기계학습 (2022년도 2학기)

SVMs and Boosting

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Overview

- Support Vector Machines
- Connection between Exponential Loss and AdaBoost

Binary Classification with a Linear Model

- Classification: Predict a discrete-valued target
- Binary classification: Targets $t \in \{-1, +1\}$
- Linear model:

$$z = \mathbf{w}^\top \mathbf{x} + b$$
$$y = sign(z)$$

- Question: How should we choose $\boldsymbol{w}$ and b?

Zero-One Loss

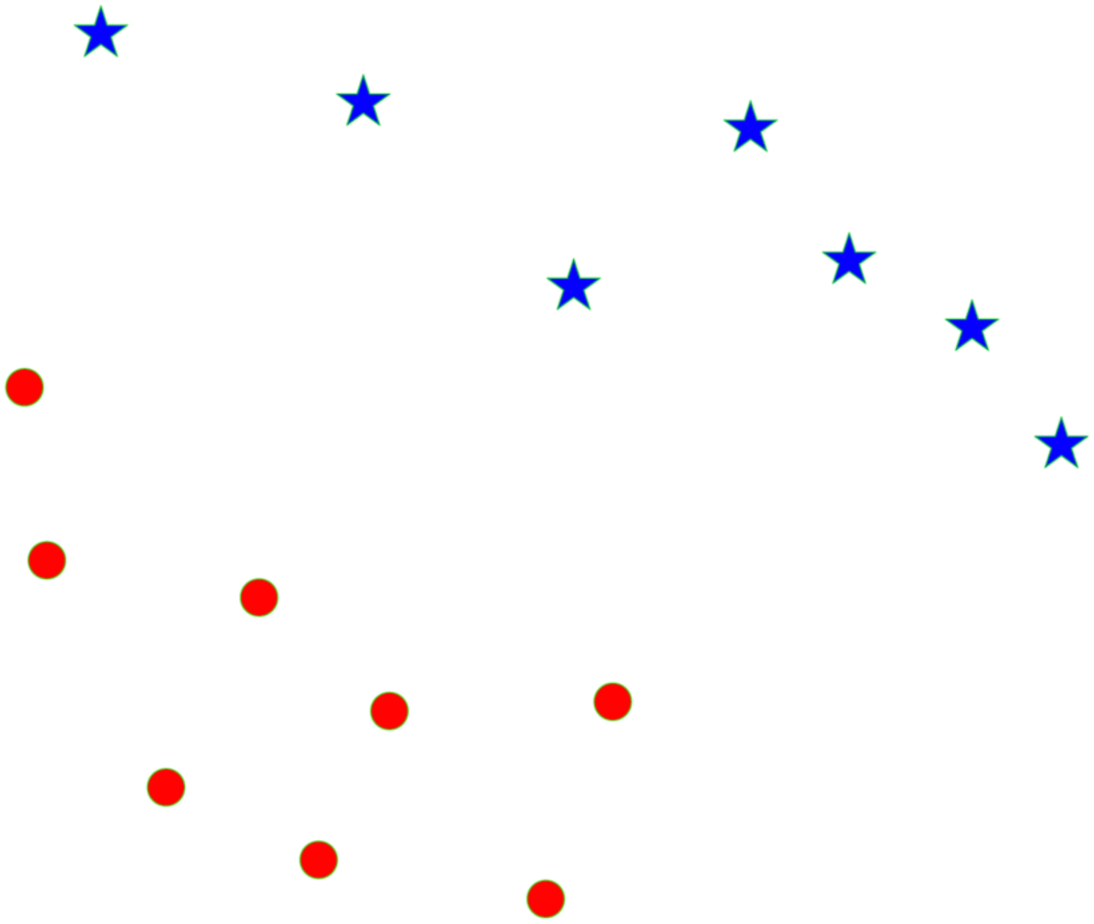
- We can use the $0-1$ loss function, and find the weights that minimize it over data points

$$\mathcal{L}_{0-1}(y,t) = \begin{cases} 0 & \text{if } y = t \\ 1 & \text{if } y \neq t \end{cases}$$
$$= \mathbb{I}\{y \neq t\}.$$

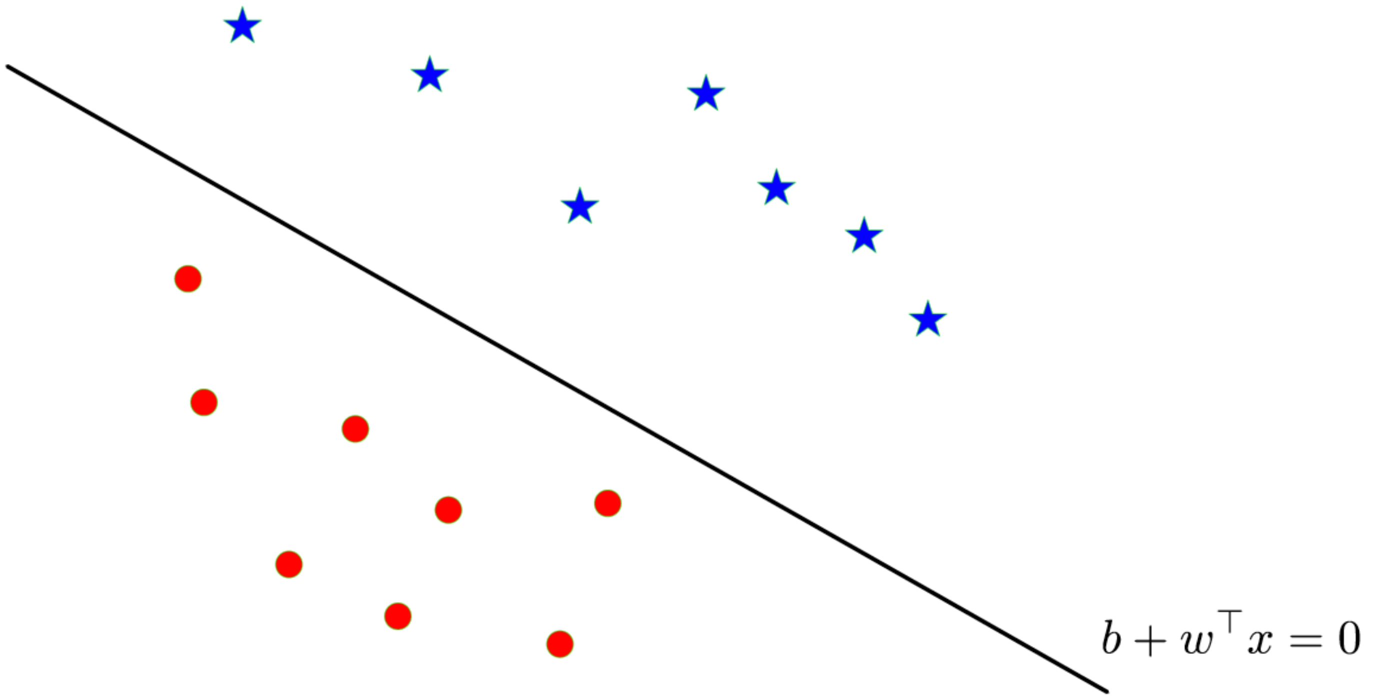
- But minimizing this loss is computationally difficult, and it can't distinguish different hypotheses that achieve the same accuracy.
- We investigated some other loss functions that are easier to minimize, e.g., logistic regression with the cross-entropy loss L_{CE}.
- Let's consider a different approach, starting from the geometry of binary classifiers.

Separating Hyperplanes

- Suppose we are given these data points from two different classes and want to find a linear classifier that separates them.

