbol{w}\|_2^2}$$

$$\frac{\partial E(\boldsymbol{w})}{\partial \boldsymbol{w}} = -\sum_{i=1}^{N}\left(\frac{\partial\Big(y_i \ln\big(h(\boldsymbol{x}_i;\boldsymbol{w})\big) + (1-y_i)\ln\big(1-h(\boldsymbol{x}_i;\boldsymbol{w})\big)\Big)}{\partial \boldsymbol{w}}\right) + \frac{\partial\left(\frac{\lambda}{2}\|\boldsymbol{w}\|_2^2\right)}{\partial \boldsymbol{w}}$$

$$= -\sum_{i=1}^{N}\big(y_i - h(\boldsymbol{x}_i;\boldsymbol{w})\big)\boldsymbol{x}_i + \lambda\boldsymbol{w}$$

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \rho\frac{\partial E(\boldsymbol{w})}{\partial \boldsymbol{w}} = \boldsymbol{w}_t + \rho\left(\sum_{i=1}^{N}\big(y_i - h(\boldsymbol{x}_i;\boldsymbol{w})\big)\boldsymbol{x}_i - \lambda\boldsymbol{w}\right)$$

Extension to Multiple Classes

- Suppose there are C classes, $\{0, 1, \ldots, C-1\}$
- Each class except class 0 is associated with a specific $\boldsymbol{w}^{(c)}, c = 1, \ldots, C-1$

For $c > 0$: $P(y = c|\boldsymbol{x}) = \dfrac{\exp\left(-\boldsymbol{w}^{(c)^T}\boldsymbol{x}\right)}{1 + \sum_{c=1}^{C-1}\exp\left(-\boldsymbol{w}^{(c)^T}\boldsymbol{x}\right)}$

For $c = 0$: $P(y = 0|\boldsymbol{x}) = \dfrac{1}{1 + \sum_{c=1}^{C-1}\exp\left(-\boldsymbol{w}^{(c)^T}\boldsymbol{x}\right)}$

$$\sum_{c=0}^{C-1} P(y = c|\boldsymbol{x}) = 1$$

- For learning each $\boldsymbol{w}^{(c)}$, the procedure is basically the same as what we derived!
- For a test data instance $\boldsymbol{x}^*$, $y^* = \arg\max_{c \in \{0,\ldots,C-1\}} P(y = c|\boldsymbol{x}^*)$

Self-reading on additional notes

Implementation using scikit-learn

- API: sklearn.linear_model: Linear Models
  https://scikit-learn.org/stable/modules/classes.html#module-sklearn.linear_model

Linear classifiers

`linear_model.LogisticRegression`([penalty, ...])	Logistic Regression (aka logit, MaxEnt) classifier.
`linear_model.LogisticRegressionCV`(*[, Cs, ...])	Logistic Regression CV (aka logit, MaxEnt) classifier.

sklearn.linear_model.LogisticRegression

class `sklearn.linear_model.LogisticRegression`(*penalty='l2', *, dual=False, tol=0.0001, C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100, multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None*) [source]

C : *float, default=1.0*

Inverse of regularization strength; must be a positive float. Like in support vector machines, smaller values specify stronger regularization.

