

10-701: Introduction to Machine Learning

Lecture 22 –Boosting

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* Slides adopted from F24 offering of 10701 by Henry Chai.

Bias-Variance Decomposition

- Suppose $y=f(x)+\varepsilon$, where ε is noise with $\mathbb{E}[\varepsilon] = 0, \text{Var}(\varepsilon) = \sigma^2$.
- The expected squared prediction error at a point x :

$$\begin{aligned}\mathbb{E}_{D,\varepsilon}[(y - \hat{f}(x))^2] &= \\ &= \underbrace{(f(x) - \mathbb{E}[\hat{f}(x)])^2}_{\text{Bias}^2} + \underbrace{\mathbb{E}[(\hat{f}(x) - \mathbb{E}[\hat{f}(x)])^2]}_{\text{Variance}} + \sigma^2\end{aligned}$$

Ensemble Learning

- **Key idea:** Different models make different errors. By aggregating their predictions, ensembles can reduce variance, bias, or both—leading to better accuracy and robustness than any single model alone.
- **Common ensemble methods**
 - **Bagging (Bootstrap Aggregating):**
Trains many models independently on different random subsets of the data to reduce variance and overfitting.
 - **Boosting:**
Trains models sequentially, with each new model focusing on the errors of the previous one to reduce bias.
 - **Stacking:**
Combines predictions from multiple models using another model (*a meta-learner*) that learns how best to blend them.

Decision Trees: Pros & Cons

- Pros
 - Interpretable
 - Efficient (computational cost and storage)
 - ...
- Cons
 - Learned greedily: each split only considers the immediate impact on the splitting criterion
 - Prone to overfit
 - High variance
 - Can be addressed via **bagging** → random forests
 - Limited expressivity (especially short trees, i.e., stumps)
 - Can be addressed via **boosting**

AdaBoost

- Intuition: iteratively reweight inputs, giving more weight to inputs that are difficult-to-predict correctly
- Analogy:
 - You all have to take a test () ...
 - ... but you're going to be taking it one at a time.
 - After you finish, you get to tell the next person the questions you struggled with.
 - Hopefully, they can cover for you because...
 - ... if “enough” of you get a question right, you'll all receive full credit for that problem

- Input: $\mathcal{D} (y^{(n)} \in \{-1, +1\}), T$
- Initialize data point weights: $\omega_0^{(1)}, \dots, \omega_0^{(N)} = \frac{1}{N}$
- For $t = 1, \dots, T$

1. Train a weak learner, h_t , by minimizing the *weighted* training error
2. Compute the *weighted* training error of h_t :

$$\epsilon_t = \sum_{n=1}^N \omega_{t-1}^{(n)} \mathbb{1}(y^{(n)} \neq h_t(\mathbf{x}^{(n)}))$$

3. Compute the **importance** of h_t :

$$\alpha_t = \frac{1}{2} \log \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$$

4. Update the data point weights:

$$\omega_t^{(n)} = \frac{\omega_{t-1}^{(n)}}{Z_t} \times \begin{cases} e^{-\alpha_t} & \text{if } h_t(\mathbf{x}^{(n)}) = y^{(n)} \\ e^{\alpha_t} & \text{if } h_t(\mathbf{x}^{(n)}) \neq y^{(n)} \end{cases} = \frac{\omega_{t-1}^{(n)} e^{-\alpha_t y^{(n)} h_t(\mathbf{x}^{(n)})}}{Z_t}$$

- Output: an aggregated hypothesis

$$g_T(\mathbf{x}) = \text{sign}(H_T(\mathbf{x}))$$

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

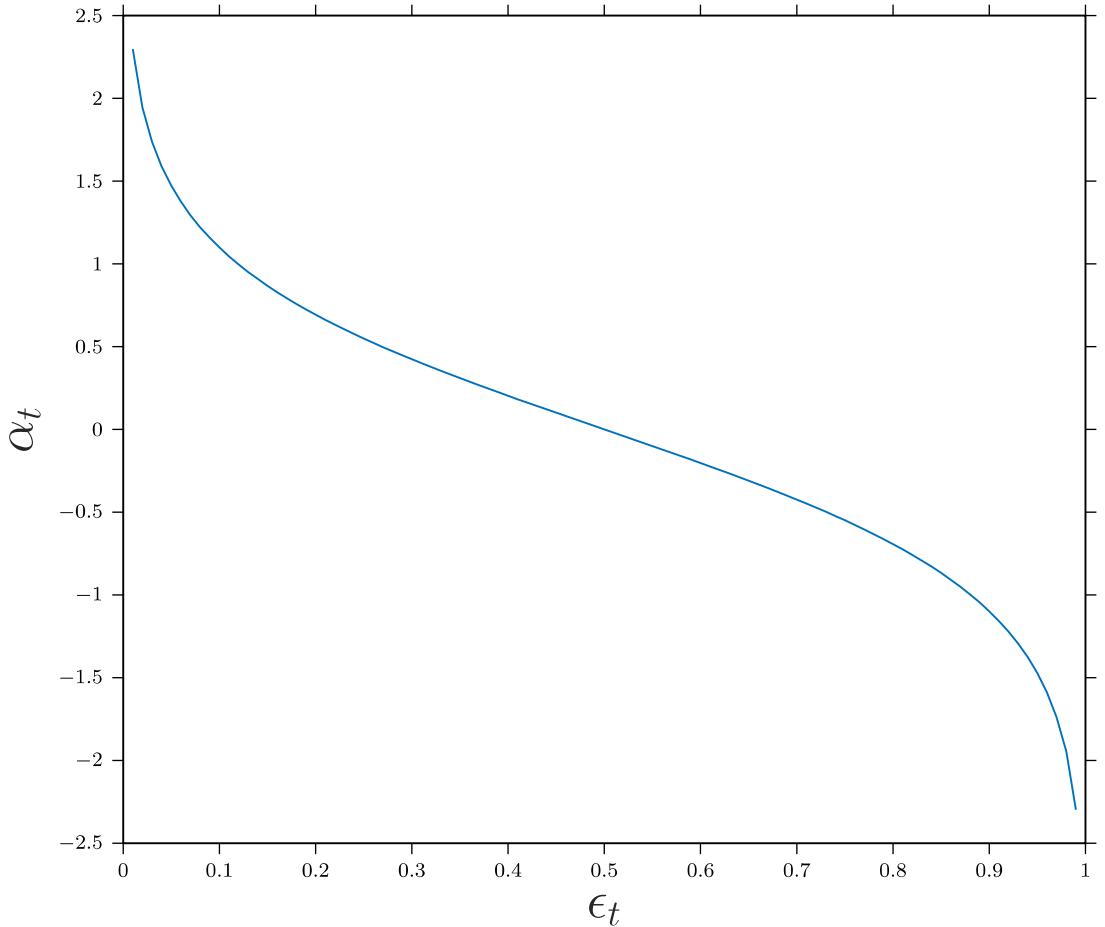
Setting α_t

α_t determines the contribution of h_t to the final, aggregated hypothesis:

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

Intuition: we want good weak learners to have high importances

$$\alpha_t = \frac{1}{2} \log \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$$



Updating $\omega^{(n)}$

- Intuition: we want incorrectly classified inputs to receive a higher weight in the next round

$$\omega_t^{(n)} = \frac{\omega_{t-1}^{(n)}}{Z_t} \times \begin{cases} e^{-\alpha_t} & \text{if } h_t(\mathbf{x}^{(n)}) = y^{(n)} \\ e^{\alpha_t} & \text{if } h_t(\mathbf{x}^{(n)}) \neq y^{(n)} \end{cases}$$