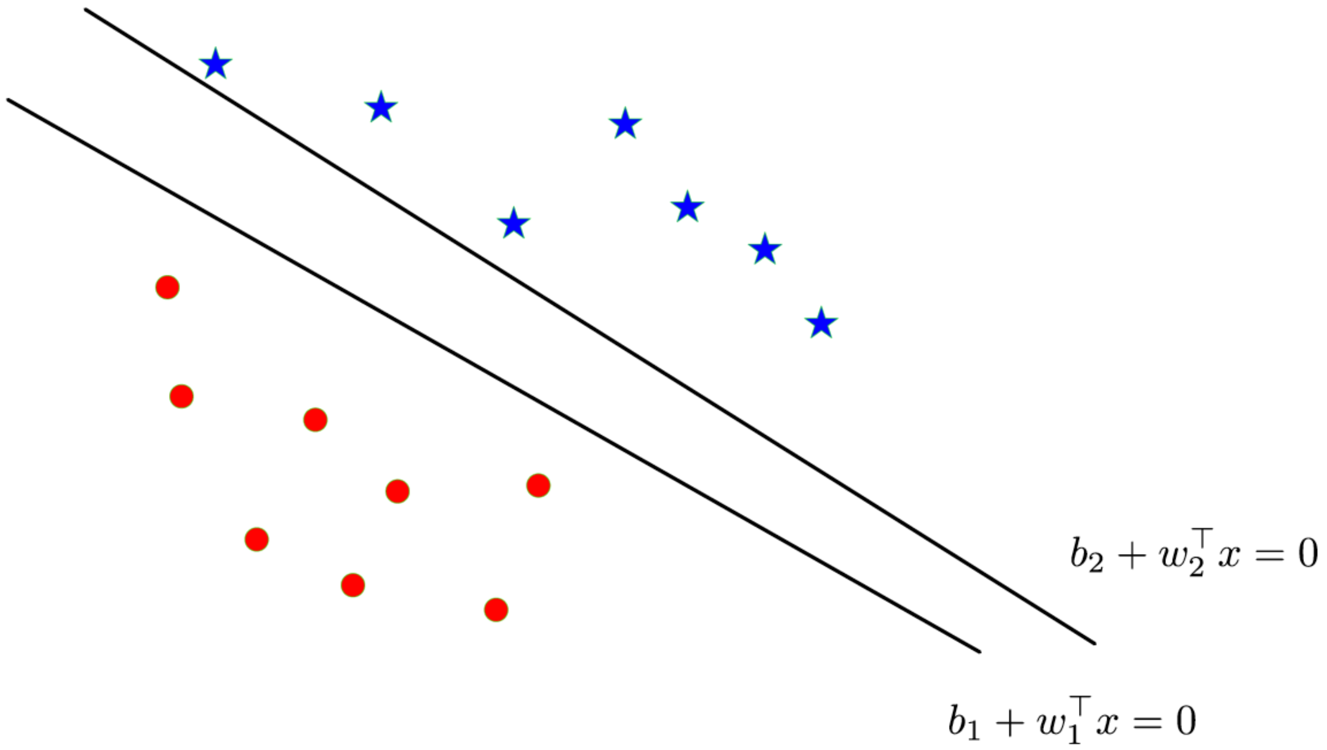


Separating Hyperplanes



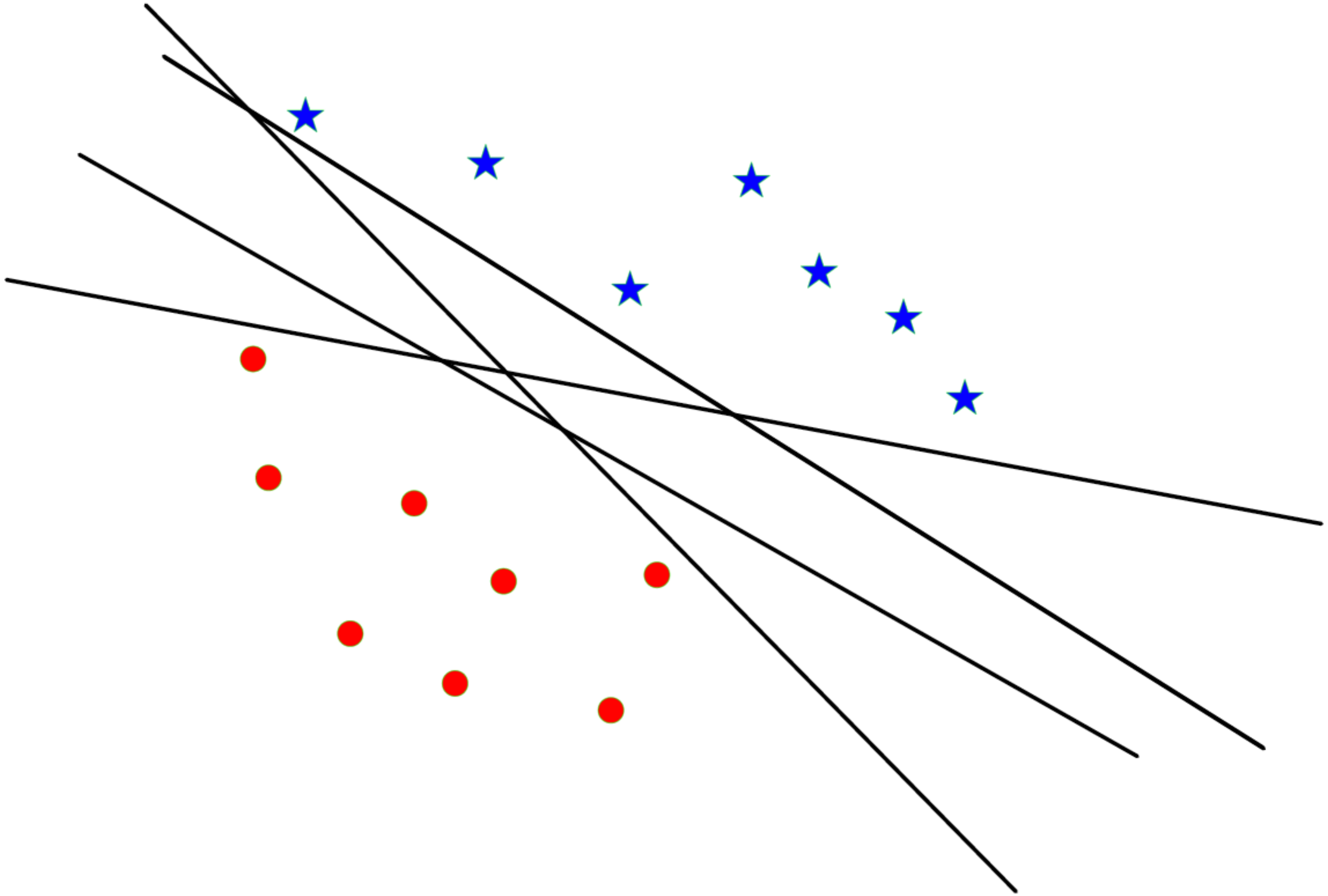
- The decision boundary looks like a line because $\boldsymbol{x} \in \mathbb{R}^2$, but think about it as a $D - 1$ dimensional hyperplane.
- Recall that a hyperplane is described by points $\boldsymbol{x} \in \mathbb{R}^D$ such that $f(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + b = 0$

Separating Hyperplanes



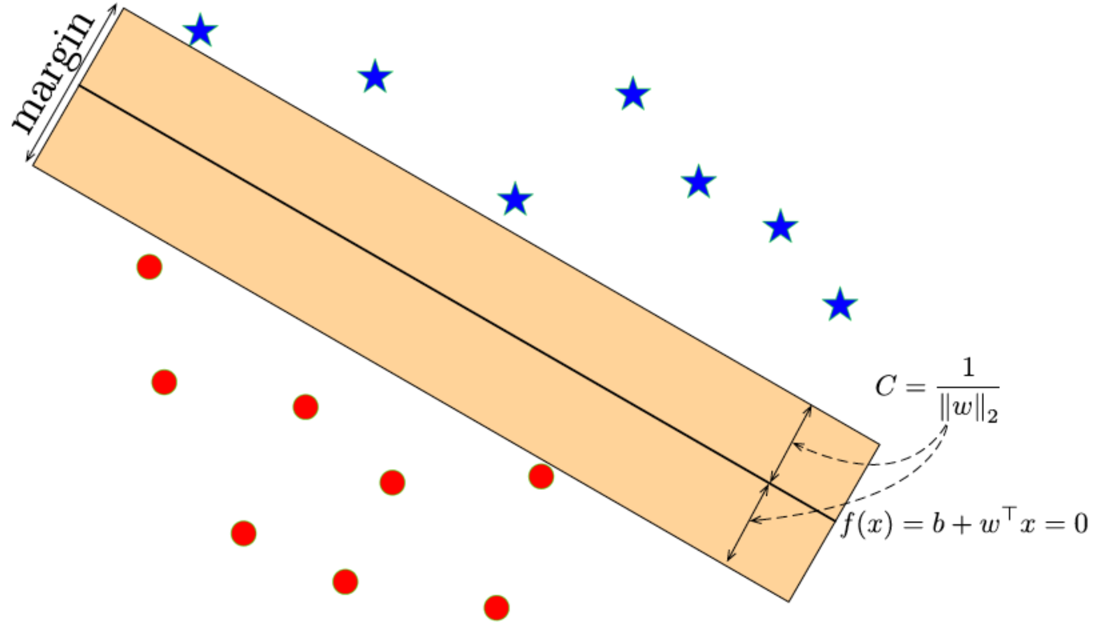
- There are multiple separating hyperplanes, described by different parameters $(\boldsymbol{w}, b)$