Example

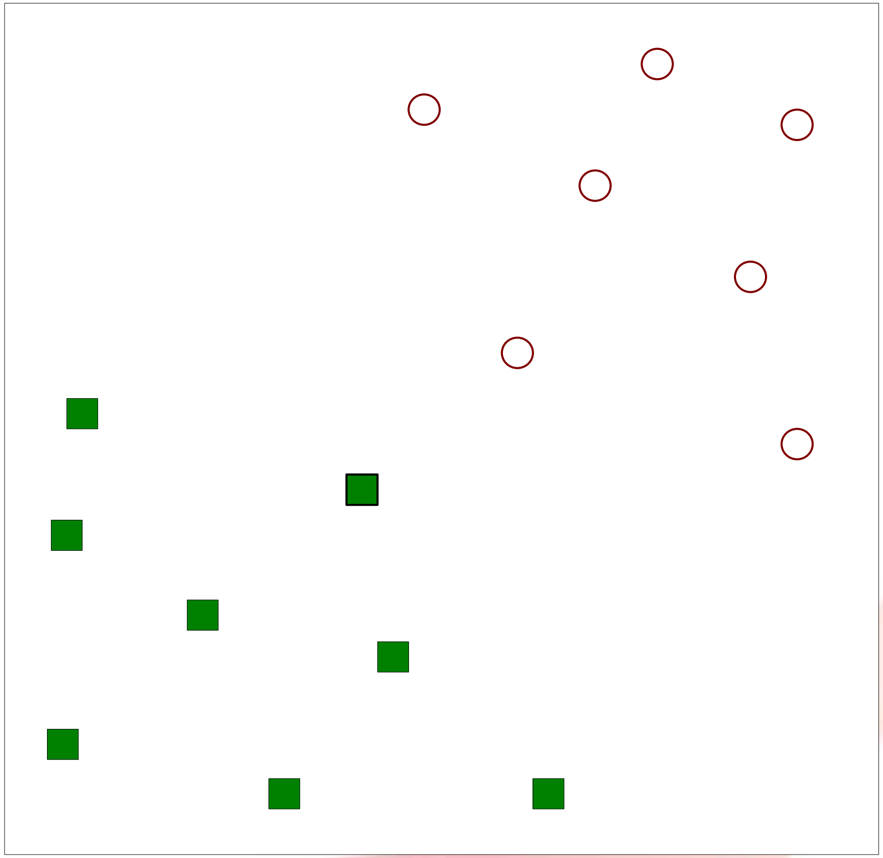
```
>>> from sklearn.linear_model import LogisticRegression
>>> import numpy as np

>>> n_samples, n_features = 10, 5
>>> rng = np.random.RandomState(0)
>>> y = rng.integers(2, n_samples)
>>> X = rng.randn(n_samples, n_features)

>>> logisticR = LogisticRegression()
>>> logisticR.fit(X, y)
>>> pred= logisticR.predict(X)
```

