

Lecture 1: Theoretical Analysis of Boosting Methods

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Algorithm 1.1
The boosting algorithm AdaBoost

Given: $(x_1, y_1), \dots, (x_m, y_m)$ where $x_i \in \mathcal{X}$, $y_i \in \{-1, +1\}$.

Initialize: $D_1(i) = 1/m$ for $i = 1, \dots, m$.

For $t = 1, \dots, T$:

- Train weak learner using distribution D_t .
- Get weak hypothesis $h_t : \mathcal{X} \rightarrow \{-1, +1\}$.
- Aim: select h_t to minimize the weighted error:

$$\epsilon_t \doteq \Pr_{i \sim D_t}[h_t(x_i) \neq y_i].$$

- Choose $\alpha_t = \frac{1}{2} \ln \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$.
- Update, for $i = 1, \dots, m$:

$$\begin{aligned} D_{t+1}(i) &= \frac{D_t(i)}{Z_t} \times \begin{cases} e^{-\alpha_t} & \text{if } h_t(x_i) = y_i \\ e^{\alpha_t} & \text{if } h_t(x_i) \neq y_i \end{cases} \\ &= \frac{D_t(i) \exp(-\alpha_t y_i h_t(x_i))}{Z_t}, \end{aligned}$$

where Z_t is a normalization factor (chosen so that D_{t+1} will be a distribution).

Output the final hypothesis:

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

Figure 1: AdaBoost Algorithm [Schapire and Freund, 2012]

1 Boosting Algorithm

1.1 AdaBoost

- **The AdaBoost algorithm** is the first boosting algorithms proposed by Freund and Schapire [Schapire and Freund, 2012]. Its basic idea is to combine multiple *weak learners* to form a *strong learner*. This strategy is called **ensemble learning**. Let $h_t \in \mathcal{H}$ be base hypothesis, and α_t be the corresponding weight at iteration $t \in [1, T]$. The *combined learner* after T iteration is

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

- **Remark** There are several other *ensemble learning algorithms* such that **bagging algorithms**, which is based on **bootstrap resampling strategy**. The idea is to *sample with replacement* on the existing dataset to create *duplicated records*. The most frequent seen records in the existing data are more likely be sampled thus this idea is equivalent to **Monte Carlo sampling** according to the empirical distribution. For each resampled dataset, we can train a classifier that reflect our understanding on the duplicated sample. Then we combine

multiple classifier to build a single classifier via **decision fusion**. The typical bagging-based algorithm is **the random forest algorithm**, which build decision trees for each bootstrapped dataset and combine them.

- **Remark (Characteristic of AdaBoost)**

AdaBoost is an *ensemble learning method*. The followings are several key characteristics:

1. **AdaBoost** trains **multiple weak learners** in **sequential manner**. Unlike *bagging methods*, *boosting methods* build weak learners *sequentially*. **The performance of the previous learners will affect how the new weak-learner is trained**. In the case of AdaBoost, it will be reflected in *the sample weights*, with misclassified samples having increased weight.

In this way, it is described as a **functional gradient descent algorithm** which *instead of computing the gradient, it learns a new base hypothesis that resembles the gradient of functional*.

2. **The performance measure** in each step of **AdaBoost** is **the training error rate** of new base learner relative to **a weighted sample distribution**; i.e.

$$\epsilon_t := \widehat{\mathbb{E}}_{\mathcal{D}_t} [h_t(X) \neq Y] = \sum_{i=1}^m \mathcal{D}_t(i) \mathbb{1} \{h_t(X_i)\}$$

The training error rate under \mathcal{D}_t has two roles:

- (a) it determine **the weight** α_t for the base hypothesis h_t . In AdaBoost,

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

It is clear that when the classifier h_t is no more than a random guess with $\epsilon_t = 1/2$, the corresponding weight $\alpha_t = 0$. In other situation, the *smaller* the ϵ_t the *larger* the α_t . Note that $\alpha_t > 0$ **if and only if** $\epsilon_t < 1/2$ meaning that the learned hypothesis h_t is a *weak-learner*.

- (b) it determines **the multiplicative factor** in the *exponential reweight strategy* for each sample. In particular, the factor is $\exp(-\alpha_t y_i h_t(x_i))$.
3. **AdaBoost** apply an **exponential reweighting strategy** at each iteration. In particular,

$$\mathcal{D}_{t+1}(i) = \frac{\mathcal{D}_t}{Z_t} \times \begin{cases} e^{-\alpha_t} & \text{if } h_t(x_i) = y_i \\ e^{\alpha_t} & \text{if } h_t(x_i) \neq y_i \end{cases}$$

where $Z_t := \sum_{i=1}^m \mathcal{D}_t(i) \exp(-\alpha_t y_i h_t(x_i))$ is the partition function that normalized the sample distribution \mathcal{D}_{t+1} . The exponential reweighting strategy **shrinks** the weight by $e^{-\alpha_t} < 1$ when *the sample is correctly labeled*, while **enlarges** the weight by $e^{\alpha_t} > 1$ when *the sample is incorrectly labeled*. This means that *misclassified samples will have higher weights* in next iteration.

4. **AdaBoost** promote the idea of **adversarial learning** that is shown great success in deep learning models such as *Generative Adversarial Network (GAN)*. The key idea comes from the **two player zero-sum game**. Unlike GAN, AdaBoost did not continually

re-train the same hypothesis but instead move on to build a new hypothesis for a few misclassified samples.

The change of sample distribution $\mathcal{D}_t \rightarrow \mathcal{D}_{t+1}$ helps the AdaBoost to **boost the impact of adversarial samples** for the *new* learner so that it will **overemphasize on the past mistakes**. The consequence is that **the later learned base hypothesis is more specialized on a few difficult samples** while **the early learned base hypothesis is more generalized for a majority of easy samples**.

In the end, when *the error rate of new classifier decreased*, the corresponding *hypothesis weight* α_t will *decrease* and the multiplicative factor will *tends to 1*, which leads to the sample distribution **converge to some stationary distribution**.

$$h_t \rightarrow \epsilon_t \downarrow \quad \Rightarrow e^{\alpha_t} \rightarrow 1 \quad \Rightarrow \mathcal{D}_t \approx \mathcal{D}_{t+1}$$

5. One of main reason behind the **popularity** of boosting is its high **computational efficiency**.

Boosting methods are highly **scalable** for large dataset with high dimensions. *AdaBoost* provides **performance guarantee both theoretically and practically** when the base learner is implemented with simple learning algorithm such as **decision trees**. Specifically, when using decision stumps (1-layer decision tree), the time complexity of each round of boosting is in $\mathcal{O}(mn)$ where n is the feature dimension and m is the sample size.