- If $\epsilon_t < \frac{1}{2}$,

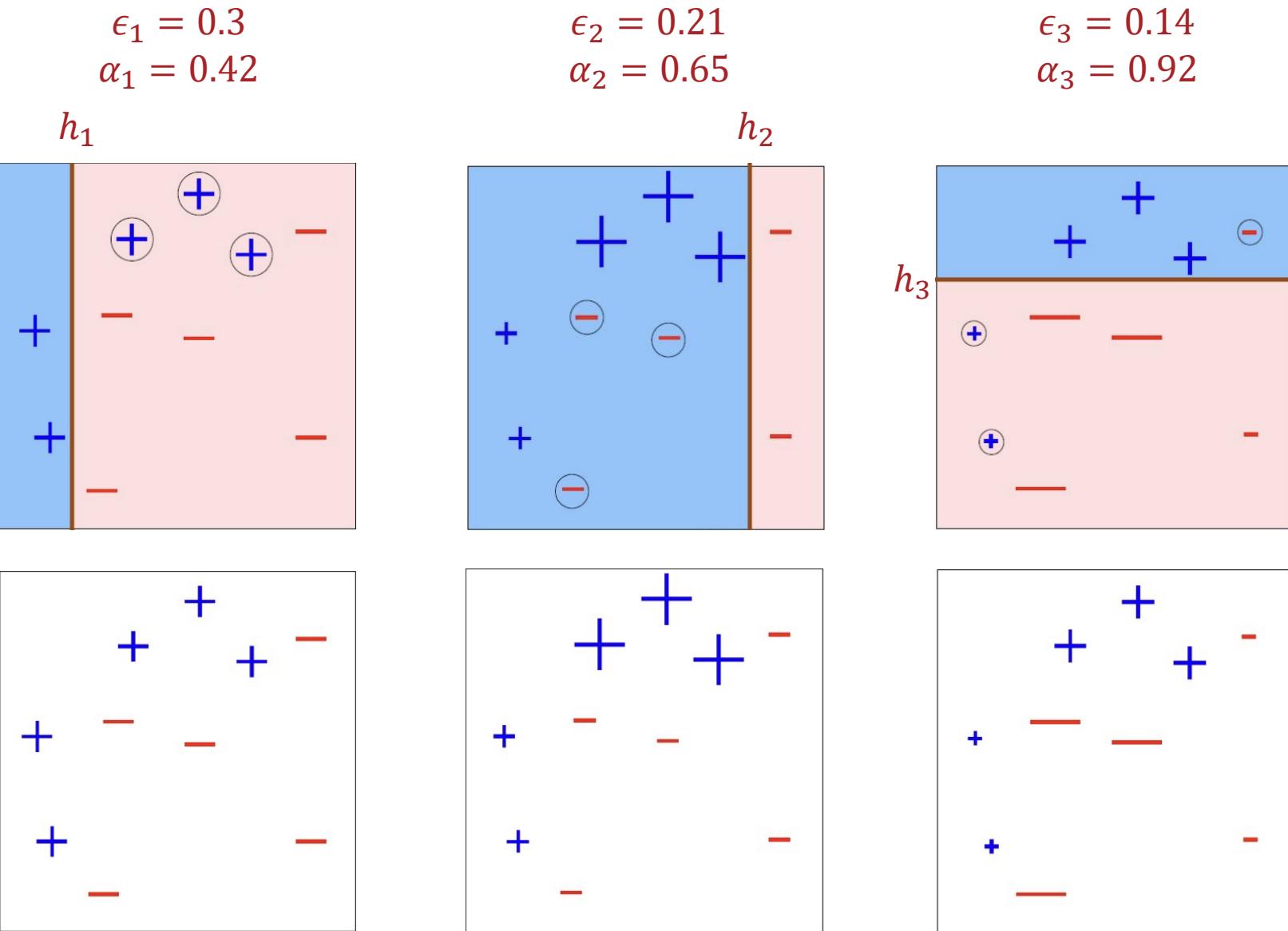
Updating $\omega^{(n)}$

- Intuition: we want incorrectly classified inputs to receive a higher weight in the next round

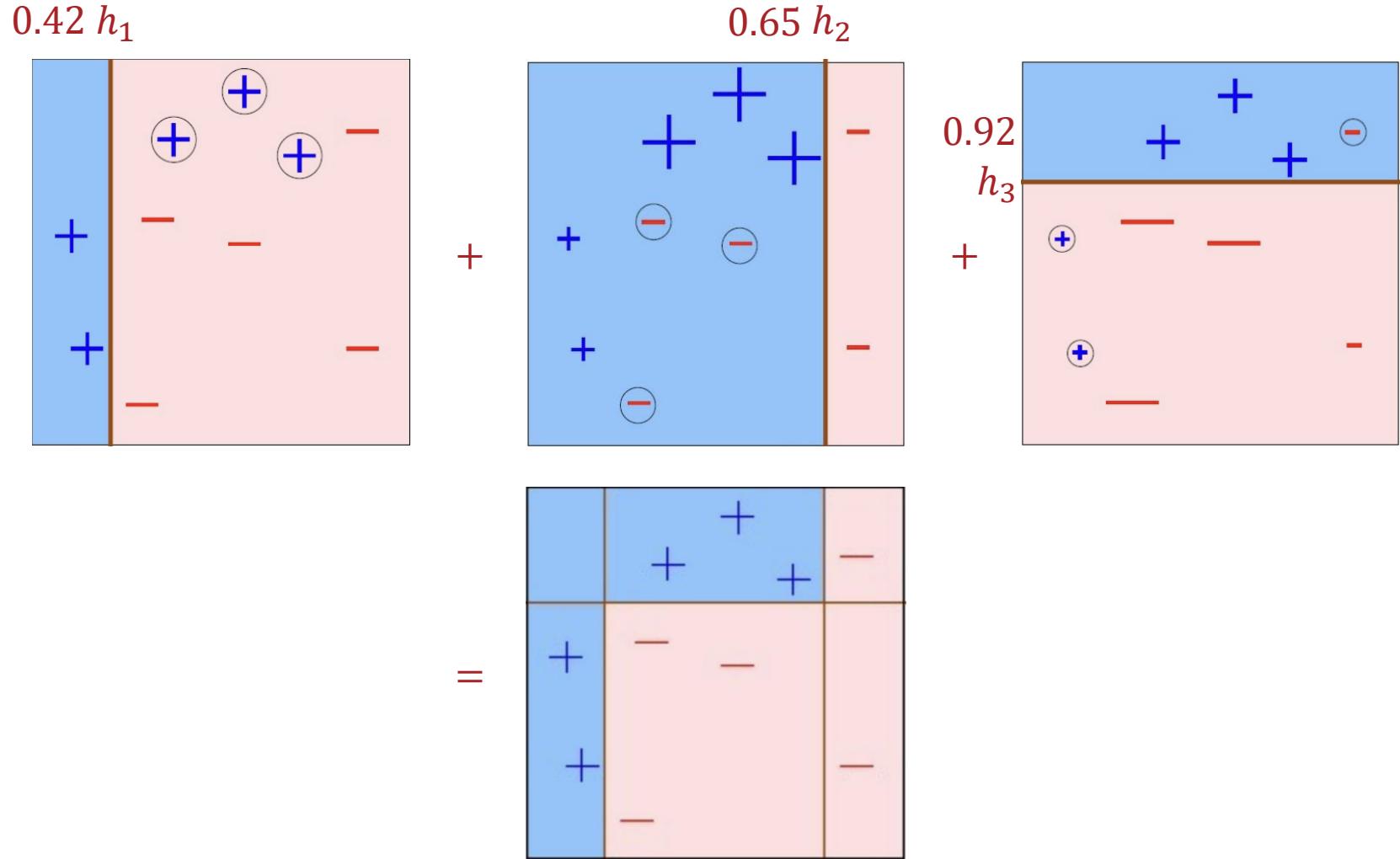
$$\omega_t^{(n)} = \frac{\omega_{t-1}^{(n)}}{Z_t} \times \begin{cases} e^{-\alpha_t} & \text{if } h_t(\mathbf{x}^{(n)}) = y^{(n)} \\ e^{\alpha_t} & \text{if } h_t(\mathbf{x}^{(n)}) \neq y^{(n)} \end{cases} = \frac{\omega_{t-1}^{(n)} e^{-\alpha_t y^{(n)} h_t(\mathbf{x}^{(n)})}}{Z_t}$$