Model training and testing

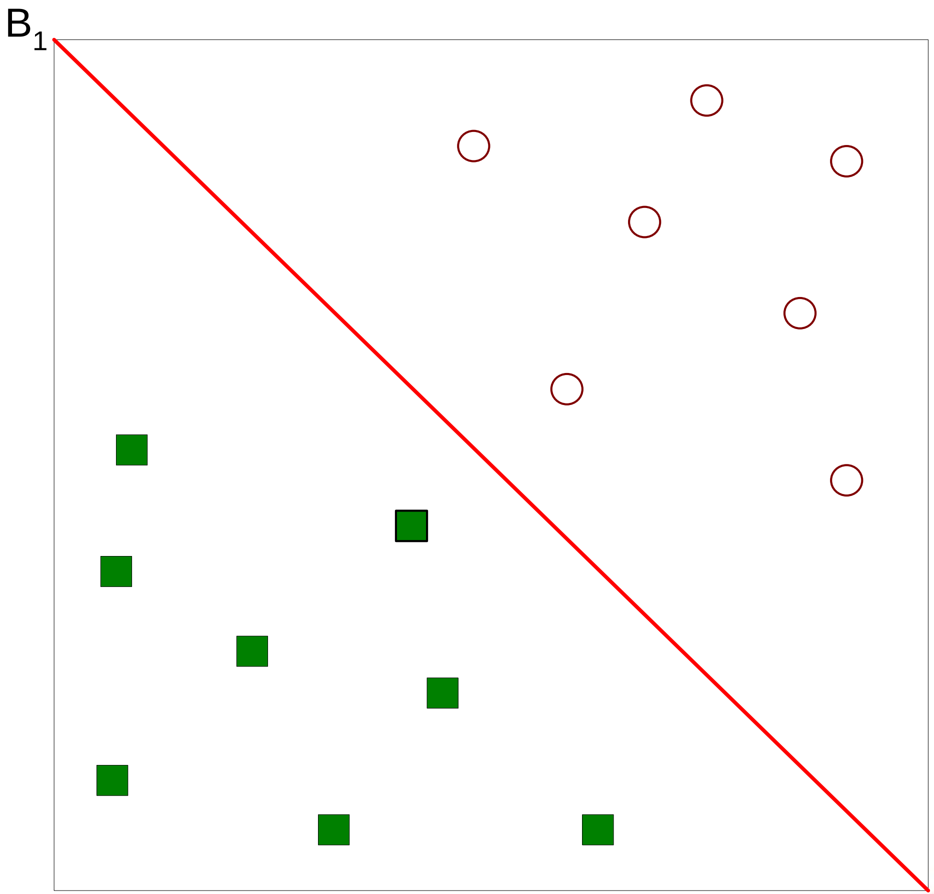
Support Vector Machines

- To learn a binary classifier

- To find a hyperplane (also known as decision boundary) such that all the squares reside on one side of the hyperplane and all the circles reside on the other side