- **Remark** *AdaBoost* is a well-studied algorithm and it provides **theoretical guarantee** based on *statistical learning theory*. This chapter focus on various aspects of theoretical guarantee of AdaBoost algorithm and its **connections** to other algorithms. In particular, we focus on following aspects:

1. We show that **the training error** of AdaBoost **will converge to zero** as iteration T increases, even if each single hypothesis only slightly better than random guess with error rate $\epsilon_t = \frac{1}{2} - \gamma_t$.
2. We develop **the generalization error bound** for AdaBoost using **VC dimension of base hypothesis class \mathcal{H}** . This allows us to provides **Probably Approximately Correct (PAC) learnability** guarantee for given hypothesis class \mathcal{H} and it helps to *quantitatively* describe the **sample complexity** of the algorithm. VC dimension theory also helps us to build intuition on the **tradeoff** between lower training error and overfitting as the number of iterations increases (i.e. **the Bias-Complexity tradeoff**).
3. The VC dimension theory is not sufficient to explain the performance of AdaBoost, esp. when the generalization error continues to improve even if the training error is zero. An alternative theory in statistical learning is called **the large margin theory**. In particular, it associated the performance of classifier with the **margin** between *the decision boundary and samples*. The idea is that for binary classification, a good classifier not only make correct decision but also make decision that is **robust to small perturbation** of samples. Leaving a margin between decision boundary and samples allows the classifier to **avoid making mistakes with highly confidence**. The idea of learning with maximal margin motivates the development of *support vector machines (SVM)*. Boosting and SVM do share some similarities here. However, **boosting is not directly optimizing the margin**. Although in practice and theory, it is observed that the learned hypothesis from AdaBoost do have a large margin, it can also be shown that

*AdaBoost's success cannot be **fully explained by large margin** either.*

4. One important aspect for AdaBoost is its connection to **game theory** via its **adversarial training style**. The *min-max theorem* helps us to understand that **the weak learnability assumption** implies a **strong assumption that the dataset is linearly separable with a margin**.
5. Other algorithms have connections with AdaBoost include
 - (a) **online learning** [Cesa-Bianchi and Lugosi, 2006], esp. when **the exponential reweighting strategy** is used; and
 - (b) **Bregman iterative projections** [Peyr and Cuturi, 2019], a generic algorithms that at each iteration projects to a subspace that is closer to the target by minimizing the **Bregman divergence**.
 - (c) The way when the sample distribution is optimized is also close to **maximum entropy learning** [Cover and Thomas, 2006].

1.2 Functional Gradient Descent

- The boosting models are summarized as a **stage-wise additive model** [Hastie et al., 2009],

$$F_M(x) := \sum_{t=1}^M \alpha_t h_t(x).$$

- The learning algorithm, at each iteration t , choose a base hypothesis $h_t \in \mathcal{H}$ and its weight $\alpha_t \in \mathbb{R}$ that *minimizes* the loss, given *the additive model in previous iterations*:

$$\min_{h_t \in \mathcal{H}, \alpha_t \in \mathbb{R}} \sum_{i=1}^m L(y_i, F_{t-1}(x_i) + \alpha_t h_t(x_i))$$

After (h_t, α_t) is selected, it *merges* with existing additive model $F_t(x) = F_{t-1}(x) + \alpha_t h_t$.

- Given sample \mathcal{D} , we treat $h_t \in \mathcal{H}$ on \mathcal{D} as a vector $h_{\mathcal{D}} := (h_t(x_1), \dots, h_t(x_m))$. Then we can find the gradient of loss function with respect to the vector $h_{\mathcal{D}}$ evaluated at F_{t-1}

$$\nabla L_{\mathcal{D}}(F_{t-1}) := \left[\frac{\partial L(y, h)}{\partial h_t(x_i)} \Big|_{h=F_{t-1}} \right]_{i=1, \dots, m} \quad (1)$$

- This step is close to the classical *gradient descent algorithm* for (unconstrained) optimization. **The major difference** is that instead of computing *the numerical gradient* ∇L , we choose to **learn a new base hypothesis** $h_t \in \mathcal{H}$ that **matches** the **negative functional gradient**

$$h_t := \arg \min_{h \in \mathcal{H}} \text{Diss}(h_{\mathcal{D}}, -\nabla L_{\mathcal{D}}(F_{t-1})), \quad (2)$$

where *Diss* is some **distance/dissimilarity measure** between two functions on given data set \mathcal{D} . Thus the new base hypothesis h_t plays role of $-\nabla L(F_{t-1})$ and it is then merging with existing function F_{t-1} to *make corrections*.

Algorithm 7.3

AnyBoost, a generic functional gradient descent algorithm

Goal: minimization of $\mathcal{L}(F)$.Initialize: $F_0 \equiv 0$.For $t = 1, \dots, T$:

- Select $h_t \in \mathcal{H}$ that maximizes $-\nabla \mathcal{L}(F_{t-1}) \cdot h_t$.
- Choose $\alpha_t > 0$.
- Update: $F_t = F_{t-1} + \alpha_t h_t$.

Output F_T .

Figure 2: A generic boosting algorithm based on functional gradient descent [Hastie et al., 2009]

- It can be shown that for AdaBoost, the loss functional is the exponential loss:

$$L(F) \equiv L(y, F) := \exp(-yF(x)) \quad (3)$$

and the functional gradient

$$\nabla L_{\mathcal{D}}(F_{t-1}) := \left[\frac{-y_i \exp(-y_i F_{t-1}(x_i))}{m} \right]_{i=1, \dots, m}. \quad (4)$$

Choose similarity measure as *the cosine similarity*, which means that the goal is to optimize

$$\begin{aligned} \max_{h \in \mathcal{H}} S(h_{\mathcal{D}}, -\nabla L_{\mathcal{D}}(F_{t-1})) &= \max_{h \in \mathcal{H}} \frac{1}{m} \sum_{i=1}^m y_i h_t(x_i) \exp(-y_i F_{t-1}(x_i)) \\ &= \max_{h \in \mathcal{H}} \sum_{i=1}^m D_t(i) y_i h_t(x_i) := 1 - 2\epsilon_t \end{aligned}$$

So the goal of the maximizing the cosine similarity is equivalent to minimizing the error rate ϵ_t on weighted sample distribution \mathcal{D}_t . The hypothesis weight α_t is chosen to minimize the exponential loss (3).

1.3 Gradient Boost

- The *gradient boosting methods* uses the negative functional gradient on samples \mathcal{D} as

$$-\nabla L_{\mathcal{D}}(F_{t-1}) := - \left[\frac{\partial L(y, h)}{\partial h_t(x_i)} \Big|_{h=F_{t-1}} \right]_{i=1, \dots, m} \equiv [r_{i,t}]_{i=1, \dots, m} \quad (5)$$

- At each iteration, it learns a base hypothesis that minimize *the mean squared error loss*. In other word, it treats *the negative functional gradient vector* $[r_{i,t}]_{i=1}^m$ as the **residual** and perform **regression tasks iteratively**. That is,

$$\min_{h_t \in \mathcal{H}} \sum_{i=1}^m (r_{i,t} - h_t(x_i))^2 = \min_{h_t \in \mathcal{H}} \sum_{i=1}^m \|-\nabla L_{\mathcal{D}}(F_{t-1}) - h_t\|_2^2 \quad (6)$$

Algorithm 10.3 *Gradient Tree Boosting Algorithm.*

1. Initialize $f_0(x) = \arg \min_{\gamma} \sum_{i=1}^N L(y_i, \gamma)$.

2. For $m = 1$ to M :

(a) For $i = 1, 2, \dots, N$ compute

$$r_{im} = - \left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)} \right]_{f=f_{m-1}}.$$

(b) Fit a regression tree to the targets r_{im} giving terminal regions

$$R_{jm}, j = 1, 2, \dots, J_m.$$

(c) For $j = 1, 2, \dots, J_m$ compute

$$\gamma_{jm} = \arg \min_{\gamma} \sum_{x_i \in R_{jm}} L(y_i, f_{m-1}(x_i) + \gamma).$$

(d) Update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} I(x \in R_{jm})$.