- If $\epsilon_t < \frac{1}{2}$, then $\frac{1-\epsilon_t}{\epsilon_t} > 1$
- If $\frac{1-\epsilon_t}{\epsilon_t} > 1$, then $\alpha_t = \frac{1}{2} \log\left(\frac{1-\epsilon_t}{\epsilon_t}\right) > 0$
- If $\alpha_t > 0$, then $e^{-\alpha_t} < 1$ and $e^{\alpha_t} > 1$

AdaBoost: Example



AdaBoost: Example



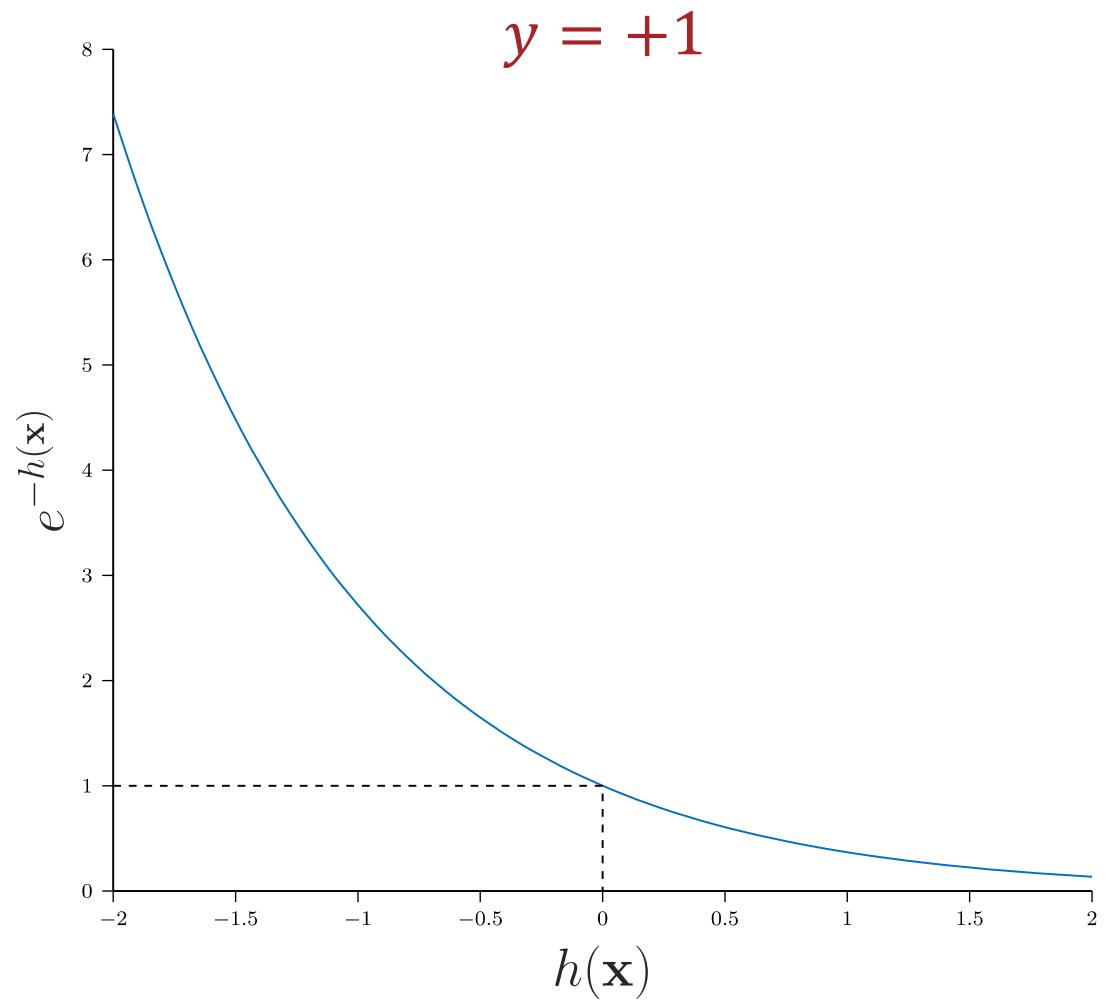
Why AdaBoost?

1. If you want to use weak learners ...
 2. ... and want your final hypothesis to be a weighted combination of weak learners, ...
 3. ... then Adaboost greedily minimizes the exponential loss:
$$e(h(\mathbf{x}), y) = e^{(-y h(\mathbf{x}))}$$
1. Because they're low variance / computational constraints
 2. Because weak learners are not great on their own
 3. Because the exponential loss upper bounds binary error!

Exponential Loss

$$e(h(\mathbf{x}), y) = e^{(-yh(\mathbf{x}))}$$

The more $h(\mathbf{x})$ “agrees with” y ,
the smaller the loss and the more
 $h(\mathbf{x})$ “disagrees with” y , the
greater the loss



Exponential Loss

- Claim:

$$\frac{1}{N} \sum_{n=1}^N e^{(-y^{(n)} h(\mathbf{x}^{(n)}))} \geq \frac{1}{N} \sum_{n=1}^N \mathbb{1}(\text{sign}(h(\mathbf{x}^{(n)})) \neq y^{(n)})$$

- Consequence:

$$\frac{1}{N} \sum_{n=1}^N e^{(-y^{(n)} h(\mathbf{x}^{(n)}))} \rightarrow 0$$

$$\Rightarrow \frac{1}{N} \sum_{n=1}^N \mathbb{1}(\text{sign}(h(\mathbf{x}^{(n)})) \neq y^{(n)}) \rightarrow 0$$

Exponential Loss

- Claim: if $g_T = \text{sign}(H_T)$ is the Adaboost hypothesis, then

$$\frac{1}{N} \sum_{n=1}^N e^{(-y^{(n)} H_T(x^{(n)}))} = \prod_{t=1}^T Z_t$$

- Proof:

Exponential Loss

- Claim: if $g_T = \text{sign}(H_T)$ is the Adaboost hypothesis, then

$$\frac{1}{N} \sum_{n=1}^N e^{-y^{(n)} H_T(x^{(n)})} = \prod_{t=1}^T Z_t$$

- Proof:

$$\omega_0^{(n)} = \frac{1}{N}, \quad \omega_1^{(n)} = \frac{e^{-\alpha_1 y^{(n)} h_1(x^{(n)})}}{NZ_1}, \quad \omega_2^{(n)} = \frac{e^{-\alpha_1 y^{(n)} h_1(x^{(n)})} e^{-\alpha_2 y^{(n)} h_2(x^{(n)})}}{NZ_1 Z_2}$$

$$\omega_T^{(n)} = \frac{\prod_{t=1}^T e^{-\alpha_t y^{(n)} h_t(x^{(n)})}}{N \prod_{t=1}^T Z_t} = \frac{e^{-y^{(n)} \sum_{t=1}^T \alpha_t h_t(x^{(n)})}}{N \prod_{t=1}^T Z_t} = \frac{e^{-y^{(n)} H_T(x^{(n)})}}{N \prod_{t=1}^T Z_t}$$

$$\sum_{n=1}^N \omega_T^{(n)} = \sum_{n=1}^N \frac{e^{-y^{(n)} H_T(x^{(n)})}}{N \prod_{t=1}^T Z_t} = 1 \Rightarrow \frac{1}{N} \sum_{n=1}^N e^{-y^{(n)} H_T(x^{(n)})} = \prod_{t=1}^T Z_t \blacksquare$$

Exponential Loss

- Claim: if $g_T = \text{sign}(H_T)$ is the Adaboost hypothesis, then

$$\frac{1}{N} \sum_{n=1}^N e^{-y^{(n)} H_T(x^{(n)})} = \prod_{t=1}^T Z_t$$

- Consequence: one way to minimize the exponential training loss is to greedily minimize Z_t , i.e., in each iteration, make the normalization constant as small as possible by tuning α_t .