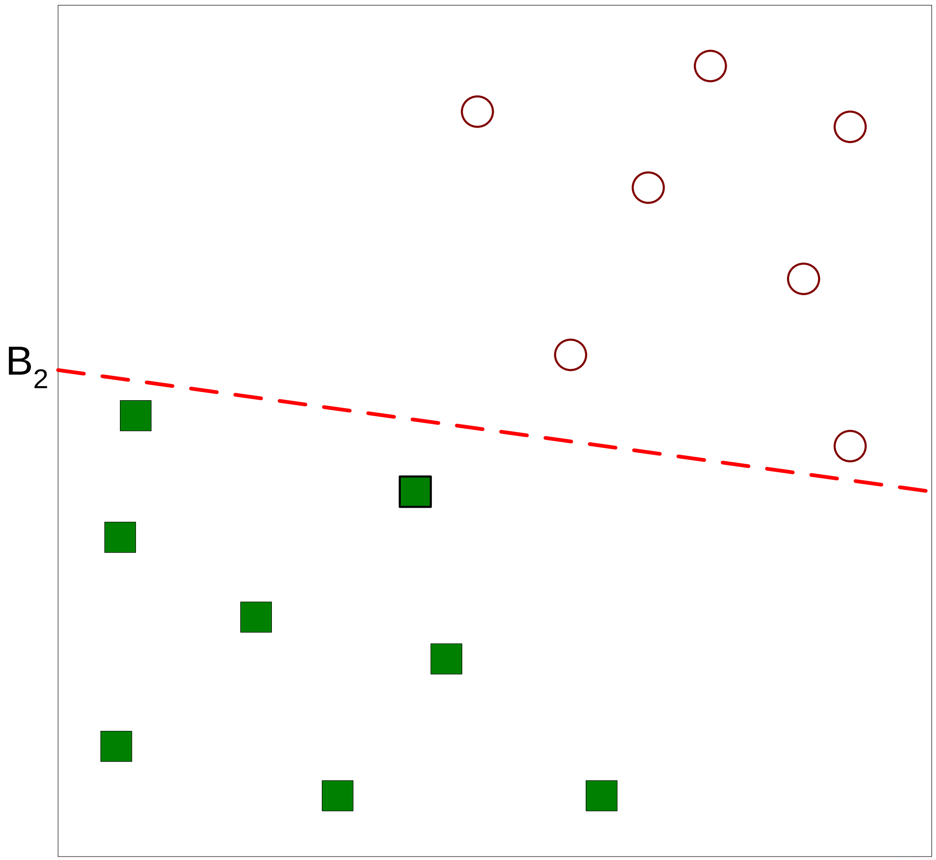


A Possible Decision Boundary



One Possible Solution

Another Possible Decision Boundary

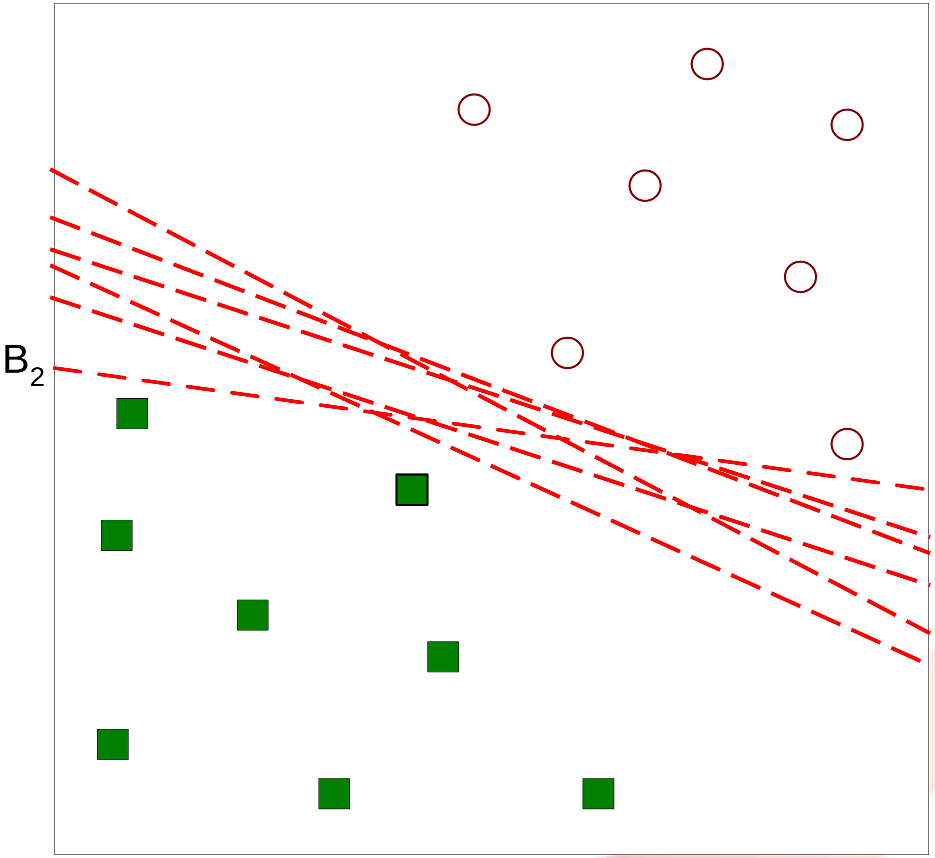


Another possible solution

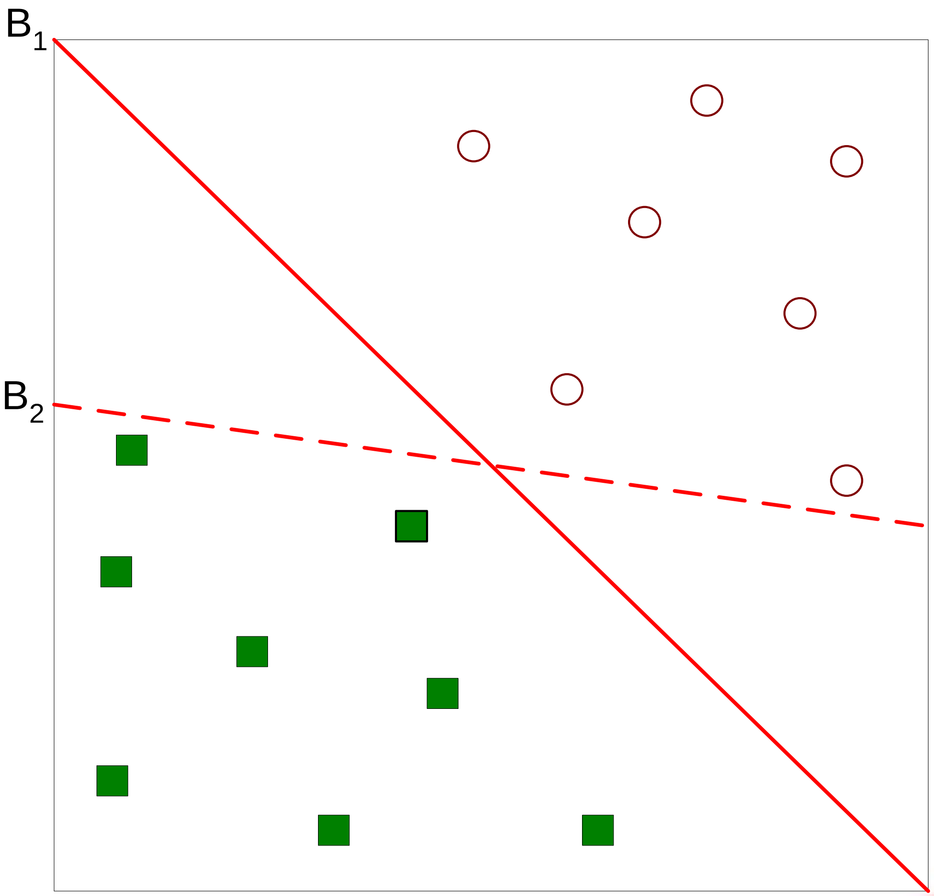
Many Possible Decision Boundary

