

Foundations of Machine Learning

Boosting

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Weak Learning

(Kearns and Valiant, 1994)


■ **Definition:** concept class C is **weakly PAC-learnable** if there exists a (**weak**) learning algorithm L and $\gamma > 0$ such that:

- for all $\delta > 0$, for all $c \in C$ and all distributions D ,

$$\Pr_{S \sim D} \left[R(h_S) \leq \frac{1}{2} - \gamma \right] \geq 1 - \delta,$$

- for samples S of size $m = \text{poly}(1/\delta)$ for a fixed polynomial.

Boosting Ideas

- Finding simple relatively accurate base classifiers often not hard  weak learner.
- Main ideas:
 - use weak learner to create a strong learner.
 - combine base classifiers returned by weak learner (ensemble method).
- But, how should the base classifiers be combined?

AdaBoost

(Freund and Schapire, 1997)

$$H \subseteq \{-1, +1\}^X.$$

ADABOOST($S = ((x_1, y_1), \dots, (x_m, y_m))$)

```
1  for  $i \leftarrow 1$  to  $m$  do
2       $D_1(i) \leftarrow \frac{1}{m}$ 
3  for  $t \leftarrow 1$  to  $T$  do
4       $h_t \leftarrow$  base classifier in  $H$  with small error  $\epsilon_t = \Pr_{i \sim D_t} [h_t(x_i) \neq y_i]$ 
5       $\alpha_t \leftarrow \frac{1}{2} \log \frac{1 - \epsilon_t}{\epsilon_t}$ 
6       $Z_t \leftarrow 2[\epsilon_t(1 - \epsilon_t)]^{\frac{1}{2}}$   $\triangleright$  normalization factor
7      for  $i \leftarrow 1$  to  $m$  do
8           $D_{t+1}(i) \leftarrow \frac{D_t(i) \exp(-\alpha_t y_i h_t(x_i))}{Z_t}$ 
9       $f_t \leftarrow \sum_{s=1}^t \alpha_s h_s$ 
10 return  $h = \text{sgn}(f_T)$ 
```

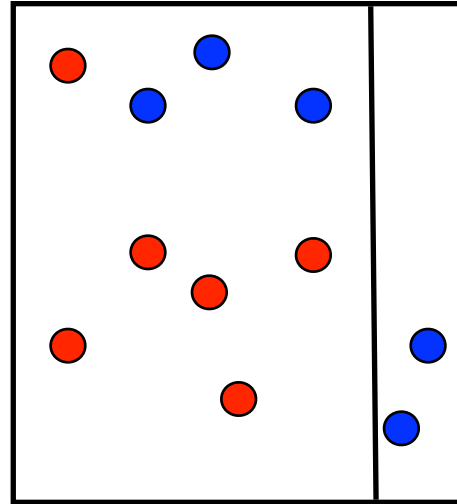
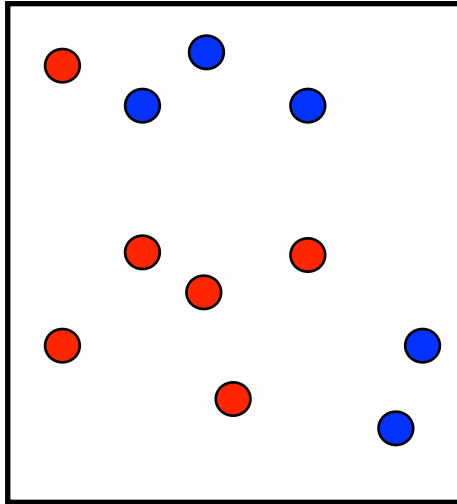
Notes

- Distributions D_t over training sample:
 - originally uniform.
 - at each round, the weight of a misclassified example is increased.
 - observation: $D_{t+1}(i) = \frac{e^{-y_i f_t(x_i)}}{m \prod_{s=1}^t Z_s}$, since

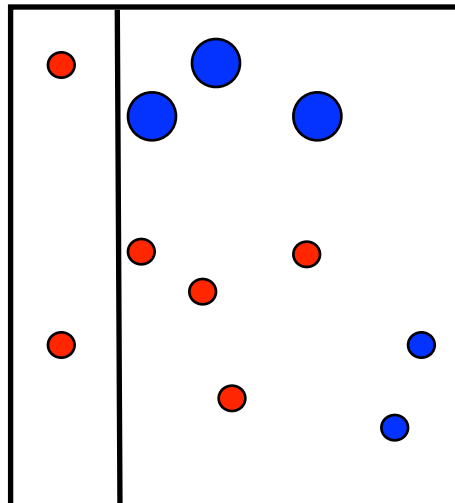
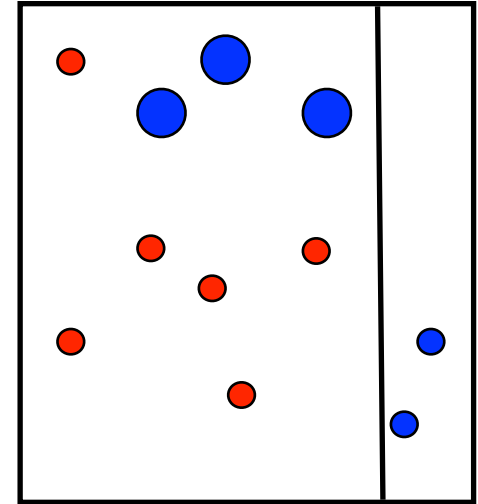
$$D_{t+1}(i) = \frac{D_t(i) e^{-\alpha_t y_i h_t(x_i)}}{Z_t} = \frac{D_{t-1}(i) e^{-\alpha_{t-1} y_i h_{t-1}(x_i)} e^{-\alpha_t y_i h_t(x_i)}}{Z_{t-1} Z_t} = \frac{1}{m} \frac{e^{-y_i \sum_{s=1}^t \alpha_s h_s(x_i)}}{\prod_{s=1}^t Z_s}.$$

- Weight assigned to base classifier h_t : α_t directly depends on the accuracy of h_t at round t .