3. Output $\hat{f}(x) = f_M(x)$.

Figure 3: Gradient Boost Tree Algorithm [Hastie et al., 2009]

Finally, choose α_t that minimize the loss function L :

$$\alpha_t := \sum_{i=1}^m r_{i,t} \frac{h_t(x_i)}{\|h_t\|_2^2}$$

- Equivalently, *the negative functional gradient* becomes *the pseudo-label* for the new hypothesis during the learning.
- Compared to *AdaBoost*, *the Gradient Boost* has several differences:
 1. Gradient boost generalized the AdaBoost by *choosing a general loss function* in the learning task, which could be more efficient and more *flexible* for some tasks.
 2. Unlike AdaBoost, *no sample reweighting is needed for Gradient Boost* since the role of error rate ϵ_t and sample distribution \mathcal{D}_t is fulfilled by *the functional gradient* $\nabla L_{\mathcal{D}}(F_{t-1})$. In particular, *correctly labeled samples have smaller functional gradients* while *misclassified samples have larger functional gradients*.

In Gradient Boosting, ‘*shortcomings*’ (of existing weak learners) are identified by *gradients*. In *AdaBoost*, ‘*shortcomings*’ are identified by *high-weight data points*.

- It tends to say that the main differences are that *Gradient Boosting is a generic algorithm to find approximate solutions to the additive modeling problem*, while *AdaBoost* can be seen as a special case with a particular loss function. Hence, *Gradient Boosting is much more flexible*.

However, as pointed by Freund and Schapire [Schapire and Freund, 2012], *optimizing the exponential loss alone cannot explain the performance of AdaBoost*. It is likely due to *large margin property* and *the adversarial training procedure* that the *AdaBoost* outperforms its counterpart in optimization only approach. It is critical to take into account *the particular dynamics of the algorithm*, not just the objective function.

2 Theoretical Guarantee for Boosting

- **Remark (Data)**

Define an **observation** as a d -dimensional vector x . The *unknown* nature of the observation is called a **class**, denoted as y . The domain of observation is called an **input space** or **feature space**, denoted as $\mathcal{X} \subset \mathbb{R}^d$, whereas the domain of class is called the **target space**, denoted as \mathcal{Y} . For **classification task**, $\mathcal{Y} = \{1, \dots, M\}$; and for **regression task**, $\mathcal{Y} = \mathbb{R}$. A **concept** $c : \mathcal{X} \rightarrow \mathcal{Y}$ is the *input-output association* from the nature and is *to be learned* by a **learning algorithm**. Denote \mathcal{C} as the set of all concepts we wish to learn as the **concept class**. The learner is requested to output a *prediction rule*, $h : \mathcal{X} \rightarrow \mathcal{Y}$. This function is also called a **predictor**, a **hypothesis**, or a **classifier**. The predictor can be used to predict the label of new domain points. Denote a collection of n **samples** as

$$\mathcal{D} \equiv \mathcal{D}_n = ((X_1, Y_1), \dots, (X_n, Y_n)) \equiv ((X_1, c(X_1)), \dots, (X_n, c(X_n))).$$

Note that \mathcal{D}_n is a finite **sub-sequence** in $(\mathcal{X} \times \mathcal{Y})^n$.

- **Definition (Generalization Error in Deterministic Scenario)** [Mohri et al., 2018]

Under a *deterministic scenario*, **generalization error** or the **risk** or simply **error** for the classifier $h \in \mathcal{H}$ is defined as

$$L(h) \equiv L_{\mathcal{P},c}(h) = \mathcal{P} \{h(X) \neq c(X)\} \equiv \mathbb{E}_X [\mathbb{1} \{h(X) \neq Y\}] \quad (7)$$

with respect to the concept $c \in \mathcal{C}$ and the *feature distribution* $\mathcal{P} \equiv \mathcal{P}_X$.

- **Definition (Empirical Error or Training Error)**

Given the data \mathcal{D} , the **training error** or the **empirical error/risk** of a hypothesis $h \in \mathcal{H}$ is defined as

$$\hat{L}(h) \equiv \hat{L}_{\mathcal{D}}(h) = \frac{1}{n} \sum_{i=1}^n \mathbb{1} \{h(X_i) \neq Y_i\} = \frac{1}{n} |\{i : h(X_i) \neq Y_i\}| := \hat{\mathbb{E}} [\mathbb{1} \{h(X) \neq Y\}]$$

where either $Y = c(X)$ or Y is a random variable associated with X .

- **Definition (The Realizable Assumption)**

There exists $h^* \in \mathcal{H}$ s.t. $L_{\mathcal{P},c}(h^*) = 0$.

- **Definition (PAC Learnability)**

A hypothesis class \mathcal{H} is **PAC learnable** if there exist a function $m_{\mathcal{H}} : (0, 1)^2 \rightarrow \mathbb{N}$ and a learning algorithm with the following property: For every $\epsilon, \delta \in (0, 1)$, for every distribution \mathcal{P} over \mathcal{X} , and for every labeling function $c : \mathcal{X} \rightarrow \{0, 1\}$, if the *realizable assumption* holds with respect to \mathcal{H} , \mathcal{P} , c , then when running the learning algorithm on $m \geq m_{\mathcal{H}}(\epsilon, \delta)$ i.i.d. examples generated by \mathcal{P} and labeled by c , the algorithm returns a hypothesis h such that, with probability of at least $1 - \delta$ (over the choice of the examples),

$$L_{\mathcal{P},c}(h) \leq \epsilon.$$

2.1 Weak Learner

- **Definition (γ -Weak Learnability)** [Schapire and Freund, 2012, Shalev-Shwartz and Ben-David, 2014]

A learning algorithm, \mathcal{A} , is a **γ -weak-learner** for a class \mathcal{H} if there exists a function $m_{\mathcal{H}} : (0, 1) \rightarrow \mathbb{N}$ such that for **every** $\delta \in (0, 1)$, **for every distribution** \mathcal{P} over \mathcal{X} , and **for every labeling function** $c : \mathcal{X} \rightarrow \{-1, +1\}$, if the realizable assumption holds with respect to \mathcal{H} , \mathcal{P} , c , then when running the learning algorithm on $m \geq m_{\mathcal{H}}(\delta)$ i.i.d. examples generated by \mathcal{P} and labeled by c , the algorithm returns a hypothesis h such that, with probability of at least $1 - \delta$,

$$L_{\mathcal{P},c}(h) \leq \frac{1}{2} - \gamma.$$

A hypothesis class \mathcal{H} is **γ -weak-learnable** if there exists a γ -weak-learner for that class.