Separating Hyperplanes



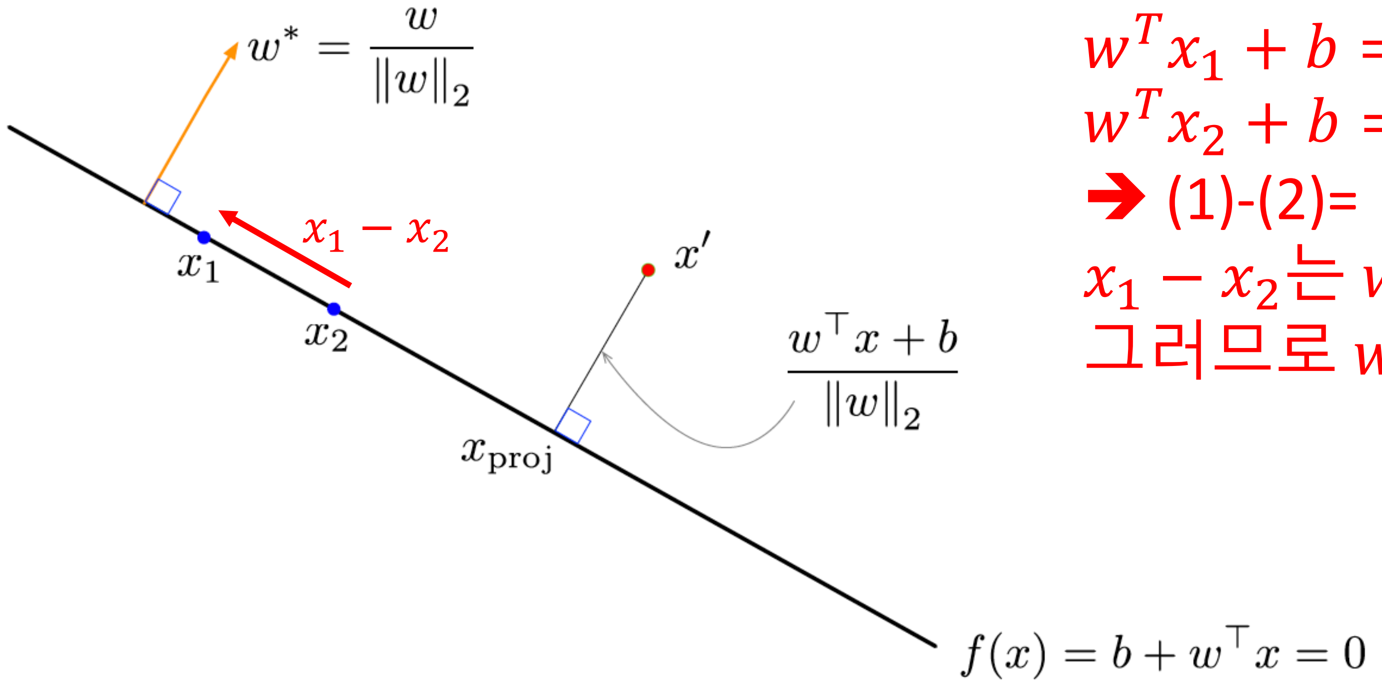
Optimal Separating Hyperplane

- **Optimal Separating Hyperplane**: A hyperplane that separates two classes and maximizes the distance to the closest point from either class, i.e., maximize the margin of the classifier.



Intuitively, ensuring that a classifier is not too close to any data points leads to better generalization on the test data.

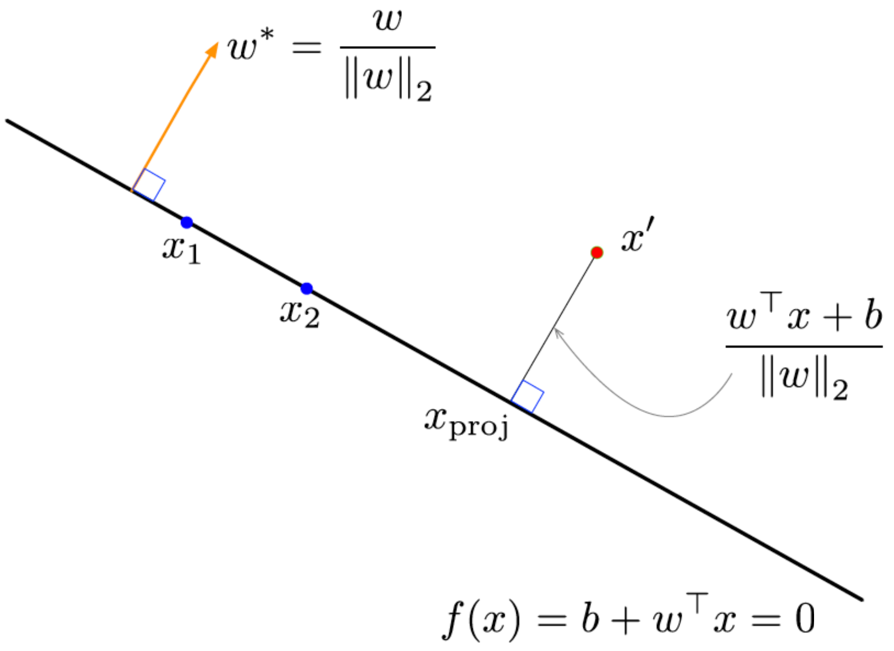
Geometry of Points and Planes



$w^T x_1 + b = 0$ (1)
$w^T x_2 + b = 0$ (2)
➔ (1)-(2)= $w^T(x_1 - x_2) = 0$
$x_1 - x_2$는 $w^T x + b = 0$의 일부분
그러므로 $w^T x + b = 0$와 w는 orthogonal

- Recall that the decision hyperplane is orthogonal (perpendicular) to $\boldsymbol{w}$.
- The vector $\boldsymbol{w}^* = \frac{\boldsymbol{w}}{||\boldsymbol{w}||_2}$ is a unit vector pointing in the same direction as $\boldsymbol{w}$.
- The same hyperplane could equivalently be defined in terms of $\boldsymbol{w}^*$

Geometry of Points and Planes



- The (signed) distance of a point $\mathbf{x}'$ to the hyperplane is

$$\frac{\mathbf{w}^\top \mathbf{x}' + b}{\|\mathbf{w}\|_2}$$

x_{proj}는 $w^T x + b = 0$ 위의 한 점이므로

$$w^T x_{proj} + b = 0 \qquad (1)$$

$x' = x_{proj} + \alpha \frac{w}{\|w\|_2}$ 라 하면, $(\alpha \in \mathbb{R})$

$$x_{proj} = x' - \alpha \frac{w}{\|w\|_2} \qquad (2)$$

(2)를 (1)에 대입하면

$$w^T \left(x' - \alpha \frac{w}{\|w\|_2}\right) + b = 0$$

$$\rightarrow w^T x' - \alpha \frac{w^T w}{\|w\|_2} + b = 0$$

$$\rightarrow w^T x' - \alpha \frac{\|w\|_2^2}{\|w\|_2} + b = 0$$

$$\rightarrow w^T x' - \alpha \|w\|_2 + b = 0$$

$\rightarrow \alpha = \frac{w^T x' + b}{\|w\|_2}$ (α의 부호는 x' 위치에 따라 달라짐)

Maximizing Margin as an Optimization Problem

- Recall: the classification for the i-th data point is correct when

$$\mathrm{sign}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) = t^{(i)}$$

- This can be rewritten as

$$t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) > 0$$

- Enforcing a margin of C:

$$t^{(i)} \cdot \underbrace{\frac{(\mathbf{w}^\top \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|_2}}_{\text{signed distance}} \geq C$$

Maximizing Margin as an Optimization Problem

- Max-margin objective:

$$\max_{\mathbf{w},b} C \quad \text{s.t.} \quad \frac{t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|_2} \geq C \qquad i = 1, \ldots, N$$