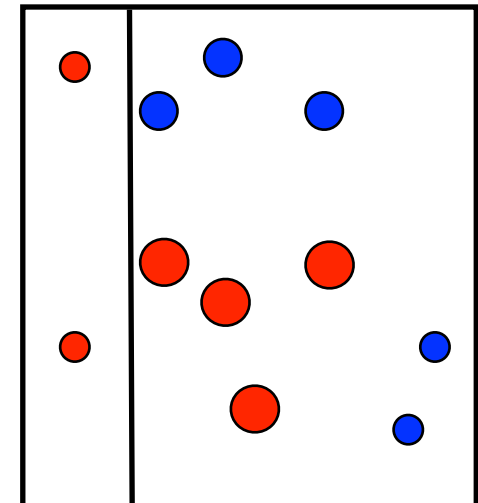
Illustration

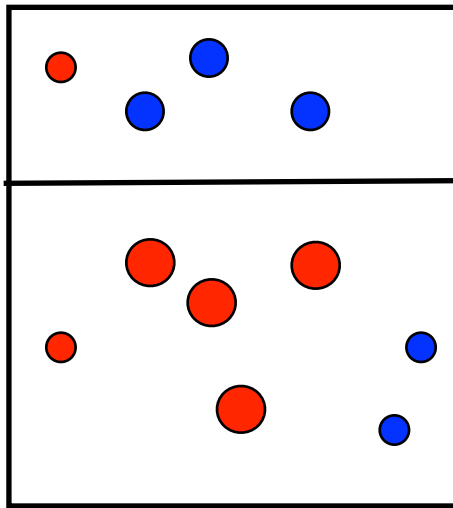


$t = 1$



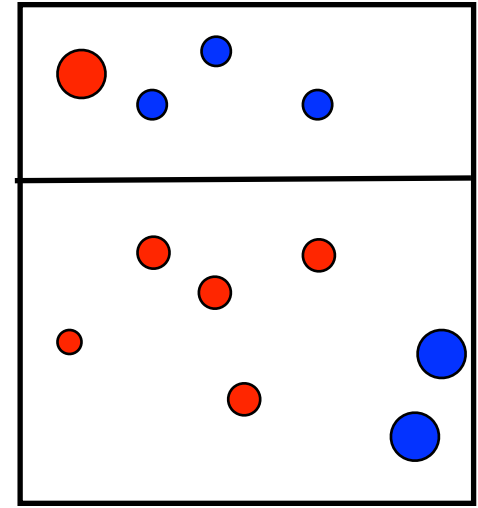
$t = 2$



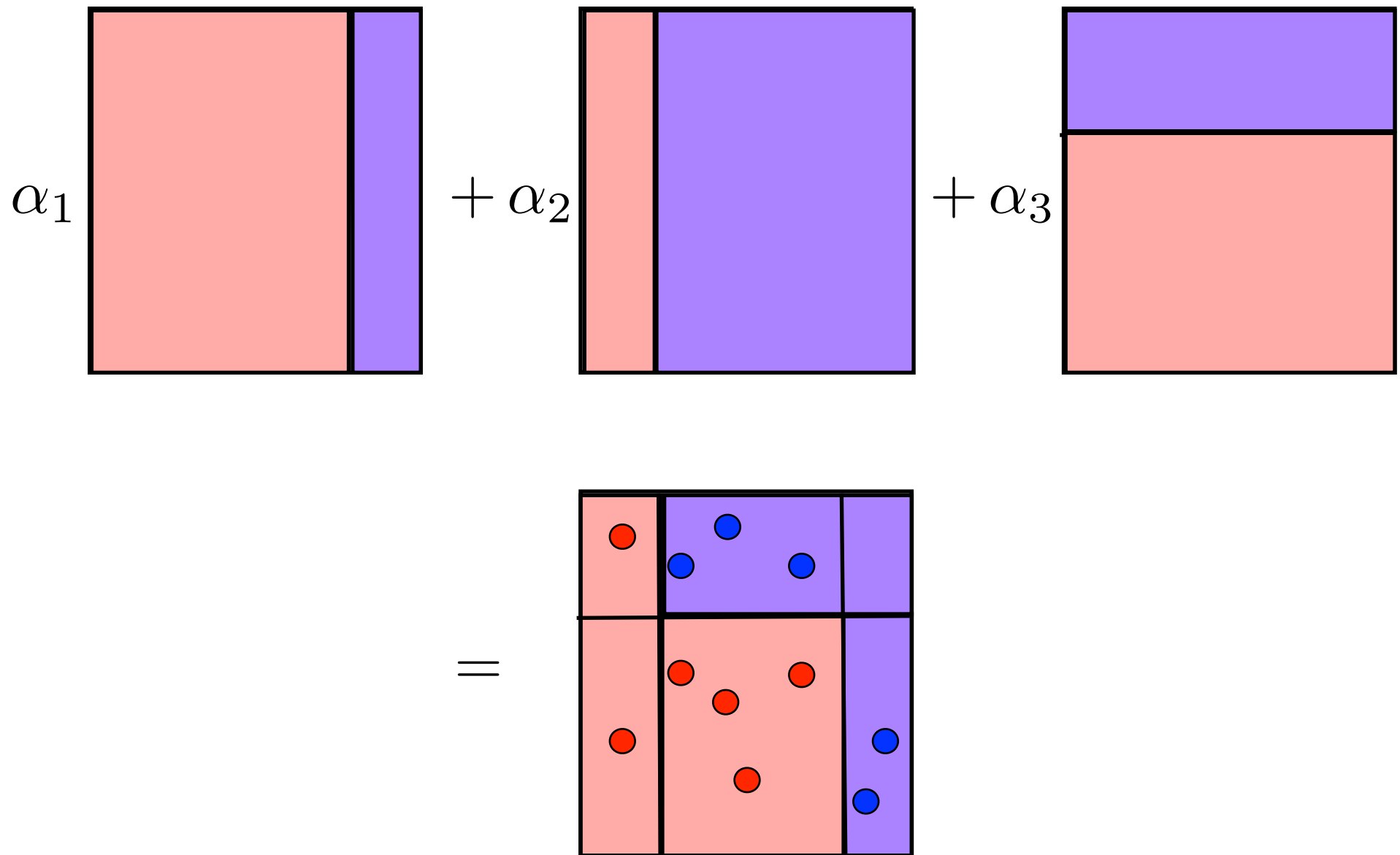


$t = 3$

...



...



Bound on Empirical Error

(Freund and Schapire, 1997)

- **Theorem:** The empirical error of the classifier output by AdaBoost verifies:

$$\hat{R}(h) \leq \exp \left[-2 \sum_{t=1}^T \left(\frac{1}{2} - \epsilon_t \right)^2 \right].$$

- If further for all $t \in [1, T]$, $\gamma \leq \left(\frac{1}{2} - \epsilon_t \right)$, then

$$\hat{R}(h) \leq \exp(-2\gamma^2 T).$$

- γ does not need to be known in advance:
adaptive boosting.

- **Proof:** Since, as we saw, $D_{t+1}(i) = \frac{e^{-y_i f_t(x_i)}}{m \prod_{s=1}^t Z_s}$,

$$\begin{aligned}\hat{R}(h) &= \frac{1}{m} \sum_{i=1}^m 1_{y_i f(x_i) \leq 0} \leq \frac{1}{m} \sum_{i=1}^m \exp(-y_i f(x_i)) \\ &\leq \frac{1}{m} \sum_{i=1}^m \left[m \prod_{t=1}^T Z_t \right] D_{T+1}(i) = \prod_{t=1}^T Z_t.\end{aligned}$$

- Now, since Z_t is a normalization factor,