- **Remark** We call PAC learnable **the strong learnable**.

- **Remark (Weak Learner Without Accuracy Guarantee)**

Unlike the PAC learner, who guarantees that with high probability the generalization error rate is less than ϵ **for all** ϵ , a γ -weak-learner guarantees that with high probability, the error rate is less than ϵ **for some** $\epsilon = 1/2 - \gamma$, i.e. *less than half with a margin γ* .

In other word, under the realizability assumption, it is expected that **with more data, a PAC learner** can learn the “true” labeling function behind the data, (i.e. **zero generalization error** with high probability). While a γ -weak-learner can only get **slightly better than random guess** and it is **not expected to have lower error rate** even if more data are available.

- **Remark (Weak Learner is as Hard as PAC Learner)**

The fundamental theorem of learning states that if a hypothesis class \mathcal{H} has a VC dimension d , then the sample complexity of PAC learning \mathcal{H} satisfies $m_{\mathcal{H}}(\epsilon, \delta) \geq C_1(d + \log(1/\delta))/\epsilon$, where C_1 is a constant. Applying this with $\epsilon = 1/2 - \gamma$ we immediately obtain that **if** $d = \infty$ **then \mathcal{H} is not γ -weak-learnable**.

This implies that from **the statistical perspective** (i.e., if we ignore *computational complexity*), **weak learnability** is also characterized by the VC dimension of \mathcal{H} and therefore is just **as hard as PAC (strong) learning**. However, when we do consider **computational complexity**, the potential advantage of weak learning is that maybe there is *an algorithm* that satisfies the requirements of weak learning and **can be implemented efficiently**.

2.2 Training Error Bounds

- **Remark** Recall that $h_t \in \mathcal{H}$ are base learners for $t \in [1, T]$, and $(\alpha_1, \dots, \alpha_T) \in \Sigma_T$. The combined learner is

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

- The space of all such combined classifiers is defined as below:

Definition (Ensemble Hypothesis Class)

Define the class of T **linear combinations of base hypotheses** from \mathcal{H} as

$$L(\mathcal{H}, T) := \left\{ \text{sgn} \left(\sum_{t=1}^T \alpha_t h_t(\cdot) \right) : \alpha \in \mathbb{R}^T, h_t \in \mathcal{H}, t = 1, \dots, T \right\} \quad (8)$$

- **Definition (*Linear Threshold Functions*)**

Define Σ_n as the space of all linear threshold functions

$$\Sigma_n := \{\text{sgn}(\langle w, x \rangle) : w \in \mathbb{R}^n\}.$$

Thus $L(\mathcal{H}, T) = \{\sigma(h_1(x), \dots, h_T(x)) : \sigma \in \Sigma_T\}$

- **Proposition 2.1 (*Training Error Bound for AdaBoost*)** [Schapire and Freund, 2012]
Given the notation of Adaboost algorithm, let $\gamma_t = 1/2 - \epsilon_t$, and let \mathcal{D}_1 be an arbitrary initial distribution over the training set. Then **the weighted training error** of the combined classifier \mathcal{H} with respect to \mathcal{D}_1 is bounded as

$$\hat{L}_{\mathcal{D}_1}(H) \leq \prod_{t=1}^T \sqrt{1 - 4\gamma_t^2} \leq \exp\left(-2 \sum_{t=1}^T \gamma_t^2\right). \quad (9)$$

Proof: Consider the linear combination of base classifiers:

$$f(x) := \sum_{t=1}^T \alpha_t h_t(x).$$

By definition of distribution \mathcal{D}_T via \mathcal{D}_{T-1} we have

$$\begin{aligned} \mathcal{D}_{T+1}(i) &= \frac{\exp(-\alpha_T y_i h_T(x_i))}{Z_T} \mathcal{D}_{T-1}(i) \\ &= \dots \\ &= \frac{\exp\left(-\sum_{t=1}^T \alpha_t y_i h_t(x_i)\right)}{\prod_{t=1}^T Z_t} \mathcal{D}_1(i) = \frac{\exp(-y_i f(x_i))}{\prod_{t=1}^T Z_t} \mathcal{D}_1(i) \end{aligned}$$

Note that $H(x) \neq y$ if and only if $y f(x) < 0$, and $\mathbb{1}_{(-\infty, 0]}(x) \leq \exp(-x)$ so

$$\mathbb{1}\{H(x_i) \neq y_i\} = \mathbb{1}_{(-\infty, 0]}(y_i f(x_i)) \leq \exp(-y_i f(x_i)).$$

By definition of training error,

$$\begin{aligned} \hat{L}_{\mathcal{D}_1}(H) &= \sum_{i=1}^m \mathbb{1}\{H(x_i) \neq y_i\} \mathcal{D}_1(i) \\ &\leq \sum_{i=1}^m \exp(-y_i f(x_i)) \mathcal{D}_1(i) \\ &= \left(\sum_{i=1}^m \mathcal{D}_{T+1}(i)\right) \prod_{t=1}^T Z_t \\ &= \prod_{t=1}^T Z_t \end{aligned} \quad (10)$$

Finally, by our choice of $\alpha_t = \frac{1}{2} \log \frac{1-\epsilon_t}{\epsilon_t} = \frac{1}{2} \log \frac{1/2+\gamma_t}{1/2-\gamma_t}$, we have that

$$\begin{aligned}
Z_t &= \sum_{i=1}^m \mathcal{D}_t(i) \exp(-\alpha_t y_i h_t(x_i)) \\
&= \exp(-\alpha_t) \sum_{i:H(x_i)=y_i} \mathcal{D}_t(i) + \exp(\alpha_t) \sum_{i:H(x_i) \neq y_i} \mathcal{D}_t(i) \\
&= \exp(-\alpha_t) (1 - \epsilon_t) + \exp(\alpha_t) \epsilon_t \quad (\text{by definition of error } \epsilon_t) \\
&= \exp(-\alpha_t) (1/2 + \gamma_t) + \exp(\alpha_t) (1/2 - \gamma_t) \quad (\text{substitute } \alpha_t) \\
&= \sqrt{(1 - 2\gamma_t)(1 + 2\gamma_t)} \tag{11}
\end{aligned}$$

Substituting (11) into (10), we have the result. \blacksquare

2.3 Generalization Error Bounds for Finite Hypothesis Class

- **Definition (*Restriction of \mathcal{H} to \mathcal{D}*).**

Let \mathcal{H} be a class of functions from \mathcal{X} to $\{0, 1\}$ and let $\mathcal{D} = \{x_1, \dots, x_m\} \subset \mathcal{X}$.

The restriction of \mathcal{H} to \mathcal{D} is the set of functions from \mathcal{D} to $\{0, 1\}$ that can be derived from \mathcal{H} . That is,

$$\mathcal{H}_{\mathcal{D}} := \{(h(x_1), \dots, h(x_m)) : h \in \mathcal{H}\},$$

where we **represent** each function from \mathcal{X} to $\{0, 1\}$ as a **vector** in $\{0, 1\}^{|\mathcal{D}|}$.