- Though all the shown decision boundaries can separate training examples perfectly, their test errors may be different

- Which one should be used to construct the classifier?

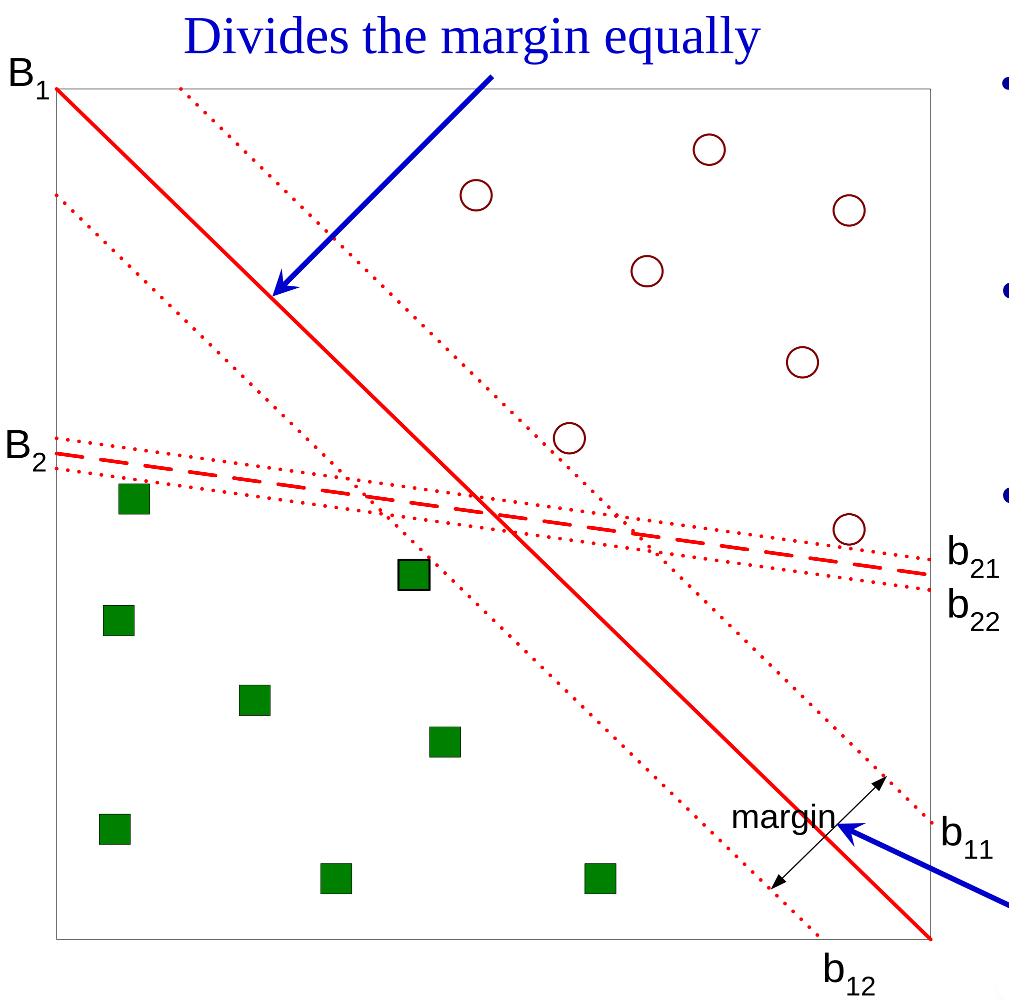


Decision Boundaries Comparison



Which one is better? B1 or B2?