$$\begin{aligned}Z_t &= \sum_{i=1}^m D_t(i) e^{-\alpha_t y_i h_t(x_i)} \\ &= \sum_{i: y_i h_t(x_i) \geq 0} D_t(i) e^{-\alpha_t} + \sum_{i: y_i h_t(x_i) < 0} D_t(i) e^{\alpha_t} \\ &= (1 - \epsilon_t) e^{-\alpha_t} + \epsilon_t e^{\alpha_t} \\ &= (1 - \epsilon_t) \sqrt{\frac{\epsilon_t}{1 - \epsilon_t}} + \epsilon_t \sqrt{\frac{1 - \epsilon_t}{\epsilon_t}} = 2 \sqrt{\epsilon_t (1 - \epsilon_t)}.\end{aligned}$$

- Thus,

$$\begin{aligned}\prod_{t=1}^T Z_t &= \prod_{t=1}^T 2\sqrt{\epsilon_t(1-\epsilon_t)} = \prod_{t=1}^T \sqrt{1 - 4\left(\frac{1}{2} - \epsilon_t\right)^2} \\ &\leq \prod_{t=1}^T \exp\left[-2\left(\frac{1}{2} - \epsilon_t\right)^2\right] = \exp\left[-2\sum_{t=1}^T \left(\frac{1}{2} - \epsilon_t\right)^2\right].\end{aligned}$$

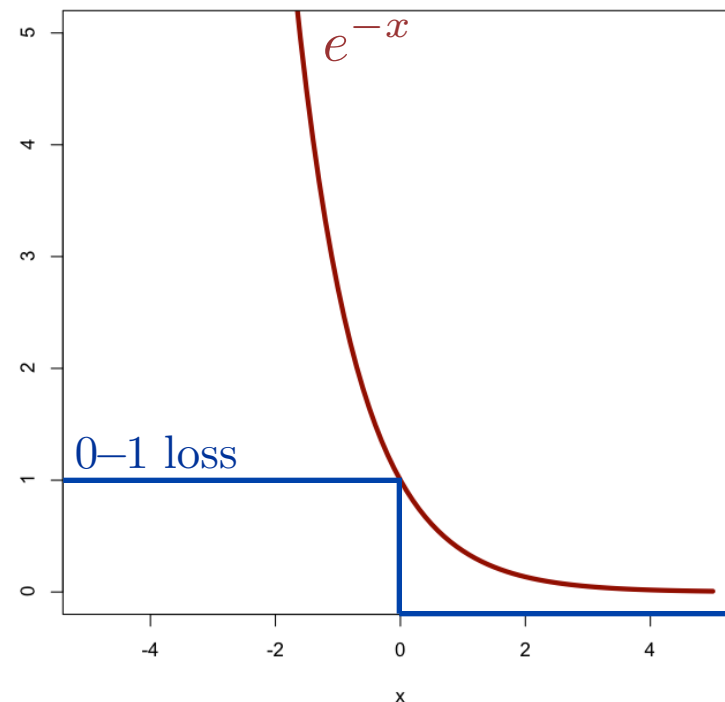
- **Notes:**

- α_t minimizer of $\alpha \mapsto (1-\epsilon_t)e^{-\alpha} + \epsilon_t e^{\alpha}$.
- since $(1-\epsilon_t)e^{-\alpha_t} = \epsilon_t e^{\alpha_t}$, at each round, AdaBoost assigns the same probability mass to correctly classified and misclassified instances.
- for base classifiers $x \mapsto [-1, +1]$, α_t can be similarly chosen to minimize Z_t .