- **Definition (*Shattering*).**

A hypothesis class \mathcal{H} **shatters** a finite set $\mathcal{D} \subset \mathcal{X}$ if the restriction of \mathcal{H} to \mathcal{D} is the set of **all functions** from \mathcal{D} to $\{0, 1\}$. That is,

$$|\mathcal{H}_{\mathcal{D}}| = 2^{|\mathcal{D}|}.$$

- **Definition (*Growth Function*).**

Let \mathcal{H} be a hypothesis class. Then the growth function of \mathcal{H} , denoted $\tau_{\mathcal{H}} : \mathbb{N} \rightarrow \mathcal{N}$, is defined as

$$\tau_{\mathcal{H}}(m) := \max_{\mathcal{D} \subset \mathcal{X} : |\mathcal{D}|=m} |\mathcal{H}_{\mathcal{D}}|.$$

In words, $\tau_{\mathcal{H}}(m)$ is **the number of different functions** from a set \mathcal{D} of **size m** to $\{0, 1\}$ that can be obtained by **restricting \mathcal{H} to \mathcal{D}** .

- **Lemma 2.2 (*Sauer's Lemma*).** [Shalev-Shwartz and Ben-David, 2014, Mohri et al., 2018]
Let \mathcal{H} be a hypothesis class with $VCdim(\mathcal{H}) \leq d < \infty$. Then, for all $m \geq d + 1$,

$$\tau_{\mathcal{H}}(m) \leq \sum_{i=0}^d \binom{m}{i} \leq \left(\frac{em}{d}\right)^d. \tag{12}$$

- **Proposition 2.3 (Generalization Bound via Growth Function)** [Mohri et al., 2018]
Let \mathcal{H} be a family of functions taking values in $\{-1, +1\}$. Then, for any $\delta > 0$, with probability at least $1 - \delta$, for any $h \in \mathcal{H}$,

$$L(h) \leq \widehat{L}_m(h) + \sqrt{\frac{2 \log \tau_{\mathcal{H}}(m)}{m}} + \sqrt{\frac{\log(1/\delta)}{2m}} \quad (13)$$

Growth function bounds can be also derived directly (without using Rademacher complexity bounds first). The resulting bound is then the following:

$$\mathcal{P} \left\{ \exists h \in \mathcal{H}, \left| L(h) - \widehat{L}_m(h) \right| > \epsilon \right\} \leq 4\tau_{\mathcal{H}}(2m) \exp \left(-\frac{m\epsilon^2}{8} \right) \quad (14)$$

which only differs from (13) by constants.

- The following lemma shows that the VC dimension of Σ_T is T .

Lemma 2.4 [Schapire and Freund, 2012, Mohri et al., 2018]
The space Σ_n of **linear threshold functions** over \mathbb{R}^n

$$\Sigma_n := \{ \text{sgn}(\langle w, x \rangle) : w \in \mathbb{R}^n \}$$

has **VC-dimension** n .

- **Remark** Note that the class Σ_n is **the class of half-spaces** $\{ \langle w, x \rangle : w \in \mathbb{R}^n \}$ whose VC dimension is n .
- **Lemma 2.5 (Growth Number of Ensemble Hypothesis Class, Finite Hypothesis Class)** [Schapire and Freund, 2012, Shalev-Shwartz and Ben-David, 2014]
Assume \mathcal{H} is **finite**. Let $m \geq T \geq 1$. For any set \mathcal{D} of m points, the number of dichotomies realizable by $L(\mathcal{H}, T)$ is bounded as follows:

$$|L(\mathcal{H}, T)_{\mathcal{D}}| \leq \tau_{L(\mathcal{H}, T)}(m) \leq \left(\frac{em}{T} \right)^T |\mathcal{H}|^T. \quad (15)$$

Proof: Consider a new sample $\mathcal{D}' := \{Z_1, \dots, Z_m\}$ where

$$Z_i := (h_1(X_i), \dots, h_T(X_i)).$$

Given that the VC dimension of Σ_T is T , the bound on the growth number becomes

$$|L(\mathcal{H}, T)_{\mathcal{D}'}| \leq \left(\frac{em}{T} \right)^T. \quad (16)$$

That is, for fixed h_1, \dots, h_T , the number of dichotomies defined by functions of the form $\sigma(h_1(x), \dots, h_T(x))$ for $\sigma \in T$ is bounded as in equation (16). Since the number of choices for h_1, \dots, h_T is equal to $|\mathcal{H}|^T$, and since for each one of these, the number of dichotomies is as in equation (16), we thus obtain the bound stated in the lemma. ■

- **Theorem 2.6 (Generalization Bound for AdaBoost, Finite Hypothesis)** [Schapire and Freund, 2012]
Suppose **AdaBoost** is run for T rounds on $m \geq T$ random examples, using base classifiers from a **finite space** \mathcal{H} . Then, with probability at least $1 - \delta$, the combined classifier H satisfies

$$L_{\mathcal{P},c}(H) \leq \widehat{L}_m(H) + \sqrt{\frac{2T(\log |\mathcal{H}| + \log(em/T))}{m}} + \sqrt{\frac{\log(1/\delta)}{2m}} \quad (17)$$

Furthermore, with probability at least $1-\delta$, if \mathcal{H} is realizable with the training set (i.e. $\hat{L}_m(h) \equiv 0$), then

$$L_{\mathcal{P},c}(H) \leq \frac{2T(\log|\mathcal{H}| + \log(2em/T)) + 2\log(2/\delta)}{m}. \quad (18)$$

2.4 Generalization Error Bounds via VC Dimension

- **Lemma 2.7 (Growth Number of Ensemble Hypothesis Class, VC Class).** [Schapire and Freund, 2012]

Assume \mathcal{H} has **finite VC-dimension** $d \geq 1$. Let $m \geq \max\{T, d\} \geq 1$. For any set \mathcal{D} of m points, the number of dichotomies realizable by $L(\mathcal{H}, T)$ is bounded as follows:

$$|L(\mathcal{H}, T)_{\mathcal{D}}| \leq \tau_{L(\mathcal{H}, T)}(m) \leq \left(\frac{em}{T}\right)^T \left(\frac{em}{d}\right)^{dT}. \quad (19)$$

- **Lemma 2.8 (VC-Dimension of Ensemble Hypothesis Class, VC Class).** [Schapire and Freund, 2012, Shalev-Shwartz and Ben-David, 2014]

Assume \mathcal{H} has **finite VC-dimension** $\nu(\mathcal{H}) = d$ and $\min\{T, d\} \geq 3$. Then the VC dimension of combined hypothesis class is bounded by

$$\nu(L(\mathcal{H}, T)) \leq T(d+1)(3\log(T(d+1)) + 2) = \mathcal{O}(Td\log(Td)). \quad (20)$$