Greedy Exponential Loss Minimization

$$Z_t = \sum_{n=1}^N \omega_{t-1}^{(n)} e^{-(a)y^{(n)} h_t(x^{(n)})}$$

Greedy Exponential Loss Minimization

$$\begin{aligned} Z_t &= \sum_{n=1}^N \omega_{t-1}^{(n)} e^{-(a)y^{(n)} h_t(x^{(n)})} \\ &= \sum_{y^{(n)} = h_t(x^{(n)})} \omega_{t-1}^{(n)} e^{-(a)} + \sum_{y^{(n)} \neq h_t(x^{(n)})} \omega_{t-1}^{(n)} e^{(a)} \\ &= e^{-(a)} \sum_{y^{(n)} = h_t(x^{(n)})} \omega_{t-1}^{(n)} + e^{(a)} \sum_{y^{(n)} \neq h_t(x^{(n)})} \omega_{t-1}^{(n)} \\ &= e^{-a}(1 - \epsilon_t) + e^a \epsilon_t \end{aligned}$$

Greedy Exponential Loss Minimization

$$Z_t = e^{-a}(1 - \epsilon_t) + e^a \epsilon_t$$

Greedy Exponential Loss Minimization

$$Z_t = e^{-a}(1 - \epsilon_t) + e^a \epsilon_t$$

$$\begin{aligned}\frac{\partial Z_t}{\partial a} &= -e^{-a}(1 - \epsilon_t) + e^a \epsilon_t \Rightarrow -e^{-\hat{a}}(1 - \epsilon_t) + e^{\hat{a}} \epsilon_t = 0 \\ &\Rightarrow e^{\hat{a}} \epsilon_t = e^{-\hat{a}}(1 - \epsilon_t) \\ &\Rightarrow e^{2\hat{a}} = \frac{1 - \epsilon_t}{\epsilon_t} \\ &\Rightarrow \hat{a} = \frac{1}{2} \log\left(\frac{1 - \epsilon_t}{\epsilon_t}\right) = \alpha_t\end{aligned}$$

$$\frac{\partial^2 Z_t}{\partial a^2} = e^{-a}(1 - \epsilon_t) + e^a \epsilon_t > 0$$

Normalizing $\omega^{(n)}$

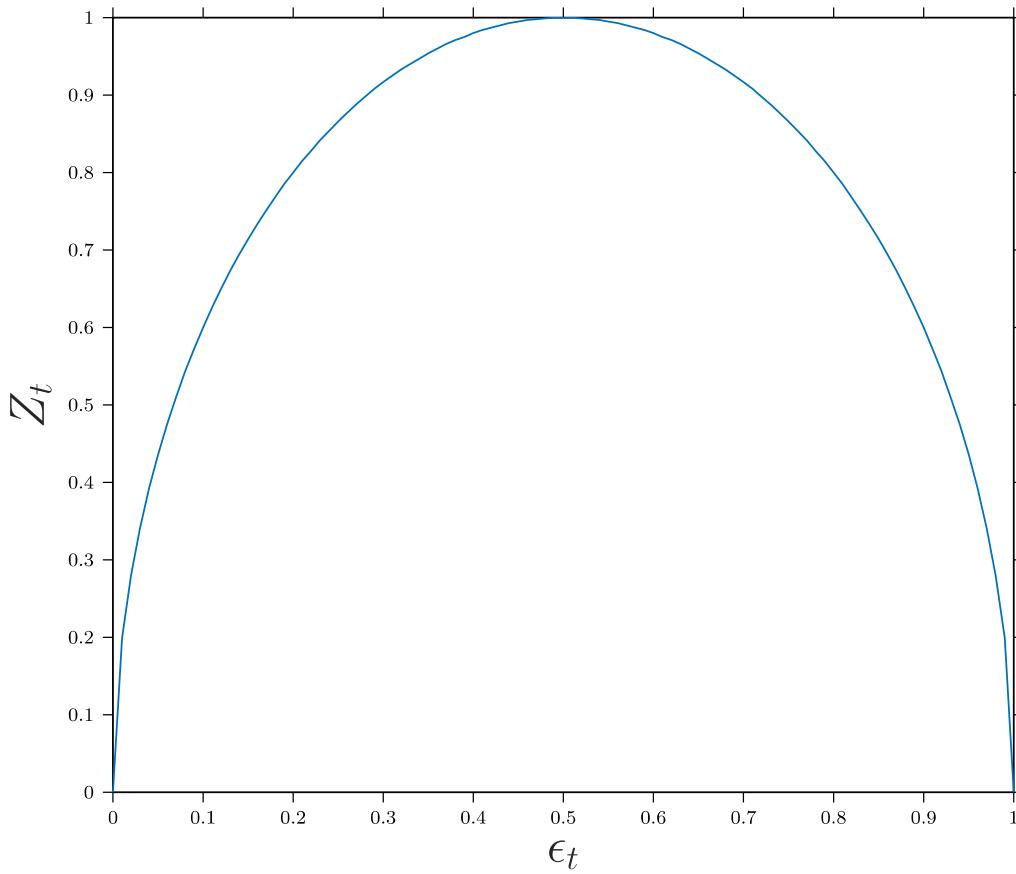
$$\begin{aligned} Z_t &= \sum_{n=1}^N \omega_{t-1}^{(n)} e^{-\alpha_t y^{(n)} h_t(x^{(n)})} \\ &= \sum_{y^{(n)} = h_t(x^{(n)})} \omega_{t-1}^{(n)} e^{-\alpha_t} + \sum_{y^{(n)} \neq h_t(x^{(n)})} \omega_{t-1}^{(n)} e^{\alpha_t} \end{aligned}$$

Normalizing $\omega^{(n)}$

$$\begin{aligned} Z_t &= \sum_{n=1}^N \omega_{t-1}^{(n)} e^{-\alpha_t y^{(n)} h_t(x^{(n)})} \\ &= \sum_{y^{(n)} = h_t(x^{(n)})} \omega_{t-1}^{(n)} e^{-\alpha_t} + \sum_{y^{(n)} \neq h_t(x^{(n)})} \omega_{t-1}^{(n)} e^{\alpha_t} \\ &= e^{-\alpha_t} \sum_{y^{(n)} = h_t(x^{(n)})} \omega_{t-1}^{(n)} + e^{\alpha_t} \sum_{y^{(n)} \neq h_t(x^{(n)})} \omega_{t-1}^{(n)} \\ &= e^{-\alpha_t} (1 - \epsilon_t) + e^{\alpha_t} \epsilon_t \\ &= e^{-\frac{1}{2}\log\left(\frac{1-\epsilon_t}{\epsilon_t}\right)} (1 - \epsilon_t) + e^{\frac{1}{2}\log\left(\frac{1-\epsilon_t}{\epsilon_t}\right)} \epsilon_t \\ &= \sqrt{\epsilon_t(1 - \epsilon_t)} + \sqrt{\epsilon_t(1 - \epsilon_t)} = 2\sqrt{\epsilon_t(1 - \epsilon_t)} \end{aligned}$$

Z_t

$$Z_t = \sum_{n=1}^N \omega_{t-1}^{(n)} e^{-\alpha_t y^{(n)} h_t(x^{(n)})} = 2\sqrt{\epsilon_t(1-\epsilon_t)} < 1 \text{ if } \epsilon_t < \frac{1}{2}$$



Training Error

$$\frac{1}{N} \sum_{n=1}^N \mathbb{1}(y^{(n)} \neq g_T(\mathbf{x}^{(n)})) \leq \frac{1}{N} \sum_{n=1}^N e^{-y^{(n)} H_T(\mathbf{x}^{(n)})}$$

$$= \prod_{t=1}^T Z_t$$

$$= \prod_{t=1}^T 2\sqrt{\epsilon_t(1 - \epsilon_t)} \rightarrow 0 \text{ as } T \rightarrow \infty$$

$\left(\text{as long as } \epsilon_t < \frac{1}{2} \forall t \right)$

True Error (Freund & Schapire, 1995)