AdaBoost = Coordinate Descent

- **Objective Function:** convex and differentiable.

$$F(\bar{\alpha}) = \frac{1}{m} \sum_{i=1}^m e^{-y_i f(x_i)} = \frac{1}{m} \sum_{i=1}^m e^{-y_i \sum_{j=1}^N \bar{\alpha}_j h_j(x_i)} .$$



- **Direction:** unit vector \mathbf{e}_k with best directional derivative:

$$F'(\bar{\alpha}_{t-1}, \mathbf{e}_k) = \lim_{\eta \rightarrow 0} \frac{F(\bar{\alpha}_{t-1} + \eta \mathbf{e}_k) - F(\bar{\alpha}_{t-1})}{\eta}.$$

- Since $F(\bar{\alpha}_{t-1} + \eta \mathbf{e}_k) = \frac{1}{m} \sum_{i=1}^m e^{-y_i \sum_{j=1}^N \bar{\alpha}_{t-1,j} h_j(x_i) - \eta y_i h_k(x_i)}$,

$$F'(\bar{\alpha}_{t-1}, \mathbf{e}_k) = -\frac{1}{m} \sum_{i=1}^m y_i h_k(x_i) e^{-y_i \sum_{j=1}^N \bar{\alpha}_{t-1,j} h_j(x_i)}$$

$$= -\frac{1}{m} \sum_{i=1}^m y_i h_k(x_i) \bar{D}_t(i) \bar{Z}_t$$

$$= -\left[\sum_{i=1}^m \bar{D}_t(i) 1_{y_i h_k(x_i)=+1} - \sum_{i=1}^m \bar{D}_t(i) 1_{y_i h_k(x_i)=-1} \right] \frac{\bar{Z}_t}{m}$$

$$= -\left[(1 - \bar{\epsilon}_{t,k}) - \bar{\epsilon}_{t,k} \right] \frac{\bar{Z}_t}{m} = \boxed{2\bar{\epsilon}_{t,k} - 1} \frac{\bar{Z}_t}{m}.$$

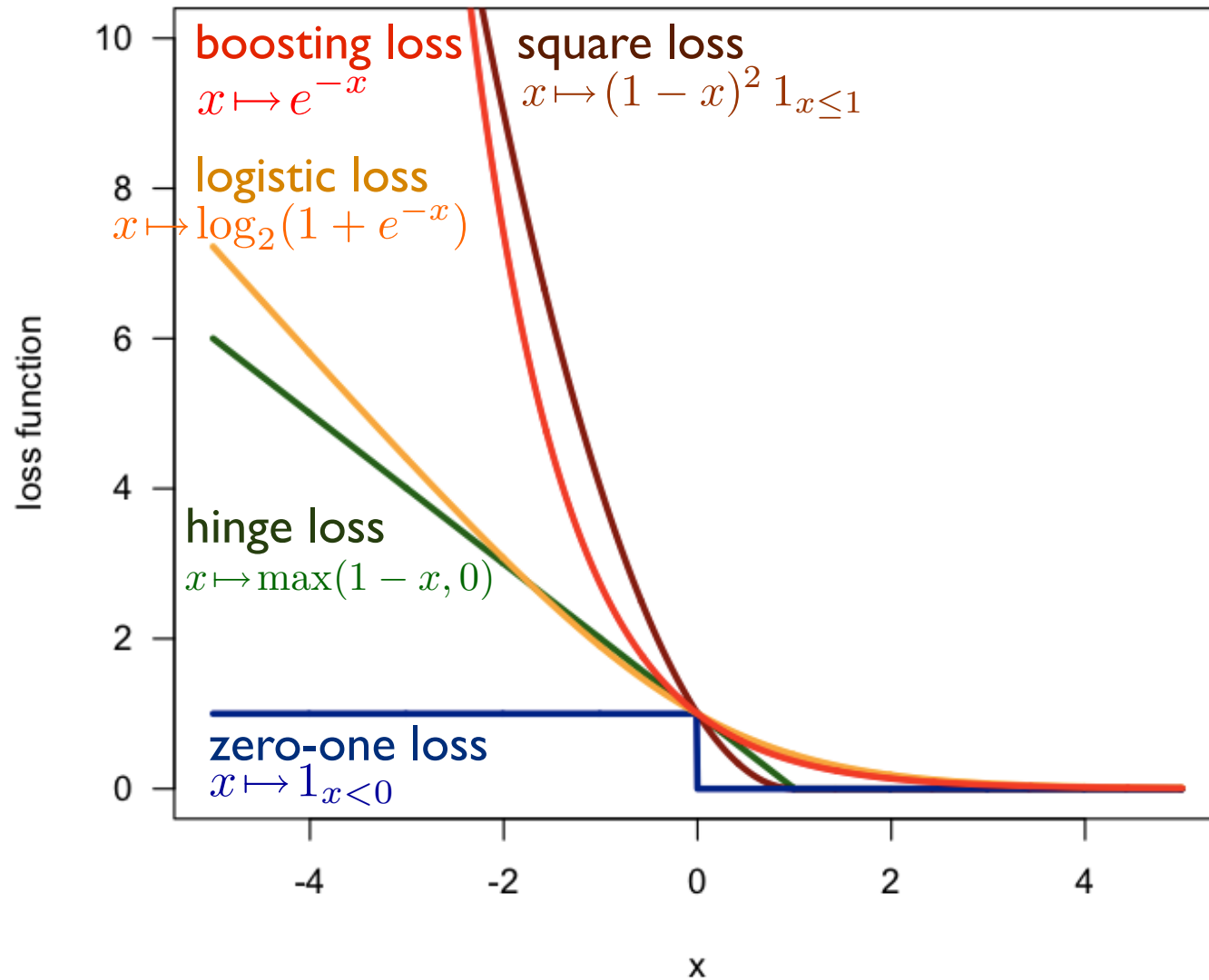
Thus, direction corresponding to base classifier with smallest error.