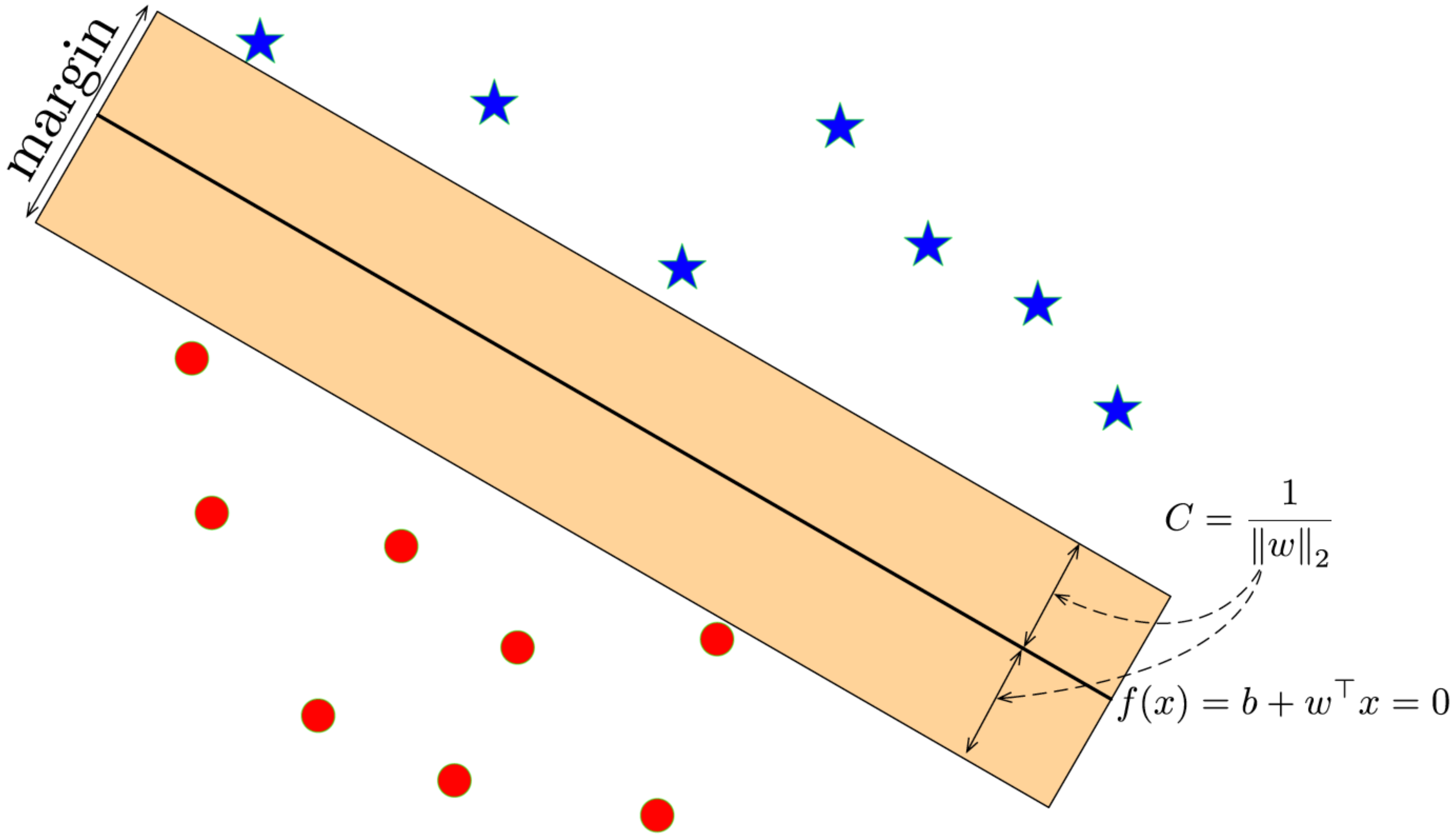
- Plug in $C = 1/\|\boldsymbol{w}\|_2$ and simplify:

$$\underbrace{\frac{t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|_2} \geq \frac{1}{\|\mathbf{w}\|_2}}_{\textbf{geometric margin constraint}} \qquad \iff \qquad \underbrace{t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1}_{\textbf{algebraic margin constraint}}$$

- Equivalent optimization objective:

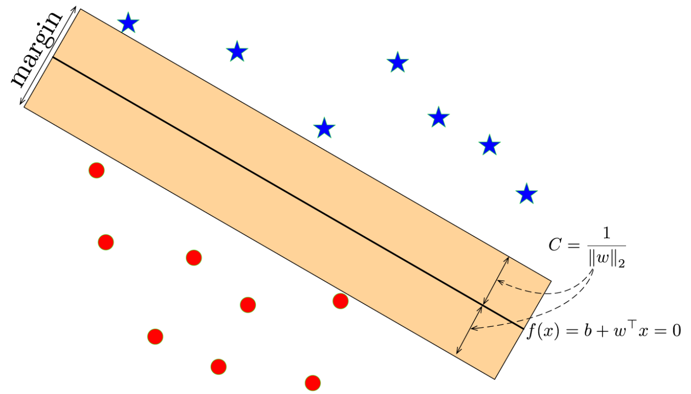
$$\min \|\mathbf{w}\|_2^2 \quad \text{s.t.} \quad t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1 \qquad i = 1, \ldots, N$$

Maximizing Margin as an Optimization Problem



Maximizing Margin as an Optimization Problem

Algebraic max-margin objective:



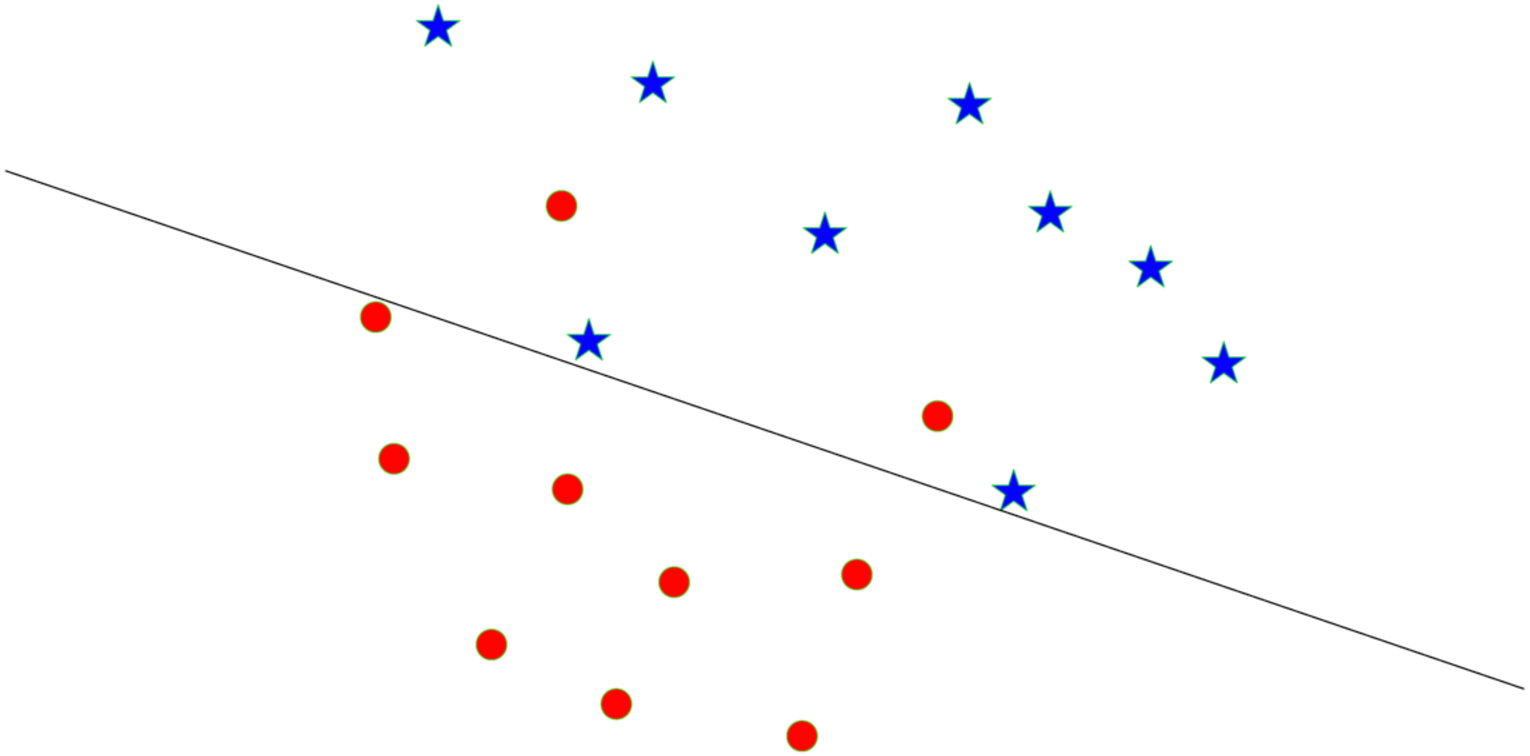
$$\min_{\mathbf{w},b} \|\mathbf{w}\|_2^2$$

$$\text{s.t. } t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1 \qquad i = 1, \ldots, N$$