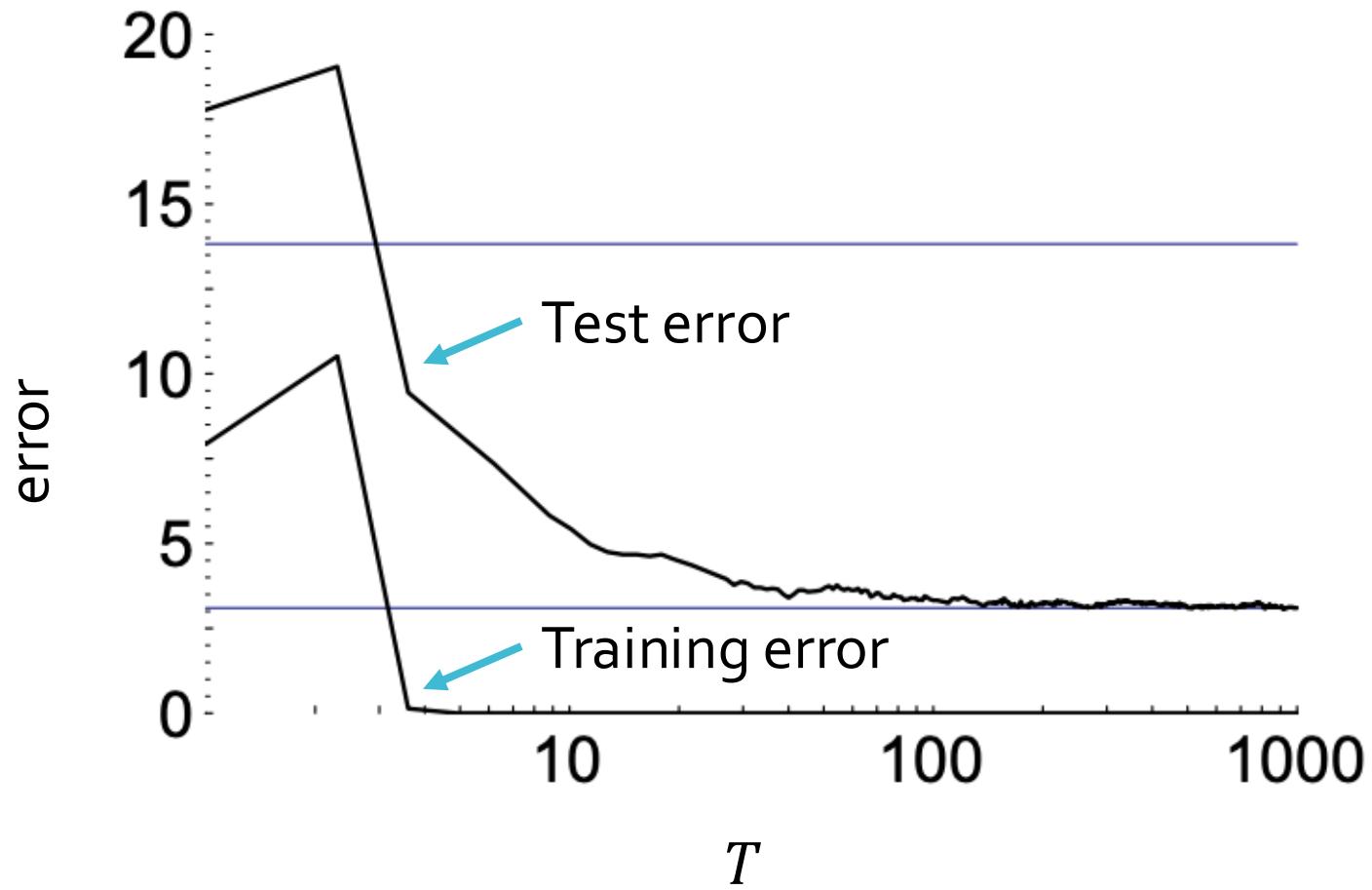
- For AdaBoost, with high probability:

$$\text{True Error} \leq \text{Training Error} + \tilde{O}\left(\sqrt{\frac{d_{vc}(\mathcal{H})T}{N}}\right)$$

where $d_{vc}(\mathcal{H})$ is the VC-dimension of the weak learners and T is the number of weak learners.

- Empirical results indicate that increasing T does not lead to overfitting as this bound would suggest!

Test Error (Schapire, 1989)

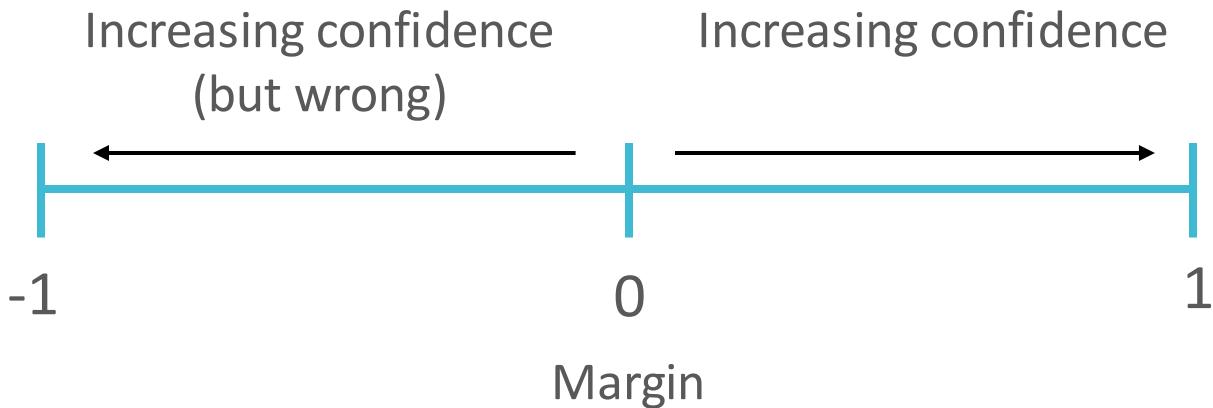


Margins

- The *margin* of training point $(\mathbf{x}^{(i)}, y^{(i)})$ is defined as:

$$m(\mathbf{x}^{(i)}, y^{(i)}) = \frac{y^{(i)} \sum_{t=1}^T \alpha_t h_t(\mathbf{x}^{(i)})}{\sum_{t=1}^T \alpha_t}$$

- The margin can be interpreted as how confident g_T is in its prediction: the bigger the margin, the more confident.



True Error (Schapire, Freund et al., 1998)

- For AdaBoost, with high probability:

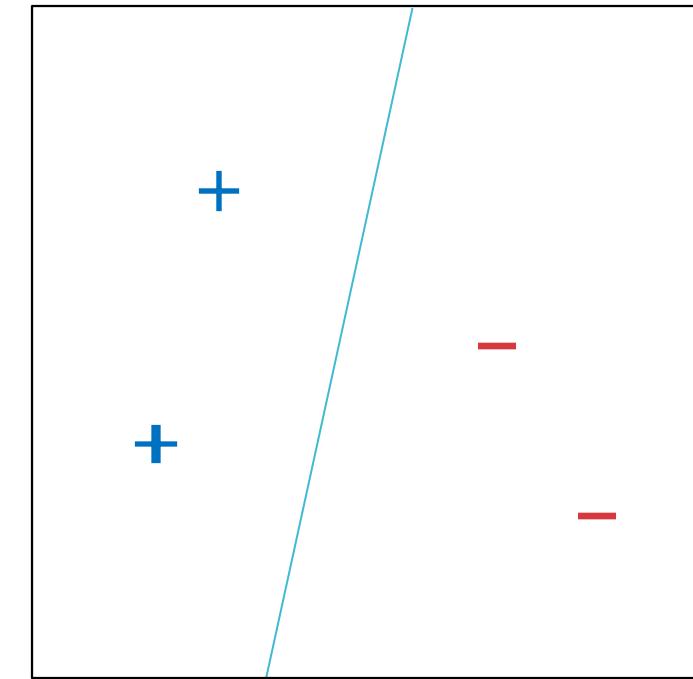
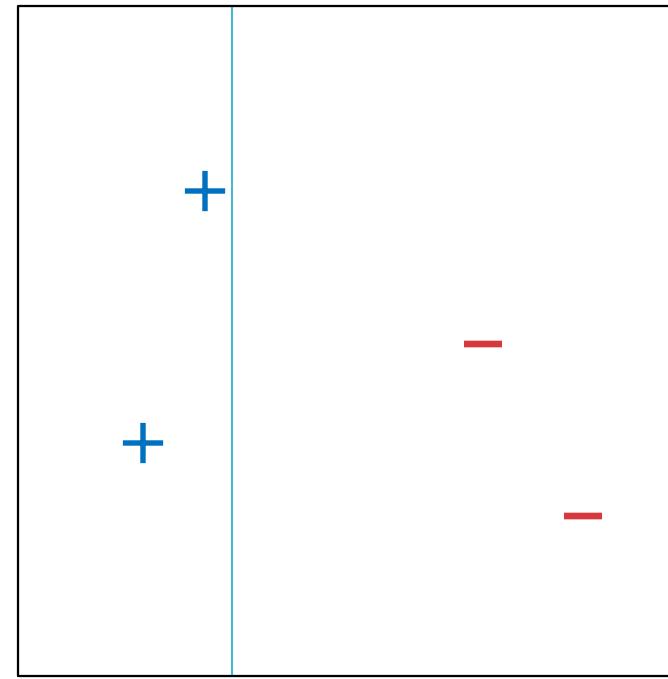
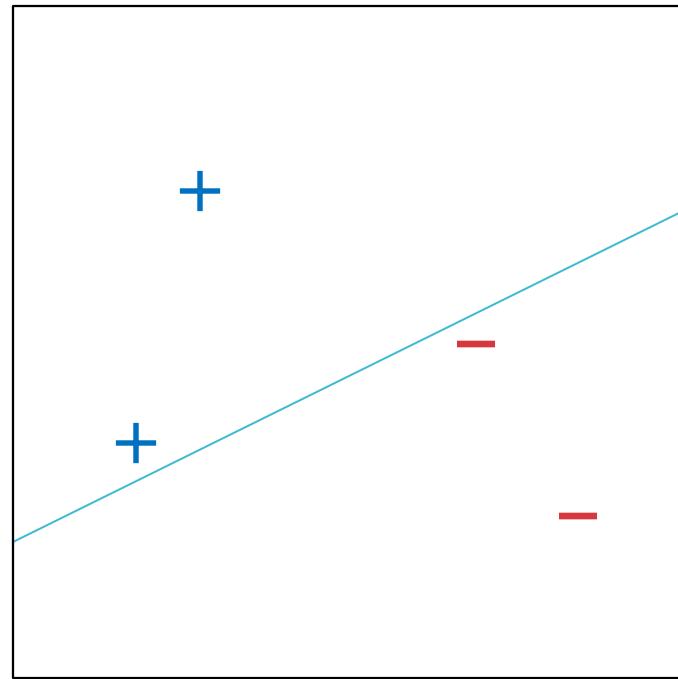
$$\text{True Error} \leq \frac{1}{N} \sum_{i=1}^N \llbracket m(\mathbf{x}^{(i)}, y^{(i)}) \leq \epsilon \rrbracket + \tilde{O}\left(\sqrt{\frac{d_{vc}(\mathcal{H})}{N\epsilon^2}}\right)$$

where $d_{vc}(\mathcal{H})$ is the VC-dimension of the weak learners and $\epsilon > 0$ is a tolerance parameter.

- Even after AdaBoost has driven the training error to 0, it continues to target the “training margin”

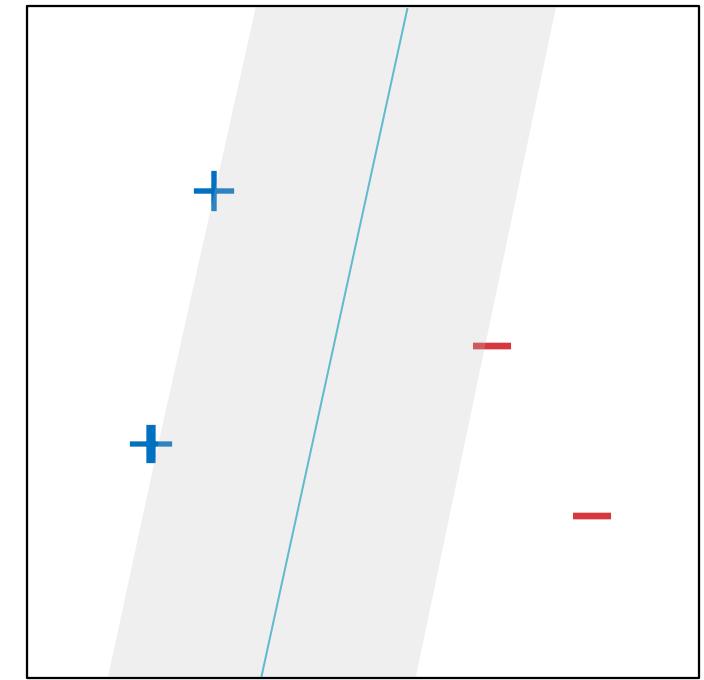
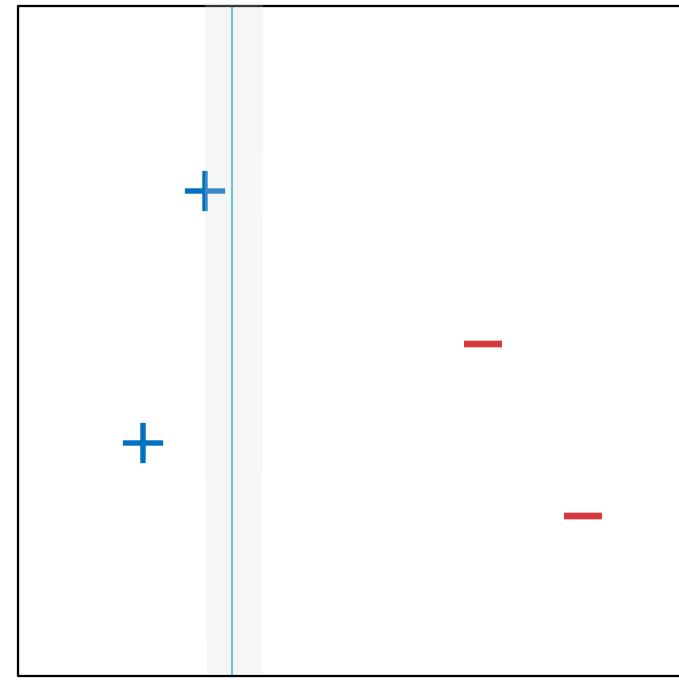
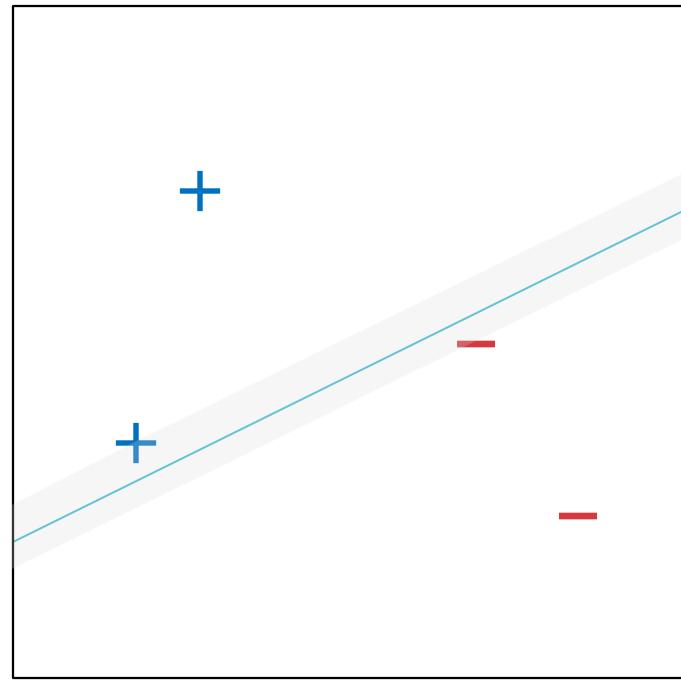
Key Takeaways

- Boosting targets simple models, i.e., weak learners
- Greedily minimizes the exponential loss, an upper bound of the classification error
- Theoretical (and empirical) results show resilience to overfitting by targeting training margin



In-class Poll:
Which linear separator is best?





Which linear separator is best?

Maximal Margin Linear Separators

- The margin of a linear separator is the distance between it and the nearest training data point
- Questions:
 1. How can we efficiently find a maximal-margin linear separator?
 2. Why are linear separators with larger margins better?
 3. What can we do if the data is not linearly separable?