- **Step size:** η chosen to minimize $F(\bar{\alpha}_{t-1} + \eta \mathbf{e}_k)$;

$$\begin{aligned}
 \frac{dF(\bar{\alpha}_{t-1} + \eta \mathbf{e}_k)}{d\eta} = 0 &\Leftrightarrow - \sum_{i=1}^m y_i h_k(x_i) e^{-y_i \sum_{j=1}^N \bar{\alpha}_{t-1,j} h_j(x_i)} e^{-\eta y_i h_k(x_i)} = 0 \\
 &\Leftrightarrow - \sum_{i=1}^m y_i h_k(x_i) \bar{D}_t(i) \bar{Z}_t e^{-\eta y_i h_k(x_i)} = 0 \\
 &\Leftrightarrow - \sum_{i=1}^m y_i h_k(x_i) \bar{D}_t(i) e^{-\eta y_i h_k(x_i)} = 0 \\
 &\Leftrightarrow - [(1 - \bar{\epsilon}_{t,k}) e^{-\eta} - \bar{\epsilon}_{t,k} e^{\eta}] = 0 \\
 &\Leftrightarrow \boxed{\eta = \frac{1}{2} \log \frac{1 - \bar{\epsilon}_{t,k}}{\bar{\epsilon}_{t,k}}}.
 \end{aligned}$$

Thus, step size matches base classifier weight of AdaBoost.

Alternative Loss Functions



Standard Use in Practice

- **Base learners:** decision trees, quite often just decision stumps (trees of depth one).
- **Boosting stumps:**
 - data in \mathbb{R}^N , e.g., $N = 2$, $(\text{height}(x), \text{weight}(x))$.
 - associate a stump to each component.
 - pre-sort each component: $O(Nm \log m)$.
 - at each round, find best component and threshold.
 - total complexity: $O((m \log m)N + mNT)$.
 - stumps **not weak learners**: think XOR example!

Overfitting?

- Assume that $\text{VCdim}(H) = d$ and for a fixed T , define

$$\mathcal{F}_T = \left\{ \text{sgn} \left(\sum_{t=1}^T \alpha_t h_t - b \right) : \alpha_t, b \in \mathbb{R}, h_t \in H \right\}.$$

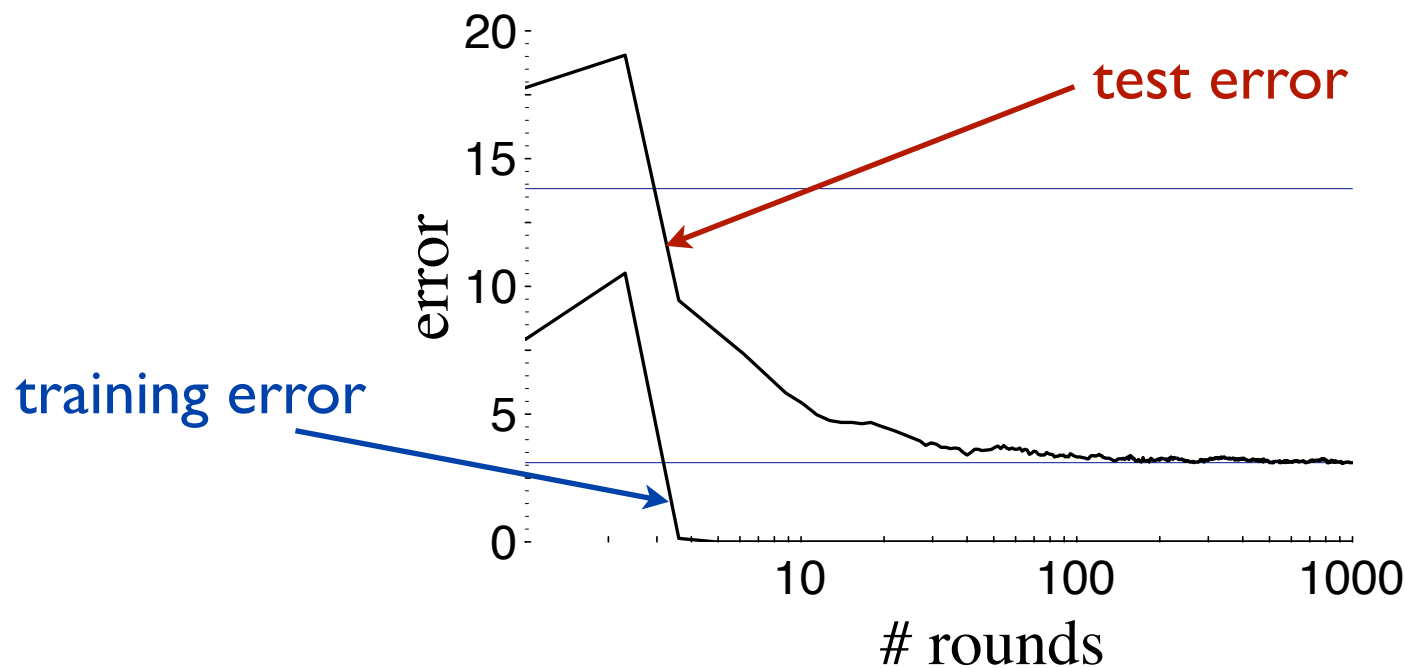
- \mathcal{F}_T can form a very rich family of classifiers. It can be shown (Freund and Schapire, 1997) that:

$$\text{VCdim}(\mathcal{F}_T) \leq 2(d + 1)(T + 1) \log_2((T + 1)e).$$

- This suggests that AdaBoost could overfit for large values of T , and that is in fact observed in some cases, but in various others it is not!

Empirical Observations

- Several empirical observations (**not all**): AdaBoost does not seem to overfit, furthermore:



C4.5 decision trees (Schapire et al., 1998).