Margin of Decision Boundary



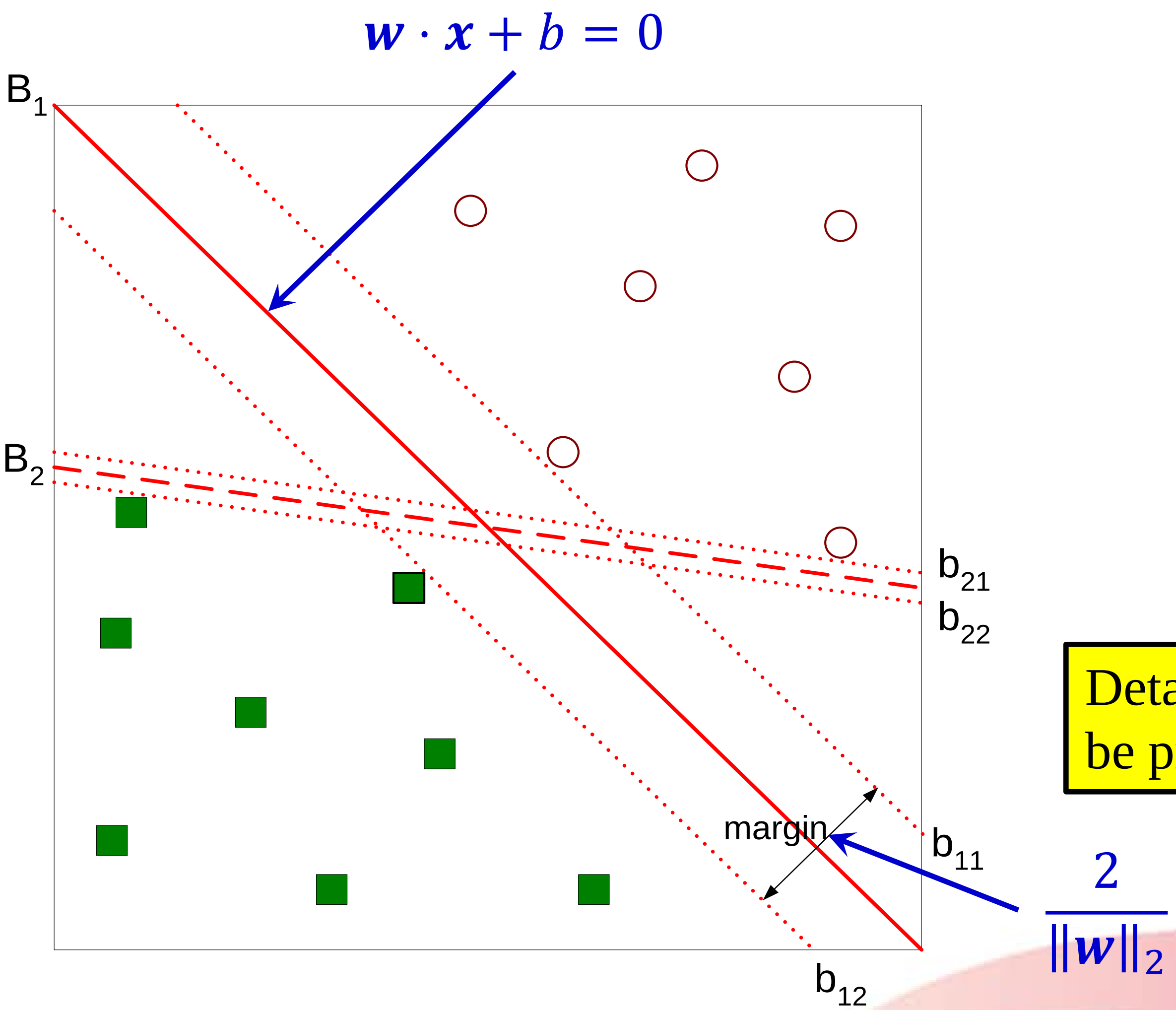
- Each decision boundary B_i is associated with a pair of parallel hyperplanes: b_{i1} and b_{i2}
- b_{i1} is obtained by moving the hyperplane until it touches the closest circle(s)
- b_{i2} is obtained by moving a hyperplane away from the decision boundary until it touches the closest square(s)