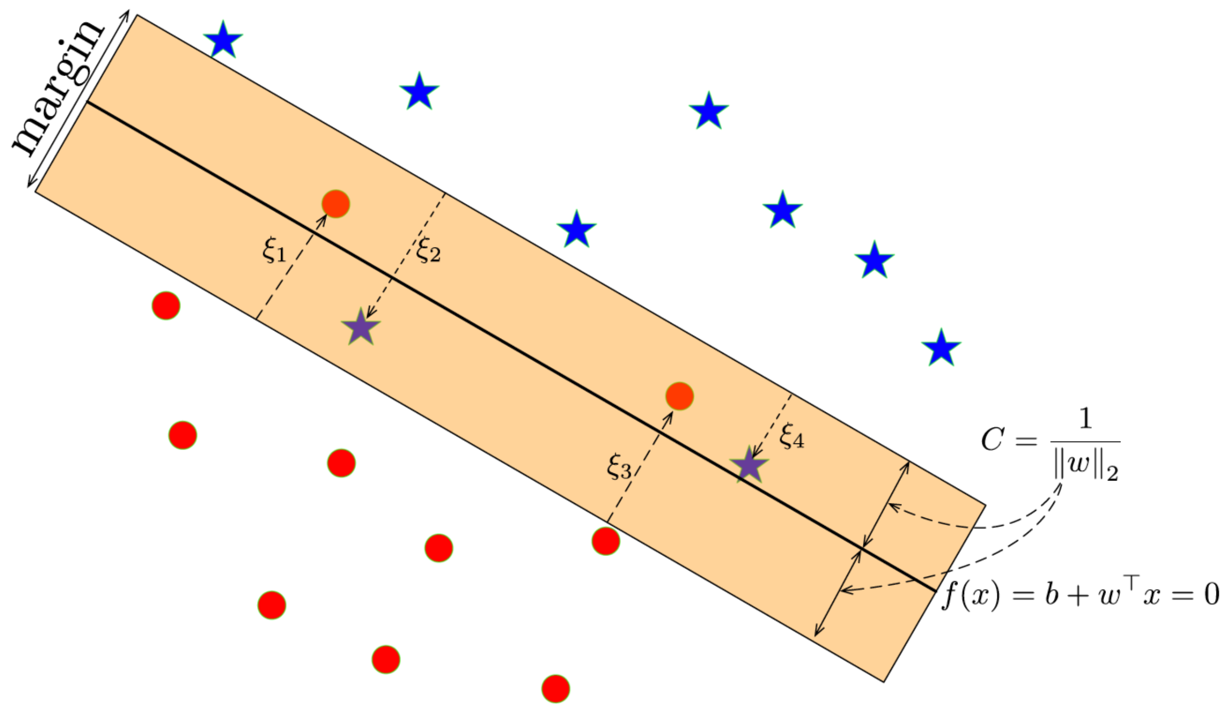
- Observe: if the margin constraint is not tight for $x^{(i)}$, we could remove it from the training set and the optimal $\boldsymbol{w}$ would be the same.
- The important training examples are the ones with algebraic margin 1, and are called support vectors.
- Hence, this algorithm is called the (hard) Support Vector Machine (SVM) (or Support Vector Classifier).
- SVM-like algorithms are often called max-margin or large-margin.

Non-Separable Data Points

- How can we apply the max-margin principle if the data are not linearly separable?



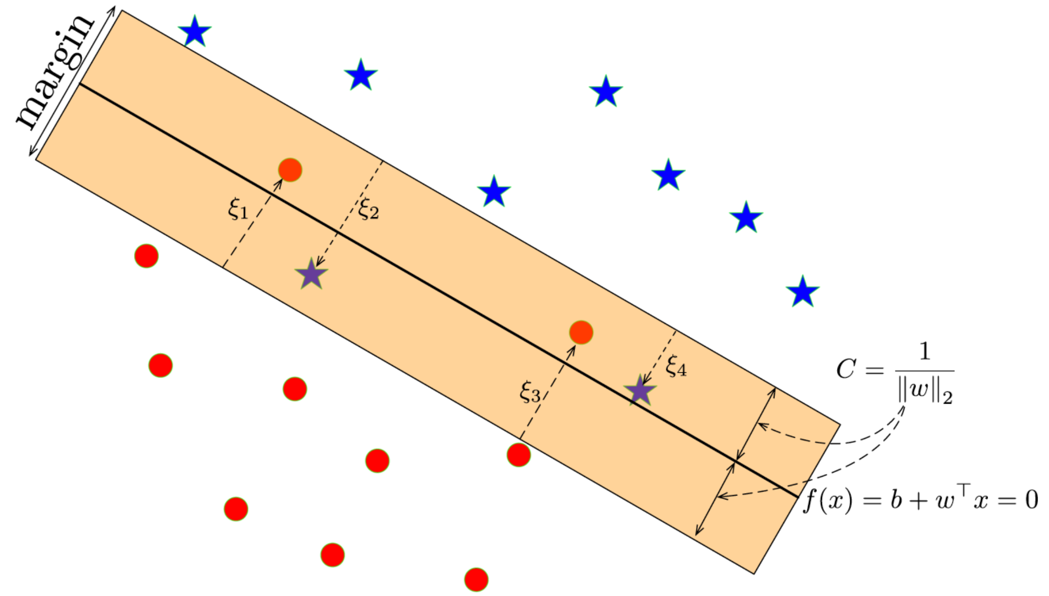
Maximizing Margin for Non-Separable Data Points



Main Idea:

- Allow some points to be within the margin or even be misclassified; we represent this with slack variables ξ_i
- But constrain or penalize the total amount of slack.

Maximizing Margin for Non-Separable Data Points



- **Soft margin constraint:**

$$\frac{t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|_2} \geq C(1 - \xi_i), \quad \text{for } \xi_i \geq 0.$$

- Penalize $\sum_i \xi_i$

Maximizing Margin for Non-Separable Data Points

Soft-margin SVM objective:

$$
\begin{aligned}
&\min_{\mathbf{w},b,\xi} \frac{1}{2}\|\mathbf{w}\|_2^2 + \gamma \sum_{i=1}^{N} \xi_i \\
&\text{s.t.} \quad t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1 - \xi_i \qquad i = 1, \ldots, N \\
&\qquad\quad \xi_i \geq 0 \qquad\qquad\qquad\qquad\quad\; i = 1, \ldots, N
\end{aligned}
$$

- γ is a hyperparameter that trades off the margin with the amount of slack.
  - For $\gamma = 0$, we'll get $\boldsymbol{w} = 0$. (Why? $\boldsymbol{w}$, b, $\boldsymbol{\xi}$를 모두 0으로 만들면 constraint를 만족)
  - As $\gamma \rightarrow \infty$, we get the hard-margin objective.
- Note: it is also possible to constrain $\sum_i \xi_i$ instead of penalizing it.