Rademacher Complexity of Convex Hulls

■ **Theorem:** Let H be a set of functions mapping from X to \mathbb{R} . Let the convex hull of H be defined as

$$\text{conv}(H) = \left\{ \sum_{k=1}^p \mu_k h_k : p \geq 1, \mu_k \geq 0, \sum_{k=1}^p \mu_k \leq 1, h_k \in H \right\}.$$

Then, for any sample S , $\hat{\mathfrak{R}}_S(\text{conv}(H)) = \hat{\mathfrak{R}}_S(H)$.

■ **Proof:**

$$\begin{aligned} \hat{\mathfrak{R}}_S(\text{conv}(H)) &= \frac{1}{m} \mathbb{E}_{\sigma} \left[\sup_{h_k \in H, \mu \geq 0, \|\mu\|_1 \leq 1} \sum_{i=1}^m \sigma_i \sum_{k=1}^p \mu_k h_k(x_i) \right] \\ &= \frac{1}{m} \mathbb{E}_{\sigma} \left[\sup_{h_k \in H} \sup_{\mu \geq 0, \|\mu\|_1 \leq 1} \sum_{k=1}^p \mu_k \left(\sum_{i=1}^m \sigma_i h_k(x_i) \right) \right] \\ &= \frac{1}{m} \mathbb{E}_{\sigma} \left[\sup_{h_k \in H} \max_{k \in [1, p]} \left(\sum_{i=1}^m \sigma_i h_k(x_i) \right) \right] \\ &= \frac{1}{m} \mathbb{E}_{\sigma} \left[\sup_{h \in H} \sum_{i=1}^m \sigma_i h(x_i) \right] = \hat{\mathfrak{R}}_S(H). \end{aligned}$$

Margin Bound - Ensemble Methods

(Koltchinskii and Panchenko, 2002)

- **Corollary:** Let H be a set of real-valued functions. Fix $\rho > 0$. For any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $h \in \text{conv}(H)$:

$$R(h) \leq \hat{R}_\rho(h) + \frac{2}{\rho} \mathfrak{R}_m(H) + \sqrt{\frac{\log \frac{1}{\delta}}{2m}}$$

$$R(h) \leq \hat{R}_\rho(h) + \frac{2}{\rho} \hat{\mathfrak{R}}_S(H) + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}.$$

- **Proof:** Direct consequence of margin bound of Lecture 4 and $\hat{\mathfrak{R}}_S(\text{conv}(H)) = \hat{\mathfrak{R}}_S(H)$.

Margin Bound - Ensemble Methods

(Koltchinskii and Panchenko, 2002); see also (Schapire et al., 1998)

- **Corollary:** Let H be a family of functions taking values in $\{-1, +1\}$ with VC dimension d . Fix $\rho > 0$. For any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $h \in \text{conv}(H)$:

$$R(h) \leq \hat{R}_\rho(h) + \frac{2}{\rho} \sqrt{\frac{2d \log \frac{em}{d}}{m}} + \sqrt{\frac{\log \frac{1}{\delta}}{2m}}.$$

- **Proof:** Follows directly previous corollary and VC dimension bound on Rademacher complexity (see lecture 3).

Notes

- All of these bounds can be generalized to hold uniformly for all $\rho \in (0, 1)$, at the cost of an additional term $\sqrt{\frac{\log \log_2 \frac{2}{\rho}}{m}}$ and other minor constant factor changes (Koltchinskii and Panchenko, 2002).

- For AdaBoost, the bound applies to the functions

$$x \mapsto \frac{f(x)}{\|\alpha\|_1} = \frac{\sum_{t=1}^T \alpha_t h_t(x)}{\|\alpha\|_1} \in \text{conv}(H).$$

- Note that T does not appear in the bound.

Margin Distribution

■ **Theorem:** For any $\rho > 0$, the following holds:

$$\widehat{\Pr} \left[\frac{y f(x)}{\|\alpha\|_1} \leq \rho \right] \leq 2^T \prod_{t=1}^T \sqrt{\epsilon_t^{1-\rho} (1 - \epsilon_t)^{1+\rho}}.$$

■ **Proof:** Using the identity $D_{t+1}(i) = \frac{e^{-y_i f(x_i)}}{m \prod_{t=1}^T Z_t}$,

$$\begin{aligned} \frac{1}{m} \sum_{i=1}^m 1_{y_i f(x_i) - \|\alpha\|_1 \rho \leq 0} &\leq \frac{1}{m} \sum_{i=1}^m \exp(-y_i f(x_i) + \|\alpha\|_1 \rho) \\ &= \frac{1}{m} \sum_{i=1}^m e^{\|\alpha\|_1 \rho} \left[m \prod_{t=1}^T Z_t \right] D_{T+1}(i) \\ &= e^{\|\alpha\|_1 \rho} \prod_{t=1}^T Z_t = 2^T \prod_{t=1}^T \left[\sqrt{\frac{1-\epsilon_t}{\epsilon_t}} \right]^\rho \sqrt{\epsilon_t (1 - \epsilon_t)}. \end{aligned}$$

Notes

- If for all $t \in [1, T]$, $\gamma \leq (\frac{1}{2} - \epsilon_t)$, then the upper bound can be bounded by

$$\widehat{\Pr} \left[\frac{y f(x)}{\|\alpha\|_1} \leq \rho \right] \leq \left[(1 - 2\gamma)^{1-\rho} (1 + 2\gamma)^{1+\rho} \right]^{T/2}.$$

For $\rho < \gamma$, $(1 - 2\gamma)^{1-\rho} (1 + 2\gamma)^{1+\rho} < 1$ and the bound decreases exponentially in T .

- For the bound to be convergent: $\rho \gg O(1/\sqrt{m})$, thus $\gamma \gg O(1/\sqrt{m})$ is roughly the condition on the edge value.