Recall: Hyperplanes

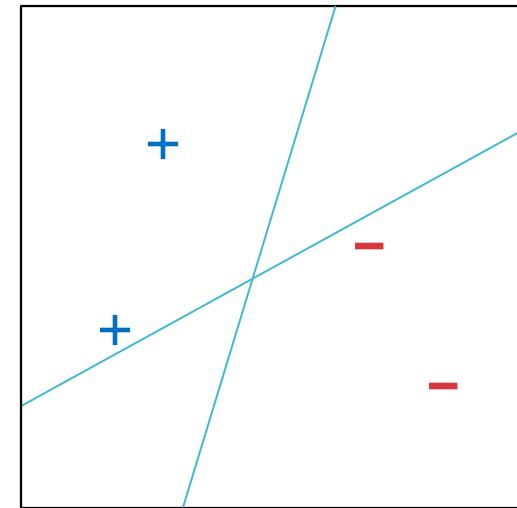
- For linear models, decision boundaries are D -dimensional **hyperplanes** defined by a weight vector, $[b, \mathbf{w}]$
$$\mathbf{w}^T \mathbf{x} + b = 0$$
- Problem: there are infinitely many weight vectors that describe the same hyperplane
 - $x_1 + 2x_2 + 2 = 0$ is the same line as
 $2x_1 + 4x_2 + 4 = 0$, which is the same line as
 $1000000x_1 + 2000000x_2 + 2000000 = 0$
 - Solution: normalize weight vectors w.r.t. *the training data*

Normalizing Hyperplanes

- Given a dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ where $y \in \{-1, +1\}$,
 $\hat{y} = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$ is a valid **linear separator** if
$$y^{(i)}(\mathbf{w}^T \mathbf{x}^{(i)} + b) > 0 \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}$$
- For SVMs, we're *only* going to consider **linear separators** in
$$\mathcal{H} = \{\hat{y} = \text{sign}(\mathbf{w}^T \mathbf{x} + b): \min_{(\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}} y^{(i)}(\mathbf{w}^T \mathbf{x}^{(i)} + b) = 1\}$$
- If $\hat{y} = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$ is a linear separator, then
$$\hat{y} = \text{sign}\left(\frac{\mathbf{w}^T}{\rho} \mathbf{x} + \frac{b}{\rho}\right) \in \mathcal{H} \text{ where}$$
$$\rho = \min_{(\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}} y^{(i)}(\mathbf{w}^T \mathbf{x}^{(i)} + b)$$

Normalizing Hyperplanes: Example

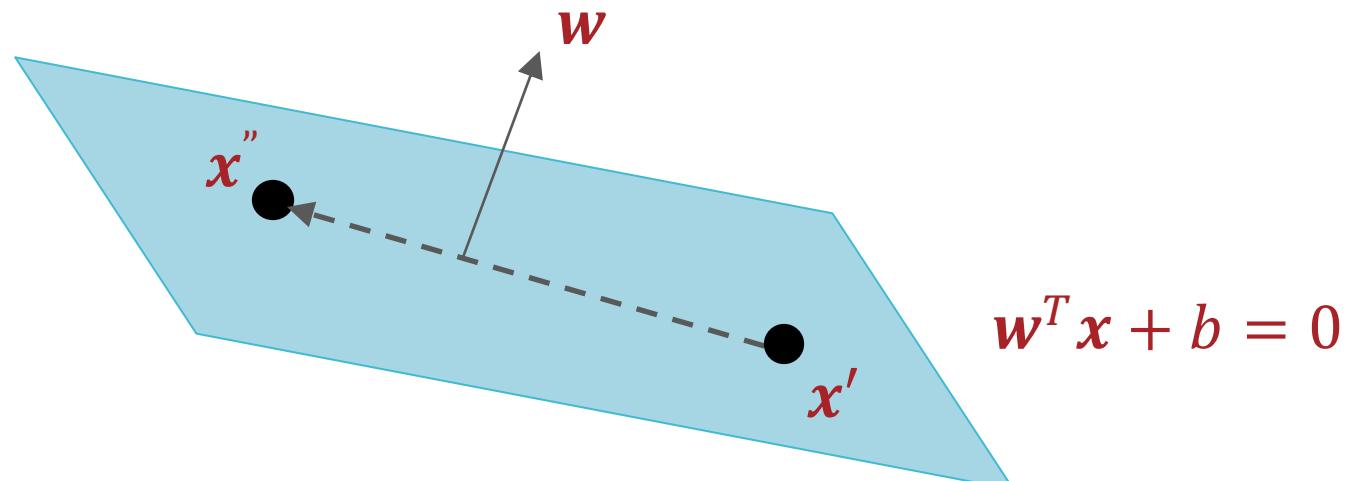
b	w_1	w_2	
-0.2	-0.6	1	$\notin \mathcal{H}$
-0.4	-1.2	2	$\notin \mathcal{H}$
-2	-6	10	$\notin \mathcal{H}$
-10	-30	50	$\in \mathcal{H}$
0.2	-0.6	0.2	$\notin \mathcal{H}$
0.1	-0.3	0.1	$\notin \mathcal{H}$
1	-3	1	$\notin \mathcal{H}$
2	-6	2	$\in \mathcal{H}$



x_1	x_2	y	$y(\mathbf{w}^T \mathbf{x} + b)$
0.2	0.4	+1	1.6
0.3	0.8	+1	1.8
0.7	0.6	-1	1
0.8	0.3	-1	2.2

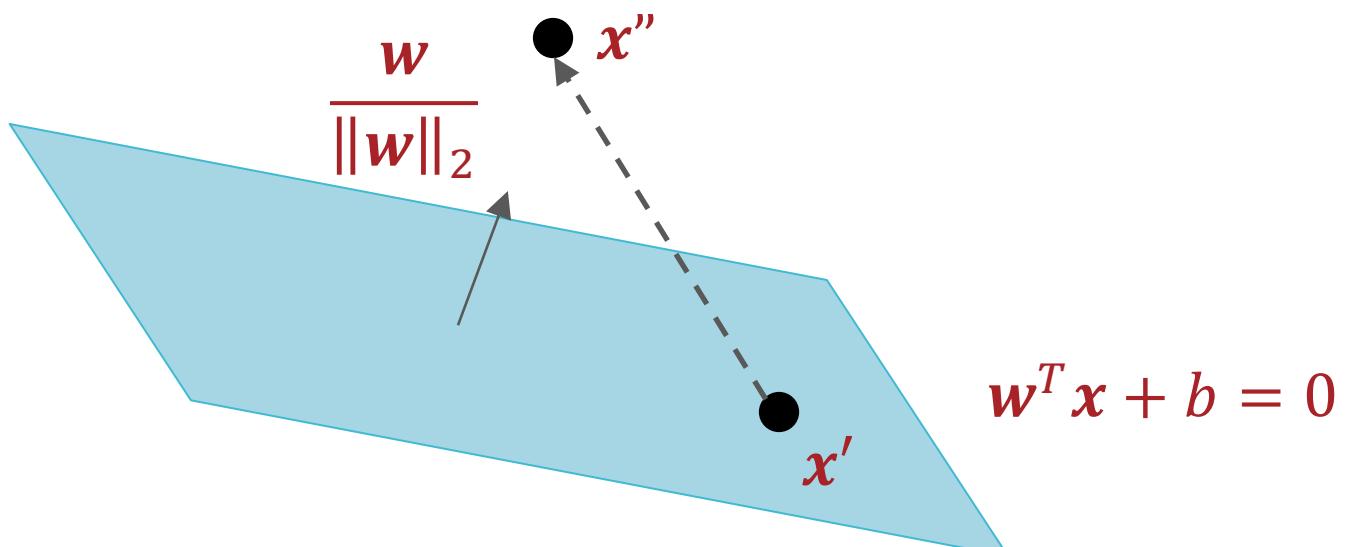
Computing the Margin

- Claim: \mathbf{w} is orthogonal to the hyperplane $\mathbf{w}^T \mathbf{x} + b = 0$ (the decision boundary)
- A vector is orthogonal to a hyperplane if it is orthogonal to every vector in that hyperplane
- Vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are orthogonal if $\boldsymbol{\alpha}^T \boldsymbol{\beta} = 0$