- **Remark (Lower Bound on VC Dimension).** [Shalev-Shwartz and Ben-David, 2014]
For some base hypothesis class \mathcal{H} , the VC-dimension of ensemble is at least Td . For instance, for \mathcal{H}_n be the class of *decision stumps* over \mathbb{R}^n , we can show that $\log(n) \leq d = \nu(\mathcal{H}) \leq 2\log(n) + 5$. In this example, for all $T \geq 1$,

$$\nu(L(\mathcal{H}_n, T)) \geq 0.5T\log(n) \asymp \Omega(Td).$$

- **Theorem 2.9 (Generalization Bound for AdaBoost via VC Dimension).** [Schapire and Freund, 2012]

Suppose **AdaBoost** is run for T rounds on $m \geq \max\{T, d\}$ random examples, using base classifiers from a **finite space** \mathcal{H} . Then, with probability at least $1-\delta$, the combined classifier H satisfies

$$L_{\mathcal{P},c}(H) \leq \hat{L}_m(H) + \sqrt{\frac{2T(d\log(em/d) + \log(em/T))}{m}} + \sqrt{\frac{\log(1/\delta)}{2m}} \quad (21)$$

Furthermore, with probability at least $1-\delta$, if \mathcal{H} is realizable with the training set (i.e. $\hat{L}_m(h) \equiv 0, \forall h \in \mathcal{H}$), then

$$L_{\mathcal{P},c}(H) \leq \frac{2T(d\log(2em/d) + \log(2em/T)) + 2\log(2/\delta)}{m}. \quad (22)$$

- **Remark (Limit of VC Dimension Analysis)**

The upper bound grows as $\mathcal{O}(dT\log(dT))$, thus the bound suggests that **AdaBoost could overfit for large values of T** , and indeed this can occur. See Figure 4. However, in many cases, it has been observed empirically that *the generalization error of AdaBoost decreases* as a function of *the number of rounds of boosting T* .

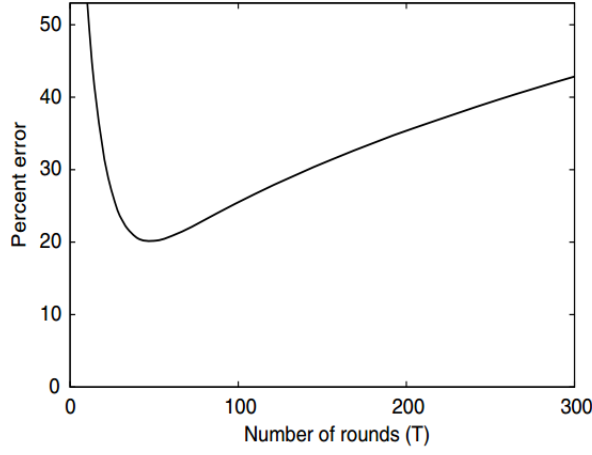


Figure 4.1

A plot of the bound on the generalization error given in equation (4.6) as a function of the number of rounds T , using the constants from theorem 4.3 with $\gamma = 0.2$, $m = 10^6$, $\ln |\mathcal{H}| = 10$, and $\delta = 0.05$.

Figure 4: AdaBoost may overfit if the number of rounds T is too large. [Schapire and Freund, 2012]

- **Corollary 2.10** [Schapire and Freund, 2012]

Assume, in addition to the assumptions of theorem 2.9, that each base classifier has weighted error $\epsilon_t \leq 1/2 - \gamma$ for some $\gamma > 0$. Let the number of rounds T be equal to

$$\inf \left\{ T \in \mathbb{N} : T \geq \frac{\log(m)}{2\gamma^2} \right\}$$

Then, with probability at least $1 - \delta$, the generalization error of the combined classifier H will be at most

$$\mathcal{O} \left(\frac{1}{m} \left[\frac{\log(m)}{\gamma^2} \left(\log(m) + d \log \left(\frac{m}{d} \right) \right) + \log \left(\frac{1}{\delta} \right) \right] \right)$$

- **Remark** Ignoring the log factor, the generalization error bound (21) can be summarized as

$$L_{\mathcal{P},c}(H) \leq \hat{L}_m(H) + \mathcal{O} \left(\sqrt{\frac{T\mathcal{C}_{\mathcal{H}}}{m}} \right)$$

where $\mathcal{C}_{\mathcal{H}}$ is some complexity measure of base class \mathcal{H} .

- **Theorem 2.11 (Strong Learnable \Leftrightarrow Weak Learnable)** [Schapire and Freund, 2012]
A target class \mathcal{H} is (efficiently) **weakly** PAC learnable **if and only if** it is (efficiently) **strongly** PAC learnable.

2.5 Generalization Error Bounds via Margin Theory

- **Definition (L_1 -Margin)** [Mohri et al., 2018, Schapire and Freund, 2012]

The L_1 -margin $\rho(x)$ of a point $x \in \mathcal{X}$ with label $y \in \{-1, +1\}$ for a linear combination of base classifiers $g = \sum_{t=1}^T \alpha_t h_t = \langle \alpha, h \rangle$ with $\alpha \neq 0$ and $h_t \in \mathcal{H}$ for all $t \in [1, T]$ is defined as

$$\rho(x) := y \frac{\langle \alpha, h(x) \rangle}{\|\alpha\|_1} = \frac{\sum_{t=1}^T \alpha_t y h_t(x)}{\|\alpha\|_1} \quad (23)$$

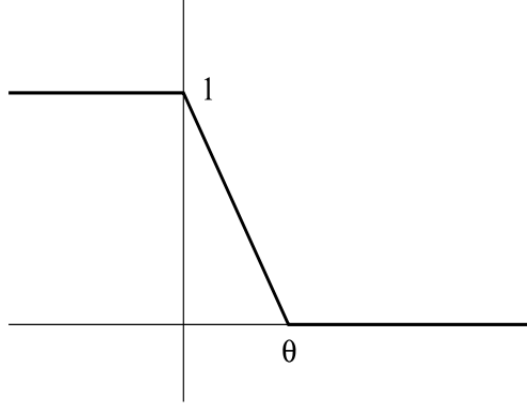


Figure 5.3
A plot of the piecewise-linear function ϕ given in equation (5.27).

Figure 5: The piecewise linear function φ_ϕ . [Schapire and Freund, 2012]

The L_1 -margin of a linear combination classifier g **with respect to a sample \mathcal{D}** is **the minimum margin** of the points within the sample:

$$\rho := \min_{i=1, \dots, m} y_i \frac{\langle \alpha, h(x_i) \rangle}{\|\alpha\|_1} = \min_{i=1, \dots, m} \frac{\sum_{t=1}^T \alpha_t y_i h_t(x_i)}{\|\alpha\|_1} \quad (24)$$

- **Definition (Margin Loss Function)** [Mohri et al., 2018, Schapire and Freund, 2012]
For any $\rho > 0$, **the ρ -margin loss** $L_\rho : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}_+$ is defined for all $y, y' \in \mathbb{R}$ by $L_\rho(y, y') = \varphi_\rho(yy')$ where φ is defined as a piecewise-linear function,

$$\varphi_\rho(x) := \begin{cases} 1 & \text{if } x \leq 0 \\ 1 - x/\rho & \text{if } 0 \leq x \leq \rho \\ 0 & \text{if } x \geq \rho \end{cases}$$

This function is **Lipschitz** with $L_\varphi = 1/\rho$.