L1-Geometric Margin

- **Definition:** the L_1 -margin $\rho_f(x)$ of a linear function $f = \sum_{t=1}^T \alpha_t h_t$ with $\alpha \neq 0$ at a point $x \in \mathcal{X}$ is defined by

$$\rho_f(x) = \frac{|f(x)|}{\|\alpha\|_1} = \frac{|\sum_{t=1}^T \alpha_t h_t(x)|}{\|\alpha\|_1} = \frac{|\alpha \cdot \mathbf{h}(x)|}{\|\alpha\|_1}.$$

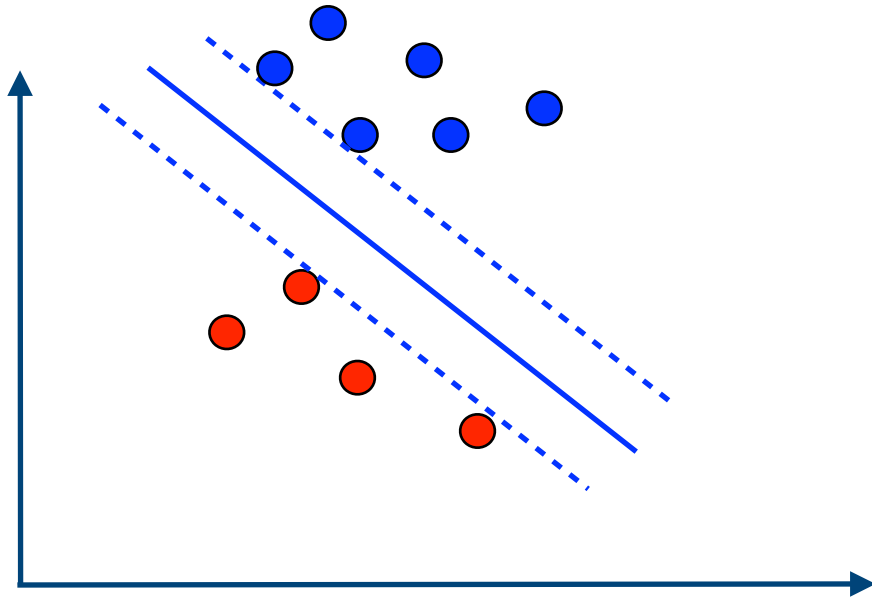
- the L_1 -margin of f over a sample $S = (x_1, \dots, x_m)$ is its minimum margin at points in that sample:

$$\rho_f = \min_{i \in [1, m]} \rho_f(x_i) = \min_{i \in [1, m]} \frac{|\alpha \cdot \mathbf{h}(x_i)|}{\|\alpha\|_1}.$$

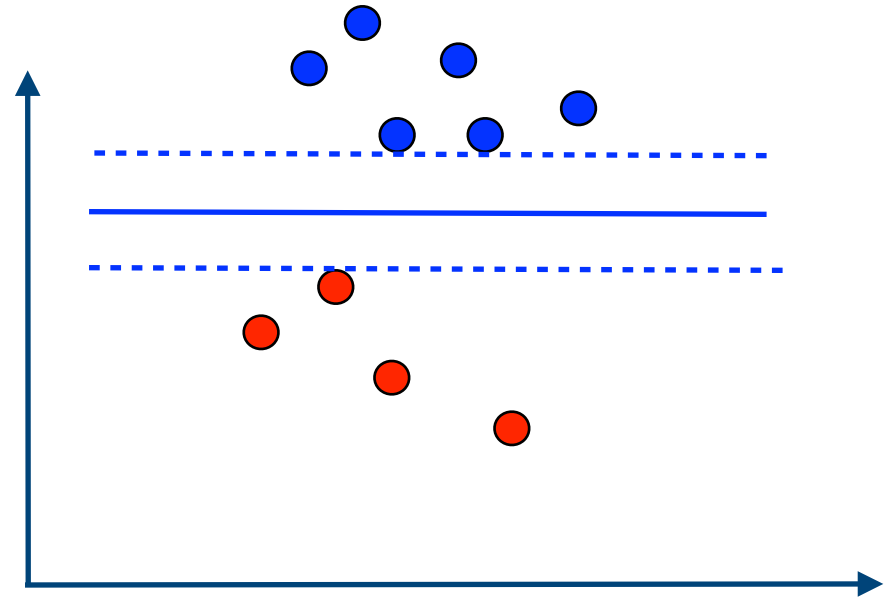
SVM vs AdaBoost

	SVM	AdaBoost
features or base hypotheses	$\Phi(x) = \begin{bmatrix} \Phi_1(x) \\ \vdots \\ \Phi_N(x) \end{bmatrix}$	$\mathbf{h}(x) = \begin{bmatrix} h_1(x) \\ \vdots \\ h_N(x) \end{bmatrix}$
predictor	$x \mapsto \mathbf{w} \cdot \Phi(x)$	$x \mapsto \boldsymbol{\alpha} \cdot \mathbf{h}(x)$
geom. margin	$\frac{ \mathbf{w} \cdot \Phi(x) }{\ \mathbf{w}\ _2} = d_2(\Phi(x), \text{hyperpl.})$	$\frac{ \boldsymbol{\alpha} \cdot \mathbf{h}(x) }{\ \boldsymbol{\alpha}\ _1} = d_\infty(\mathbf{h}(x), \text{hyperpl.})$
conf. margin	$y(\mathbf{w} \cdot \Phi(x))$	$y(\boldsymbol{\alpha} \cdot \mathbf{h}(x))$
regularization	$\ \mathbf{w}\ _2$	$\ \boldsymbol{\alpha}\ _1$ (L1-AB)

Maximum-Margin Solutions



Norm $\| \cdot \|_2$.