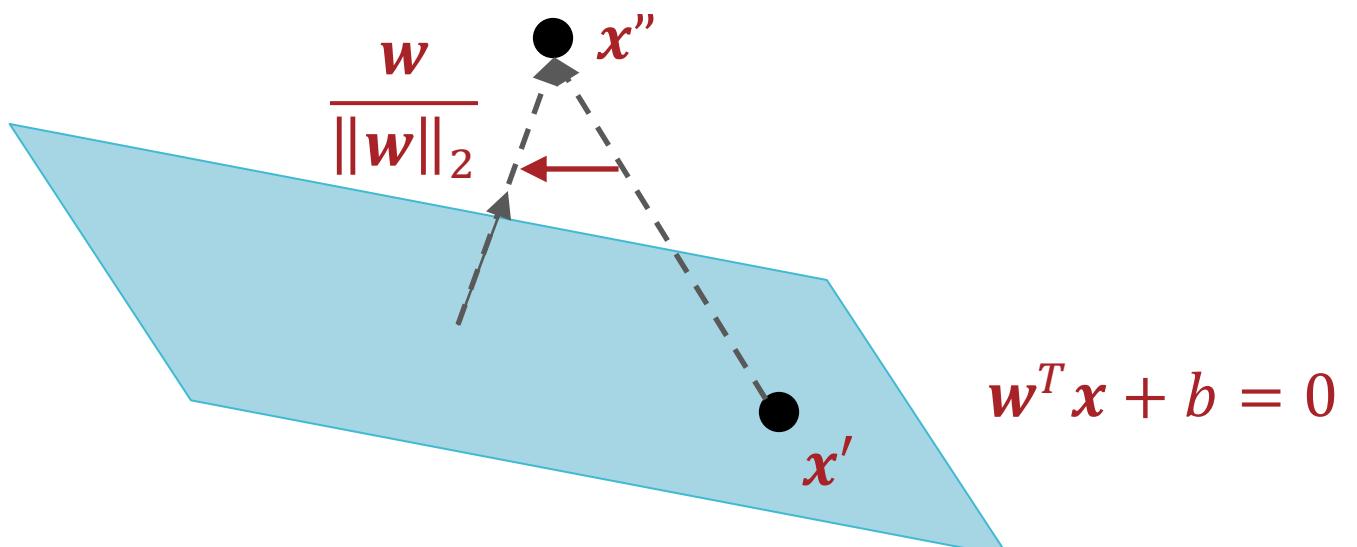
Computing the Margin

- Let \mathbf{x}' be an arbitrary point on the hyperplane $\mathbf{w}^T \mathbf{x} + b = 0$ and let \mathbf{x}'' be an arbitrary point
- The distance between \mathbf{x}'' and $\mathbf{w}^T \mathbf{x} + b = 0$ is equal to the magnitude of the projection of $\mathbf{x}'' - \mathbf{x}'$ onto $\frac{\mathbf{w}}{\|\mathbf{w}\|_2}$, the unit vector orthogonal to the hyperplane



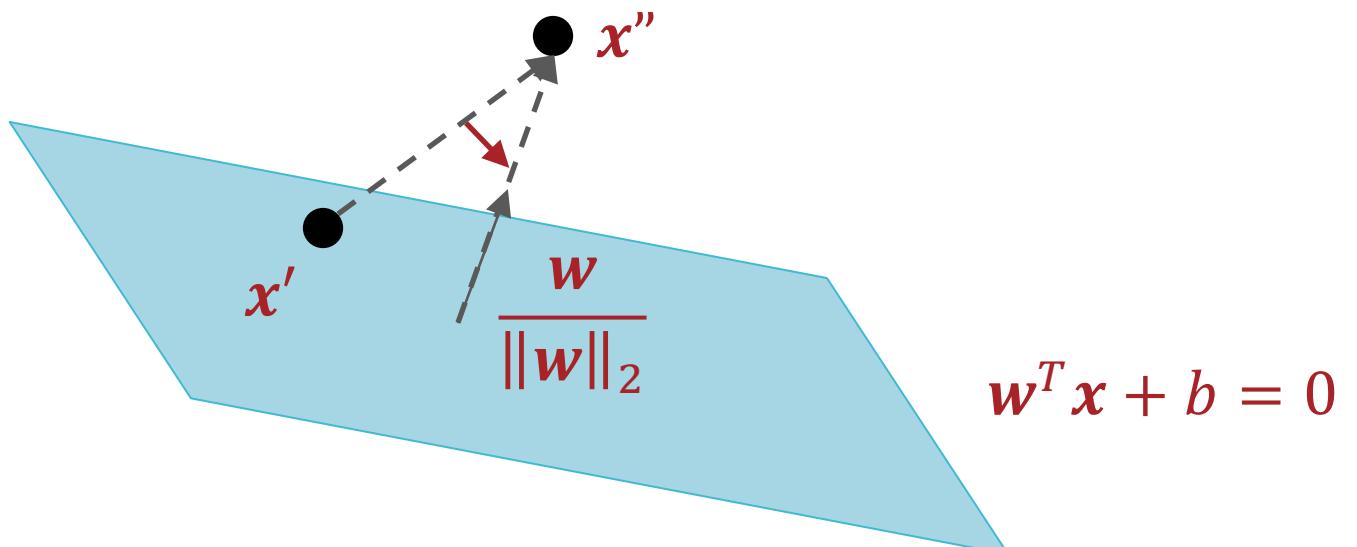
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Computing the Margin

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Computing the Margin

- Let \mathbf{x}' be an arbitrary point on the hyperplane $h(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = 0$ and let \mathbf{x}'' be an arbitrary point
- The distance between \mathbf{x}'' and $h(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = 0$ is equal to the magnitude of the projection of $\mathbf{x}'' - \mathbf{x}'$ onto $\frac{\mathbf{w}}{\|\mathbf{w}\|_2}$, the unit vector orthogonal to the hyperplane

$$\begin{aligned} d(\mathbf{x}'', h) &= \left| \frac{\mathbf{w}^T (\mathbf{x}'' - \mathbf{x}')}{\|\mathbf{w}\|_2} \right| = \frac{|\mathbf{w}^T \mathbf{x}'' - \mathbf{w}^T \mathbf{x}'|}{\|\mathbf{w}\|_2} \\ &= \frac{|\mathbf{w}^T \mathbf{x}'' + b|}{\|\mathbf{w}\|_2} \end{aligned}$$

Computing the Margin

- The margin of a linear separator is the distance between it and the nearest training data point

$$\begin{aligned} \min_{(\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}} d(\mathbf{x}^{(i)}, h) &= \min_{(\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}} \frac{|\mathbf{w}^T \mathbf{x}^{(i)} + b|}{\|\mathbf{w}\|_2} \\ &= \frac{1}{\|\mathbf{w}\|_2} \min_{(\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}} |\mathbf{w}^T \mathbf{x}^{(i)} + b| \\ &= \frac{1}{\|\mathbf{w}\|_2} \min_{(\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}} y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + b) \\ &= \frac{1}{\|\mathbf{w}\|_2} \end{aligned}$$

Maximizing the Margin

$$\begin{aligned} & \text{maximize} \quad \frac{1}{\|\mathbf{w}\|_2} \\ & \text{subject to} \quad \min_{(\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}} y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + b) = 1 \\ & \qquad \Updownarrow \\ & \text{minimize} \quad \|\mathbf{w}\|_2 \\ & \text{subject to} \quad \min_{(\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}} y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + b) = 1 \\ & \qquad \Updownarrow \\ & \text{minimize} \quad \frac{1}{2} \|\mathbf{w}\|_2^2 \\ & \text{subject to} \quad \min_{(\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}} y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + b) = 1 \\ & \qquad \Updownarrow \\ & \text{minimize} \quad \frac{1}{2} \mathbf{w}^T \mathbf{w} \\ & \text{subject to} \quad y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + b) \geq 1 \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D} \end{aligned}$$