- **Definition (Empirical Margin Loss)** [Schapire and Freund, 2012, Mohri et al., 2018]
Given a sample \mathcal{D}_m and a hypothesis h , **the empirical margin loss** is defined by

$$\hat{L}_{m,\rho}(h) = \frac{1}{m} \sum_{i=1}^m \varphi_\rho(Y_i h(X_i)) \quad (25)$$

Note that for any $i \in [1, m]$, $\mathbb{1}\{y_i h(x_i) \leq 0\} \leq \varphi_\rho(y_i h(x_i)) \leq \mathbb{1}\{y_i h(x_i) \leq \rho\}$. Thus, the empirical margin loss can be bounded as follows:

$$\begin{aligned} \hat{L}(h) &= \frac{1}{m} \sum_{i=1}^m \mathbb{1}\{h(X_i) \neq Y_i\} = \frac{1}{m} \sum_{i=1}^m \mathbb{1}\{Y_i h(X_i) \leq 0\} \\ &\leq \hat{L}_{m,\rho}(h) \leq \frac{1}{m} \sum_{i=1}^m \mathbb{1}\{Y_i h(X_i) \leq \rho\}. \end{aligned} \quad (26)$$

- **Remark** In all the results that follow, the empirical margin loss can be replaced by this upper bound, which admits a simple interpretation: it is *the fraction of the points in the training sample \mathcal{D} that have been misclassified or classified with confidence less than ρ* .

- **Remark** When the coefficients α_t are **non-negative**, as in the case of *AdaBoost*, $\rho(x)$ is a **convex combination** of the base classifier values $h_t(x)$. In particular, if the base classifiers h_t take values in $[-1, +1]$, then $\rho(x)$ is in $[-1, +1]$. The **absolute value** $|\rho(x)|$ can be interpreted as **the confidence of the classifier g** in that label.

- **Definition (Convex Hull of Hypothesis Class)**

For any hypothesis class \mathcal{H} , **the convex hull** of set \mathcal{H} , denoted as $\text{conv}(\mathcal{H})$, is defined as

$$\text{conv}(\mathcal{H}) := \left\{ \sum_{k=1}^T \lambda_k h_k(\cdot) : T \geq 1, \forall k \in [1, T], \lambda_k \geq 0, h_k \in \mathcal{H}, \sum_{k=1}^T \lambda_k = 1 \right\}.$$

- **Remark** Let \mathcal{H} be our space of base classifiers, and let \mathcal{M} be the space of all “**margin functions**” of the form $yf(x)$ where f is any convex combination of base classifiers:

$$\mathcal{M} := \{(x, y) \rightarrow yf(x) : f \in \text{conv}(\mathcal{H})\}$$

Note that $\hat{\mathfrak{R}}_{\mathcal{D}}(\mathcal{M}) = \hat{\mathfrak{R}}_{\mathcal{D}}(\text{conv}(\mathcal{H}))$ since $y_i \sigma_i$ has the same distribution as σ_i .

- **Definition (Empirical Rademacher Complexity)**

Let \mathcal{G} be a family of functions mapping from $\mathcal{Z} := \mathcal{X} \times \mathcal{Y}$ to $[a, b]$ and $\mathcal{D} = (z_1, \dots, z_n)$ a fixed *sample* of size n with elements in \mathcal{Z} . Then, **the empirical Rademacher complexity** of \mathcal{G} with respect to the sample \mathcal{D} is defined as:

$$\hat{\mathfrak{R}}_{\mathcal{D}}(\mathcal{G}) = \mathbb{E}_{\sigma} \left[\sup_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^n \sigma_i g(z_i) \right] \quad (27)$$

where $\sigma := (\sigma_1, \dots, \sigma_n)$ are **independent uniform random variables** taking values in $\{-1, +1\}$. The random variables σ_i are called **Rademacher variables**.

- **Proposition 2.12 (Empirical Rademacher Complexity of a Convex Hull of Function Class)**

Let \mathcal{H} be a set of functions mapping from \mathcal{X} to \mathbb{R} . Then, for any sample \mathcal{D} , the empirical Rademacher complexity

$$\hat{\mathfrak{R}}_{\mathcal{D}}(\text{conv}(\mathcal{H})) = \hat{\mathfrak{R}}_{\mathcal{D}}(\mathcal{H}) \quad (28)$$

where $\text{conv}(\mathcal{H})$ is **the convex hull** of set \mathcal{H} .

- **Theorem 2.13 (Uniform Bound via Rademacher Complexity)** [Mohri et al., 2018]
Let \mathcal{G} be a family of functions mapping from \mathcal{Z} to $[0, 1]$. Then, for any $\delta > 0$, **with probability at least $1 - \delta$** , each of the following holds for all $g \in \mathcal{G}$:

$$\mathbb{E}[g(Z)] \leq \frac{1}{m} \sum_{i=1}^m g(Z_i) + 2\mathfrak{R}_m(\mathcal{G}) + \sqrt{\frac{\log(1/\delta)}{2m}} \quad (29)$$

and

$$\mathbb{E}[g(Z)] \leq \frac{1}{m} \sum_{i=1}^m g(Z_i) + 2\hat{\mathfrak{R}}_m(\mathcal{G}) + 3\sqrt{\frac{\log(2/\delta)}{2m}} \quad (30)$$

- Based on the theorem above, we can have the generalization error bound via margin:

Theorem 2.14 (Ensemble Rademacher Margin Bound) [Schapire and Freund, 2012, Mohri et al., 2018]

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

$$L(h) \leq \widehat{L}_{m,\rho}(h) + \frac{2}{\rho} \mathfrak{R}_m(\mathcal{H}) + \sqrt{\frac{\log(1/\delta)}{2m}} \quad (31)$$

$$L(h) \leq \widehat{L}_{m,\rho}(h) + \frac{2}{\rho} \widehat{\mathfrak{R}}_m(\mathcal{H}) + 3\sqrt{\frac{\log(2/\delta)}{2m}} \quad (32)$$

Proof: Consider the family of functions taking values in $[0, 1]$:

$$\varphi_\rho \circ \mathcal{M} := \{\varphi_\rho \circ f : f \in \mathcal{M}\}$$

where $\mathcal{M} := \{(x, y) \rightarrow yh(x) : h \in \text{conv}(\mathcal{H})\}$. By the generalization bound via Rademacher complexity,

$$\mathbb{E} [\varphi_\rho(Yh(X))] \leq \frac{1}{m} \sum_{i=1}^m \varphi_\rho(Y_i h(X_i)) + 2\mathfrak{R}_m(\varphi_\rho \circ \mathcal{M}) + \sqrt{\frac{\log(1/\delta)}{2m}}$$