The distance between the parallel hyperplanes is known as the margin of the decision boundary

Support Vector Machines

- Support Vector Machines (SVMs) aim to learn a linear decision boundary whose margin is largest over the training data instances
- SVMs are one of the most classical machine learning methods
- In the past (in 90’s and 00’s), SVMs have shown promising empirical results in many practical applications, such as computer vision, sensor networks and text mining

How to Represent A Margin?



Detailed induction will be presented next week

Optimization Problem

Detailed induction will be presented next week

- Optimization problem of linear SVMs (separable case)

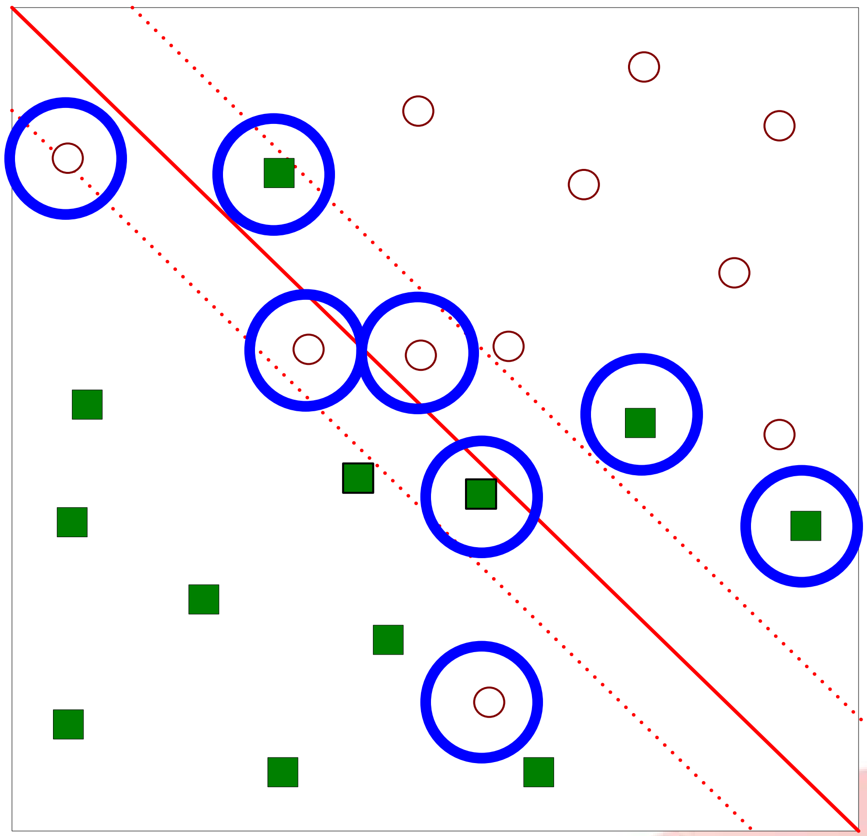
$$
\begin{aligned}
&\min_{\boldsymbol{w},b} \ \frac{\|\boldsymbol{w}\|_2^2}{2} \\
&\text{s.t.} \quad \boldsymbol{w}\cdot\boldsymbol{x}_i + b \ge 1, \text{if } y_i = 1, \\
&\qquad\ \ \boldsymbol{w}\cdot\boldsymbol{x}_i + b \le -1, \text{if } y_i = -1, \\
&\qquad\ \ i = 1, \ldots, N
\end{aligned}
$$

$$\Downarrow$$

$$
\begin{aligned}
&\min_{\boldsymbol{w},b} \ \frac{\|\boldsymbol{w}\|_2^2}{2} \\
&\text{s.t.} \quad y_i \times (\boldsymbol{w}\cdot\boldsymbol{x}_i + b) \ge 1,\ i = 1, \ldots, N
\end{aligned}
$$

Linear SVMs: Non-separable Case

- What if data instances of the two class are not separable?