Norm $\| \cdot \|_\infty$.

But, Does AdaBoost Maximize the Margin?

- **No:** AdaBoost may converge to a margin that is significantly below the maximum margin (Rudin et al., 2004) (e.g., $1/3$ instead of $3/8$)!
- **Lower bound:** AdaBoost can achieve **asymptotically** a margin that is at least $\frac{\rho_{\max}}{2}$ if the data is separable and some conditions on the base learners hold (Rätsch and Warmuth, 2002).
- Several boosting-type margin-maximization algorithms: but, performance in practice not clear or not reported.

AdaBoost's Weak Learning Condition

- **Definition:** the **edge** of a base classifier h_t for a distribution D over the training sample is

$$\gamma(t) = \frac{1}{2} - \epsilon_t = \frac{1}{2} \sum_{i=1}^m y_i h_t(x_i) D(i).$$

- **Condition:** there exists $\gamma > 0$ for any distribution D over the training sample and any base classifier

$$\gamma(t) \geq \gamma.$$

Zero-Sum Games

■ Definition:

- payoff matrix $\mathbf{M} = (\mathbf{M}_{ij}) \in \mathbb{R}^{m \times n}$.
- m possible actions (**pure strategy**) for row player.
- n possible actions for column player.
- \mathbf{M}_{ij} payoff for row player (= loss for column player) when row plays i , column plays j .

■ Example:

	rock	paper	scissors
rock	0	-1	1
paper	1	0	-1
scissors	-1	1	0

Mixed Strategies

(von Neumann, 1928)

- **Definition:** player row selects a distribution \mathbf{p} over the rows, player column a distribution \mathbf{q} over columns. The expected payoff for row is

$$\mathbb{E}_{\substack{i \sim \mathbf{p} \\ j \sim \mathbf{q}}} [\mathbf{M}_{ij}] = \sum_{i=1}^m \sum_{j=1}^n p_i \mathbf{M}_{ij} q_j = \mathbf{p}^\top \mathbf{M} \mathbf{q}.$$

- **von Neumann's minimax theorem:**

$$\max_{\mathbf{p}} \min_{\mathbf{q}} \mathbf{p}^\top \mathbf{M} \mathbf{q} = \min_{\mathbf{q}} \max_{\mathbf{p}} \mathbf{p}^\top \mathbf{M} \mathbf{q}.$$

- **equivalent form:**

$$\max_{\mathbf{p}} \min_{j \in [1, n]} \mathbf{p}^\top \mathbf{M} \mathbf{e}_j = \min_{\mathbf{q}} \max_{i \in [1, m]} \mathbf{e}_i^\top \mathbf{M} \mathbf{q}.$$

John von Neumann (1903 - 1957)



AdaBoost and Game Theory

■ Game:

- Player A: selects point $x_i, i \in [1, m]$.
- Player B: selects base hypothesis $h_t, t \in [1, T]$.
- Payoff matrix $\mathbf{M} \in \{-1, +1\}^{m \times T}$: $\mathbf{M}_{it} = y_i h_t(x_i)$.

■ von Neumann's theorem: assume finite H .

$$2\gamma^* = \min_D \max_{h \in H} \sum_{i=1}^m D(i) y_i h(x_i) = \max_{\alpha} \min_{i \in [1, m]} y_i \sum_{t=1}^T \frac{\alpha_t h_t(x_i)}{\|\alpha\|_1} = \rho^*.$$

Consequences

- Weak learning condition \implies non-zero margin.
 - thus, possible to search for non-zero margin.
 - AdaBoost = (suboptimal) search for corresponding α ; achieves at least half of the maximum margin.
- Weak learning = strong condition:
 - the condition implies linear separability with margin $2\gamma^* > 0$.

Linear Programming Problem

- Maximizing the margin:

$$\rho = \max_{\alpha} \min_{i \in [1, m]} y_i \frac{(\alpha \cdot \mathbf{x}_i)}{\|\alpha\|_1}.$$

- This is equivalent to the following convex optimization LP problem:

$$\begin{aligned} & \max_{\alpha} \rho \\ & \text{subject to : } y_i(\alpha \cdot \mathbf{x}_i) \geq \rho \\ & \|\alpha\|_1 = 1. \end{aligned}$$

- Note that:

$$\frac{|\alpha \cdot \mathbf{x}|}{\|\alpha\|_1} = \|\mathbf{x} - H\|_{\infty}, \text{ with } H = \{\mathbf{x} : \alpha \cdot \mathbf{x} = 0\}.$$

Advantages of AdaBoost

- **Simple**: straightforward implementation.
- **Efficient**: complexity $O(mNT)$ for stumps:
 - when N and T are not too large, the algorithm is quite fast.
- **Theoretical guarantees**: but still many questions.
 - AdaBoost not designed to maximize margin.
 - regularized versions of AdaBoost.

Outliers

- AdaBoost assigns larger weights to harder examples.
- **Application:**
 - Detecting mislabeled examples.
 - Dealing with noisy data: regularization based on the average weight assigned to a point (soft margin idea for boosting) (Meir and Rätsch, 2003).

Weaker Aspects

■ Parameters:

- need to determine T , the number of rounds of boosting: **stopping criterion**.
- need to determine base learners: risk of overfitting or low margins.

■ Noise: severely damages the accuracy of Adaboost (Dietterich, 2000).

Other Boosting Algorithms

- **arc-gv** (Breiman, 1996): designed to maximize the margin, but outperformed by AdaBoost in experiments (Reyzin and Schapire, 2006).
- **L1-regularized AdaBoost** (Raetsch et al., 2001): outperforms AdaBoost in experiments (Cortes et al., 2014).
- **DeepBoost** (Cortes et al., 2014): more favorable learning guarantees, outperforms both AdaBoost and L1-regularized AdaBoost in experiments.

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