From Margin Violation to Hinge Loss

- Let's simplify the soft margin constraint by eliminating ξ_i. Recall:

$$t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1 - \xi_i \qquad i = 1, \ldots, N$$
$$\xi_i \geq 0 \qquad i = 1, \ldots, N$$

- Rewrite as $\xi_i \geq 1 - t^{(i)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(\boldsymbol{i})} + b\right)$
- Case 1: $1 - t^{(i)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(\boldsymbol{i})} + b\right) \leq 0$
  - The smallest non-negative ξ_i that satisfies the constraint is $\xi_i = 0$.
- Case 2: $1 - t^{(i)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(\boldsymbol{i})} + b\right) > 0$
  - The smallest ξ_i that satisfies the constraint is $\xi_i = 1 - t^{(i)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(\boldsymbol{i})} + b\right)$
- Hence, $\xi_i = \max\{0, 1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)\}$
- Therefore, the slack penalty can be written as

$$\sum_{i=1}^{N} \xi_i = \sum_{i=1}^{N} \max\{0, 1 - t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b)\}$$

From Margin Violation to Hinge Loss

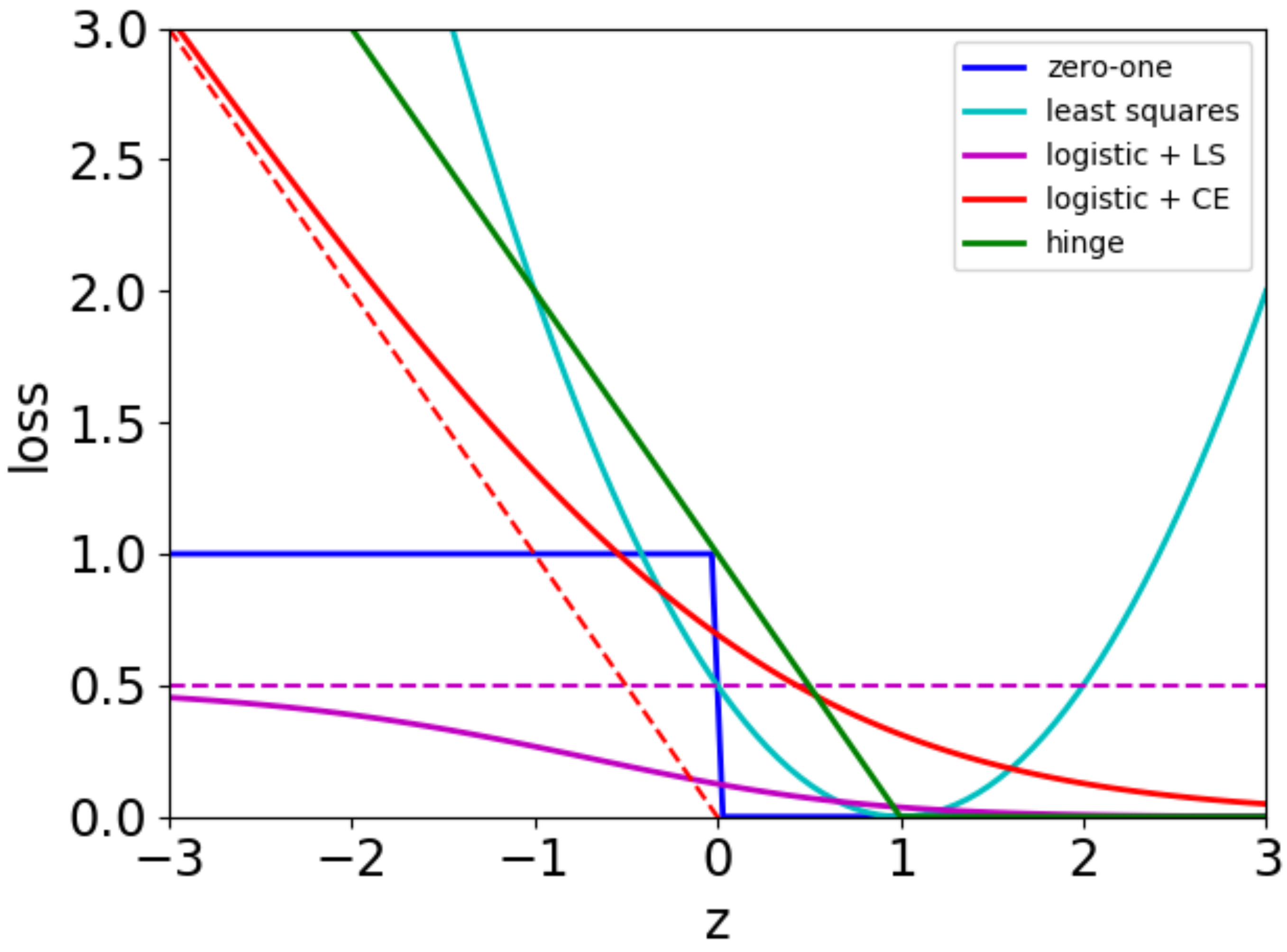
If we write $y^{(i)}(\mathbf{w}, b) = \mathbf{w}^\top \mathbf{x} + b$, then the optimization problem can be written as

$$\min_{\mathbf{w},b,\xi} \sum_{i=1}^{N} \max\{0, 1 - t^{(i)} y^{(i)}(\mathbf{w}, b)\} + \frac{1}{2\gamma} \|\mathbf{w}\|_2^2$$

- The loss function $L_H(\mathbf{y}, \boldsymbol{t}) = \max\{0,1 - \boldsymbol{t}\mathbf{y}\}$ is called the hinge loss.
- The second term is the L_2-norm of the weights.
- Hence, the soft-margin SVM can be seen as a linear classifier with hinge loss and an L_2 regularizer.

Revisiting Loss Functions for Classification

Hinge loss compared with other loss functions



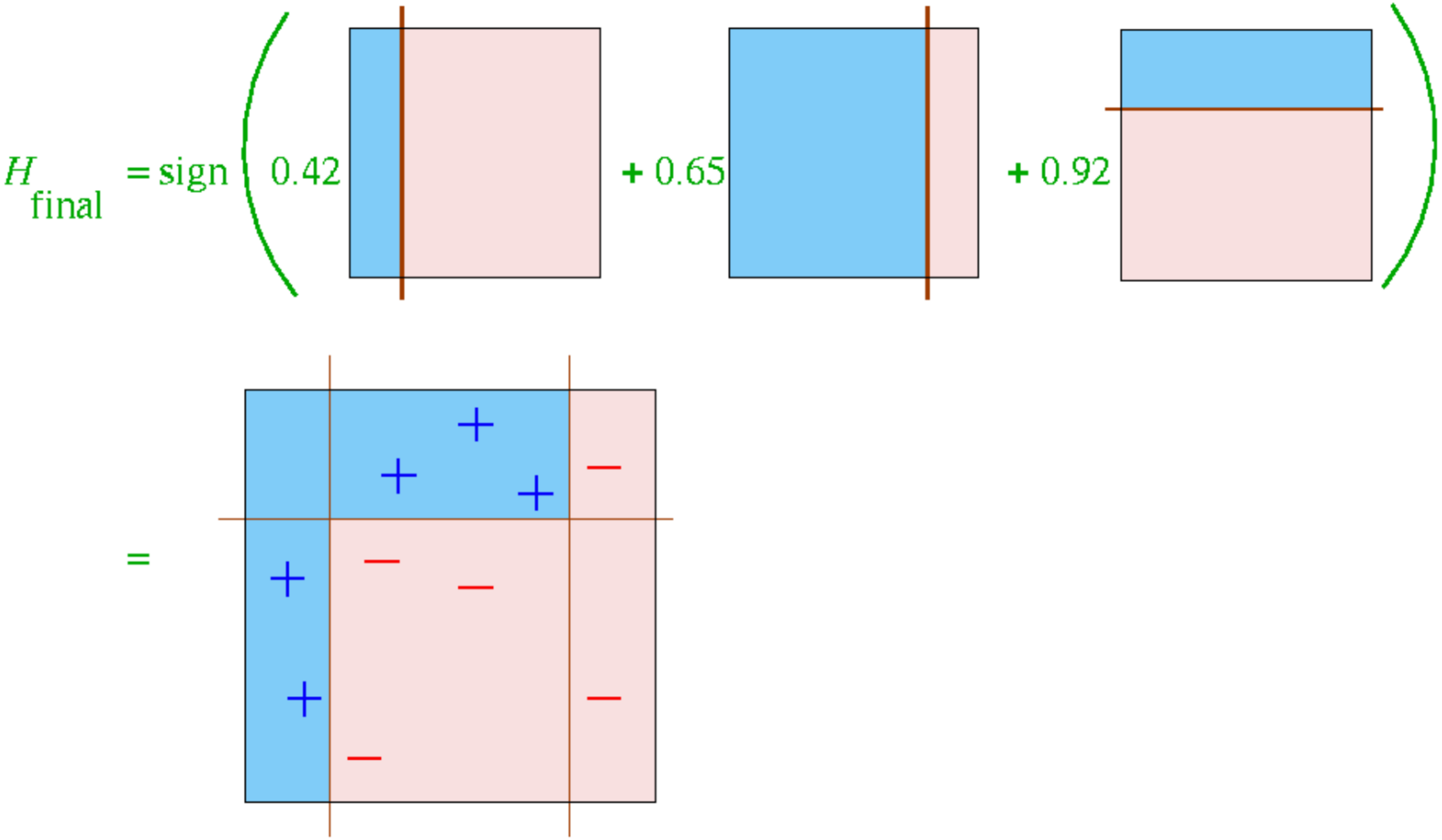
SVMs: What we Left Out

What we left out:

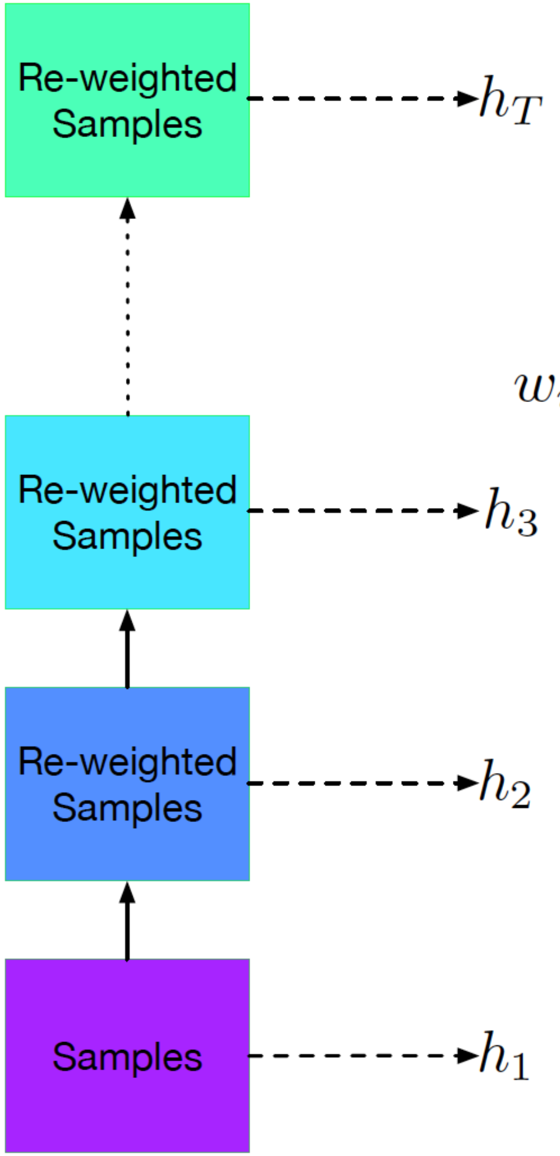
- How to fit $\boldsymbol{w}$:
  - One option: gradient descent
  - Can reformulate with the Lagrange dual
- The "kernel trick" converts it into a powerful nonlinear classifier. We'll cover this later in the course.
- Classic results from learning theory show that a large margin implies good generalization.

AdaBoost Revisited

- **Part 2**: reinterpreting AdaBoost in terms of what we've learned about loss functions.



AdaBoost Revisited



$$H(x) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$$

$$w_i \leftarrow w_i \exp\left(2\alpha_t \mathbb{I}\{h_t(\mathbf{x}^{(\mathbf{i})}) \neq \mathbf{t}^{(\mathbf{i})}\}\right)$$

$$\alpha_t = \frac{1}{2}\log\left(\frac{1-\text{err}_t}{\text{err}_t}\right)$$

$$\text{err}_t = \frac{\sum_{i=1}^{N} w_i \mathbb{I}\{h_t(\mathbf{x}^{(\mathbf{i})} \neq \mathbf{t}^{(\mathbf{i})}\}}{\sum_{i=1}^{N} w_i}$$

Additive Models

- Consider a hypothesis class $\mathcal{H}$ with each $h_i\colon \boldsymbol{x} \longmapsto \{-1, +1\}$ within $\mathcal{H}$, i.e., $h_i \in \mathcal{H}$. These are the "weak learners", and in this context they're also called bases.
- An additive model with m terms is given by

$$H_m(x) = \sum_{i=1}^{m} \alpha_i h_i(\mathbf{x}), \quad \text{where } (\alpha_1, \cdots, \alpha_m) \in \mathbb{R}^m$$

- Observe that we're taking a linear combination of base classifiers, just like in boosting.
- We'll now interpret AdaBoost as a way of fitting an additive model.

Stagewise Training of Additive Models

A greedy approach to fitting additive models, known as stagewise training:

1. Initialize $H_0(x) = 0$
2. For $m = 1$ to T:
   - Compute the m-th hypothesis and its coefficient

$$(h_m, \alpha_m) \leftarrow \underset{h \in \mathcal{H}, \alpha}{\operatorname{argmin}} \sum_{i=1}^{N} \mathcal{L}\left(H_{m-1}(\mathbf{x}^{(i)}) + \alpha h(\mathbf{x}^{(i)}), t^{(i)}\right)$$

   - Add it to the additive model

$$H_m = H_{m-1} + \alpha_m h_m$$

Additive Models with Exponential Loss

- Consider the exponential loss

$$\mathcal{L}_{\mathrm{E}}(y, t) = \exp(-ty)$$

- We want to see how the stagewise training of additive models can be done.

$$\begin{aligned}
(h_m, \alpha_m) \leftarrow \underset{h \in \mathcal{H}, \alpha}{\operatorname{argmin}} \sum_{i=1}^{N} \exp\left(-\left[H_{m-1}(\mathbf{x}^{(i)}) + \alpha h(\mathbf{x}^{(i)})\right] t^{(i)}\right) \\
= \sum_{i=1}^{N} \exp\left(-H_{m-1}(\mathbf{x}^{(i)}) t^{(i)} - \alpha h(\mathbf{x}^{(i)}) t^{(i)}\right) \\
= \sum_{i=1}^{N} \exp\left(-H_{m-1}(\mathbf{x}^{(i)}) t^{(i)}\right) \exp\left(-\alpha h(\mathbf{x}^{(i)}) t^{(i)}\right) \\
= \sum_{i=1}^{N} w_i^{(m)} \exp\left(-\alpha h(\mathbf{x}^{(i)}) t^{(i)}\right).
\end{aligned}$$

- Here we defined $w_i^{(m)} \triangleq \exp\left(-H_{m-1}(\mathbf{x}^{(i)}) t^{(i)}\right)$

Additive Models with Exponential Loss

We want to solve the following minimization problem:

$$(h_m, \alpha_m) \leftarrow \underset{h \in \mathcal{H}, \alpha}{\operatorname{argmin}} \sum_{i=1}^{N} w_i^{(m)} \exp\left(-\alpha h(\mathbf{x}^{(i)}) t^{(i)}\right)$$

- If $h(\mathbf{x}^{(i)}) = t^{(i)}$, we have $\exp\left(-\alpha h(\mathbf{x}^{(i)}) t^{(i)}\right) = \exp(-\alpha)$
- If $h(\mathbf{x}^{(i)}) \neq t^{(i)}$, we have $\exp\left(-\alpha h(\mathbf{x}^{(i)}) t^{(i)}\right) = \exp(+\alpha)$

(recall that we are in the binary classification case with {-1,+1} output values).

We can divide the summation to two parts:

$$\begin{aligned}
\sum_{i=1}^{N} w_i^{(m)} \exp\left(-\alpha h(\mathbf{x}^{(i)}) t^{(i)}\right) =& e^{-\alpha} \sum_{i=1}^{N} w_i^{(m)} \mathbb{I}\{h(\mathbf{x}^{(i)}) = t_i\} + e^{\alpha} \sum_{i=1}^{N} w_i^{(m)} \mathbb{I}\{h(\mathbf{x}^{(i)}) \neq t_i\} \\
=& (e^{\alpha} - e^{-\alpha}) \sum_{i=1}^{N} w_i^{(m)} \mathbb{I}\{h(\mathbf{x}^{(i)}) \neq t_i\} + \\
& e^{-\alpha} \sum_{i=1}^{N} w_i^{(m)} \left[\mathbb{I}\{h(\mathbf{x}^{(i)}) \neq t_i\} + \mathbb{I}\{h(\mathbf{x}^{(i)}) = t_i\}\right]
\end{aligned}$$