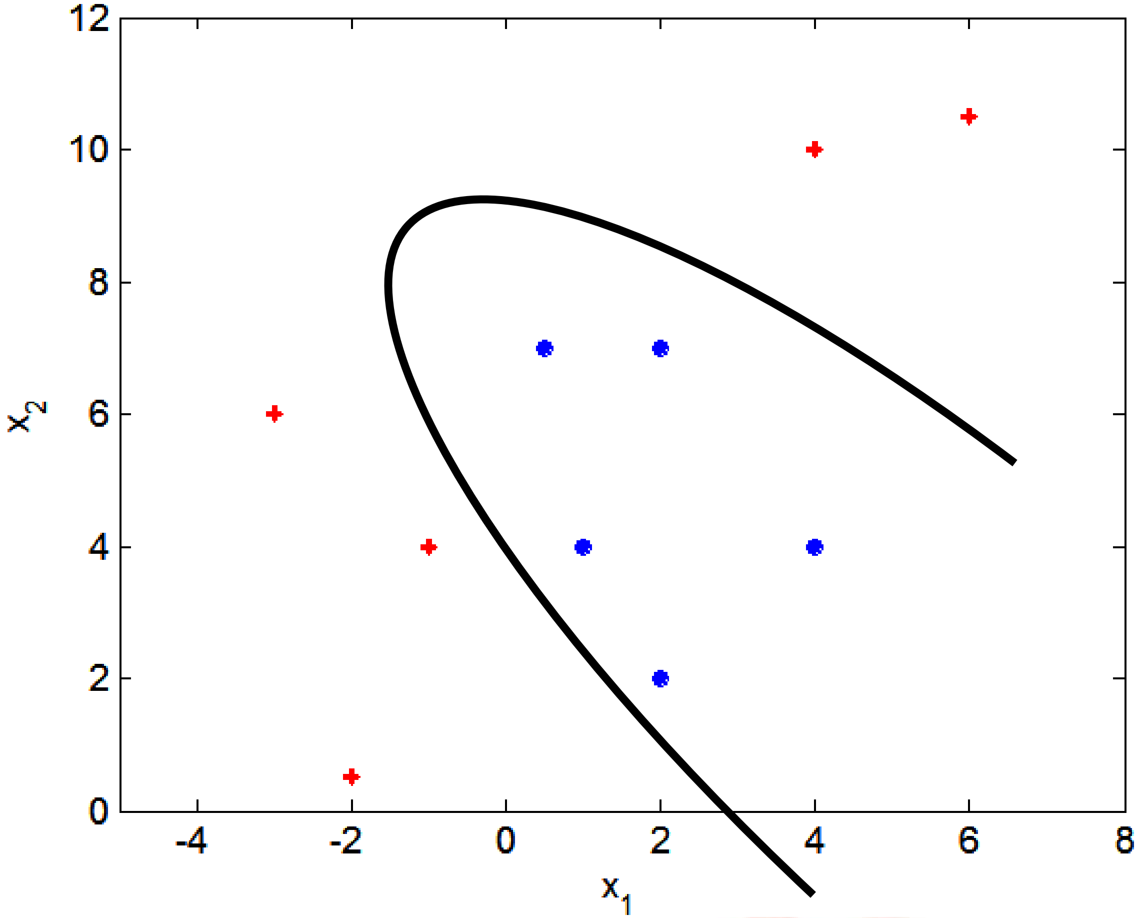
Slack variables $\xi_i \geq 0$ need to be introduced to absorb errors

Detailed induction will be presented next week

Nonlinear SVMs

Detailed induction will be presented next week

- What if the decision boundary is not linear?



Kernel methods

Thank you!