Additive Models with Exponential Loss

$$\begin{aligned}\sum_{i=1}^{N} w_i^{(m)} \exp\left(-\alpha h(\mathbf{x}^{(i)}) t^{(i)}\right) =& (e^{\alpha} - e^{-\alpha}) \sum_{i=1}^{N} w_i^{(m)} \mathbb{I}\{h(\mathbf{x}^{(i)} \neq t_i\} + \\ & e^{-\alpha} \sum_{i=1}^{N} w_i^{(m)} \left[\mathbb{I}\{h(\mathbf{x}^{(i)} \neq t_i\} + \mathbb{I}\{h(\mathbf{x}^{(i)}) = t_i\}\right] \\ =& (e^{\alpha} - e^{-\alpha}) \sum_{i=1}^{N} w_i^{(m)} \mathbb{I}\{h(\mathbf{x}^{(i)}) \neq t_i\} + e^{-\alpha} \sum_{i=1}^{N} w_i^{(m)}.\end{aligned}$$

Let us first optimize h:

The second term on the RHS does not depend on h. So we get

$$h_m \leftarrow \underset{h \in \mathcal{H}}{\operatorname{argmin}} \sum_{i=1}^{N} w_i^{(m)} \exp\left(-\alpha h(\mathbf{x}^{(i)}) t^{(i)}\right) \equiv \underset{h \in \mathcal{H}}{\operatorname{argmin}} \sum_{i=1}^{N} w_i^{(m)} \mathbb{I}\{h(\mathbf{x}^{(i)}) \neq t_i\}$$

This means that h_m is the minimizer of the weighted 0/1-loss.

Additive Models with Exponential Loss

- Now that we obtained h_m, we want to find α: Define the weighted classification error:

$$\mathrm{err}_m = \frac{\sum_{i=1}^N w_i^{(m)} \mathbb{I}\{h_m(\mathbf{x}^{(i)}) \neq t^{(i)}\}}{\sum_{i=1}^N w_i^{(m)}}$$

- With this definition and

$\min_{h \in \mathcal{H}} \sum_{i=1}^N w_i^{(m)} \exp\left(-\alpha h(\mathbf{x}^{(i)}) t^{(i)}\right) = \sum_{i=1}^N w_i^{(m)} \mathbb{I}\{h_m(\mathbf{x}^{(i)}) \neq t_i\}$, we have

$$\min_{\alpha} \min_{h \in \mathcal{H}} \sum_{i=1}^N w_i^{(m)} \exp\left(-\alpha h(\mathbf{x}^{(i)}) t^{(i)}\right) =$$

$$\min_{\alpha} \left\{ (e^{\alpha} - e^{-\alpha}) \sum_{i=1}^N w_i^{(m)} \mathbb{I}\{h_m(\mathbf{x}^{(i)}) \neq t_i\} + e^{-\alpha} \sum_{i=1}^N w_i^{(m)} \right\}$$

$$= \min_{\alpha} \left\{ (e^{\alpha} - e^{-\alpha}) \mathrm{err}_m \left(\sum_{i=1}^N w_i^{(m)} \right) + e^{-\alpha} \left(\sum_{i=1}^N w_i^{(m)} \right) \right\}$$

- Take derivative w.r.t. α and set it to zero. We get that

$$e^{2\alpha} = \frac{1 - \mathrm{err}_m}{\mathrm{err}_m} \Rightarrow \alpha = \frac{1}{2} \log\left(\frac{1 - \mathrm{err}_m}{\mathrm{err}_m} \right)$$

Additive Models with Exponential Loss

- The updated weights for the next iteration is

$$
\begin{aligned}
w_i^{(m+1)} &= \exp\left(-H_m(\mathbf{x}^{(i)})t^{(i)}\right) \\
&= \exp\left(-\left[H_{m-1}(\mathbf{x}^{(i)}) + \alpha_m h_m(\mathbf{x}^{(i)})\right] t^{(i)}\right) \\
&= \exp\left(-H_{m-1}(\mathbf{x}^{(i)})t^{(i)}\right) \exp\left(-\alpha_m h_m(\mathbf{x}^{(i)})t^{(i)}\right) \\
&= w_i^{(m)} \exp\left(-\alpha_m h_m(\mathbf{x}^{(i)})t^{(i)}\right) \\
&= w_i^{(m)} \exp\left(-\alpha_m \left(2\mathbb{I}\{h_m(\mathbf{x}^{(i)}) = t^{(i)}\} - 1\right)\right) \\
&= \exp(\alpha_m) w_i^{(m)} \exp\left(-2\alpha_m \mathbb{I}\{h_m(\mathbf{x}^{(i)}) = t^{(i)}\}\right).
\end{aligned}
$$

- The term $\exp(\alpha_m)$ multiplies the weight corresponding to all samples, so it does not affect the minimization of h_{m+1} or α_{m+1}.

Additive Models with Exponential Loss

- To summarize, we obtain the additive model $H_m(x) = \sum_{i=1}^{m} \alpha_i h_i(\mathbf{x})$ with

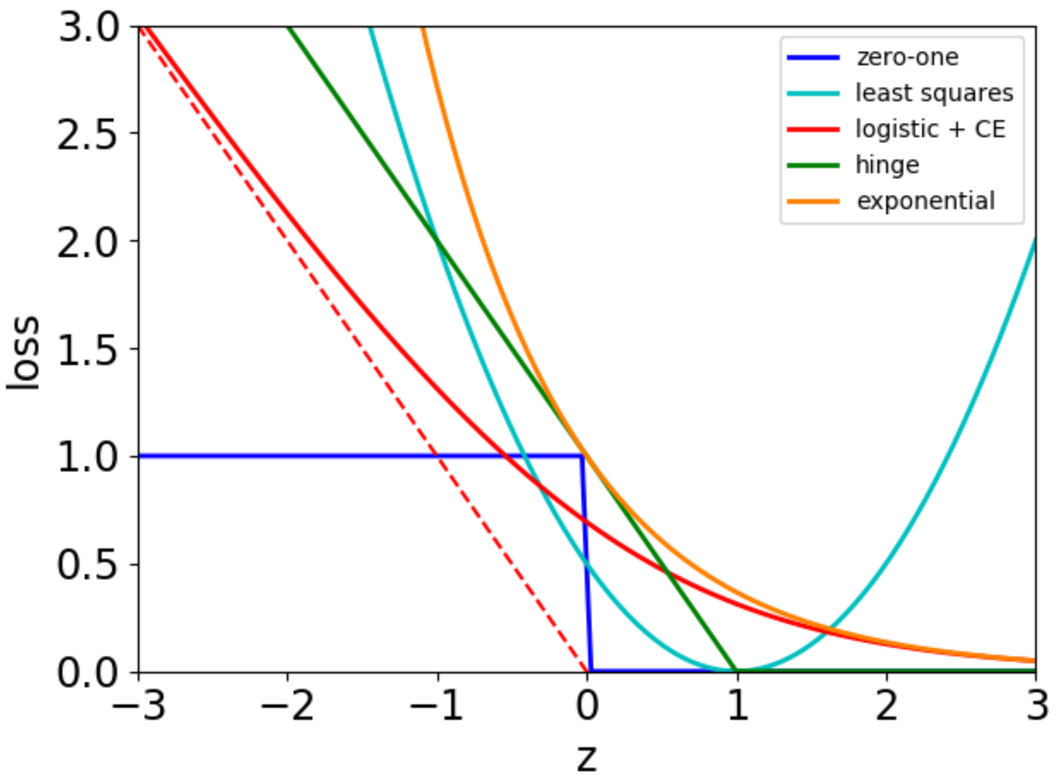
$$h_m \leftarrow \underset{h \in \mathcal{H}}{\operatorname{argmin}} \sum_{i=1}^{N} w_i^{(m)} \mathbb{I}\{h(\mathbf{x}^{(i)}) \neq t_i\},$$

$$\alpha = \frac{1}{2} \log \left(\frac{1 - \text{err}_m}{\text{err}_m} \right), \qquad \text{where } \text{err}_m = \frac{\sum_{i=1}^{N} w_i^{(m)} \mathbb{I}\{h_m(\mathbf{x}^{(i)}) \neq t^{(i)}\}}{\sum_{i=1}^{N} w_i^{(m)}},$$

$$w_i^{(m+1)} = w_i^{(m)} \exp\left(-\alpha_m h_m(\mathbf{x}^{(i)}) t^{(i)} \right).$$

- We derived the AdaBoost algorithm!

Revisiting Loss Functions for Classification



- If AdaBoost is minimizing exponential loss, what does that say about its behavior (compared to, say, logistic regression)?
- This interpretation allows boosting to be generalized to lots of other loss functions.