By inequality (26)

$$L(h) = \mathbb{E} [\mathbb{1} \{Y \neq h(X)\}] \leq \mathbb{E} [\varphi_\rho(Yh(X))]$$

thus

$$L(h) \leq \widehat{L}_{m,\rho}(h) + 2\mathfrak{R}_m(\varphi_\rho \circ \mathcal{M}) + \sqrt{\frac{\log(1/\delta)}{2m}}$$

Note that φ_ρ is $(\frac{1}{\rho})$ -Lipschitz function.

$$\begin{aligned} \mathfrak{R}_m(\varphi_\rho \circ \mathcal{M}) &\leq \frac{1}{\rho} \mathfrak{R}_m(\mathcal{M}) && \text{(by contraction principle)} \\ &= \frac{1}{\rho} \mathfrak{R}_m(\text{conv}(\mathcal{H})) && \text{(since } y_i \text{ is absorbed by } \sigma_i) \\ &= \frac{1}{\rho} \mathfrak{R}_m(\mathcal{H}). && \text{(by (28))} \end{aligned}$$

This complete the proof. ■

- **Theorem 2.15 (Ensemble VC-Dimension Margin Bound)** [Schapire and Freund, 2012, Mohri et al., 2018]

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

$$L(h) \leq \widehat{L}_{m,\rho}(h) + \frac{2}{\rho} \sqrt{\frac{2d \log(em/d)}{m}} + \sqrt{\frac{\log(1/\delta)}{2m}} \quad (33)$$

- **Remark** Note that from the point of view of binary classification, g and $g/\|\alpha\|_1$ are equivalent since $\text{sgn}(g) = \text{sgn}(g/\|\alpha\|_1)$, thus $L(g) = L(g/\|\alpha\|_1)$, but their empirical margin loss are

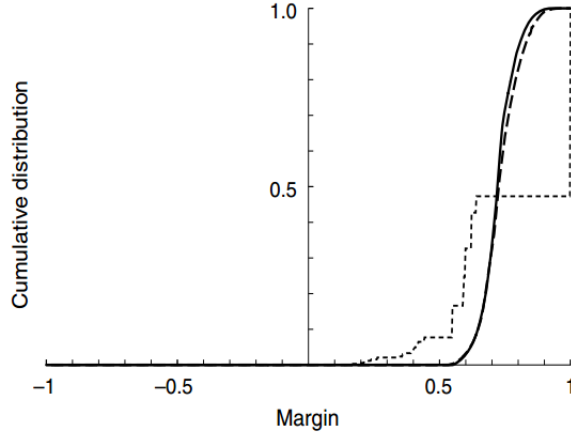


Figure 5.2

The margin distribution graph for boosting C4.5 on the letter dataset showing the cumulative distribution of margins of the training instances after 5, 100, and 1000 iterations, indicated by short-dashed, long-dashed (mostly hidden), and solid curves, respectively. (Reprinted with permission of the Institute of Mathematical Statistics.)

Figure 6: Distribution of margin for AdaBoost on one example dataset. [Schapire and Freund, 2012]

distinct. Let $g = \sum_{t=1}^T \alpha_t h_t$ denote the function defining the classifier returned by AdaBoost after T rounds of boosting when trained on sample \mathcal{D} . Then, in view of (31), for any $\delta > 0$, with probability at least $1 - \delta$

$$L(g) \leq \widehat{L}_{m,\rho}(g/\|\alpha\|_1) + \frac{2}{\rho} \mathfrak{R}_m(\mathcal{H}) + \sqrt{\frac{\log(1/\delta)}{2m}} \quad (34)$$

- **Remark (Generalization Guarantee by Large Margin Only)**

Remarkably, *the number of rounds of boosting T does not appear in the generalization bound (34)*. The bound depends only on *the margin ρ , the sample size m , and the Rademacher complexity of the family of base classifiers \mathcal{H}* . Thus, the bound guarantees an effective generalization if the margin loss $\widehat{L}_{m,\rho}(g/\|\alpha\|_1)$ is small for a relatively large ρ .

- **Proposition 2.16 (Empirical Margin Loss Bound for AdaBoost) [Schapire and Freund, 2012, Mohri et al., 2018]**

Let $f = \sum_{t=1}^T \alpha_t h_t$ denote the function defining the classifier returned by AdaBoost after T rounds of boosting and assume for all $t \in [1, T]$ that $\epsilon_t < 1/2$, which implies $\alpha_t > 0$. Then, for any $\rho > 0$, the following holds:

$$\widehat{L}_{m,\rho}(f) \leq 2^T \prod_{t=1}^T \sqrt{\epsilon_t^{1-\rho} (1 - \epsilon_t)^{1+\rho}} \leq [(1 - 2\gamma)^{1-\rho} (1 + 2\gamma)^{1+\rho}]^{T/2} \quad (35)$$

where $\gamma \leq 1/2 - \epsilon_t$ for all t . Note that $\gamma > 0$ so $[(1 - 2\gamma)^{1-\rho} (1 + 2\gamma)^{1+\rho}] < 1$.

Proof: Consider the linear combination of base classifiers:

$$f(x) := \sum_{t=1}^T \alpha_t h_t(x).$$

Note that $yf(x) \leq \rho$ if and only if

$$y \sum_{t=1}^T \alpha_t h_t(x) \leq \rho \sum_{t=1}^T \alpha_t.$$

This implies that

$$\exp \left(-y \sum_{t=1}^T \alpha_t h_t(x) + \rho \sum_{t=1}^T \alpha_t \right) \geq 1 \geq \mathbb{1} \{yf(x) \leq \rho\}$$

Thus

$$\begin{aligned} \hat{L}_{m,\rho}(f) &= \frac{1}{m} \sum_{i=1}^m \mathbb{1} \{y_i f(x_i) \leq \rho\} \leq \exp \left(\rho \sum_{t=1}^T \alpha_t \right) \left[\frac{1}{m} \sum_{i=1}^m \exp \left(-y_i \sum_{t=1}^T \alpha_t h_t(x_i) \right) \right] \\ &= \exp \left(\rho \sum_{t=1}^T \alpha_t \right) \left(\prod_{t=1}^T Z_t \right) \quad (\text{See proof in Proposition 2.1}) \end{aligned}$$

Plugging in the values of $\alpha_t = \frac{1}{2} \log \frac{1-\epsilon_t}{\epsilon_t}$ and $Z_t = 2\sqrt{\epsilon_t(1-\epsilon_t)}$ and the derivation follows the same as in Proposition 2.1, which gives the final result. \blacksquare

- **Remark** This bound implies that the fraction of training examples with $yf(x) \leq \rho$ decreases to zero *exponentially fast* with T , and must actually be equal to zero at some point since this fraction must always be a multiple of $1/m$.

- **Remark** (*AdaBoost Maximize the Margin?*)

The margin bounds combined with the bound on the empirical margin loss suggest that under some conditions, *AdaBoost can achieve a large margin on the training sample*. They could also serve as a theoretical explanation of the empirical observation that *in some tasks the generalization error decreases as a function of T even after the error on the training sample is zero: the margin would continue to increase*.

But does *AdaBoost* maximize the L_1 -margin? **No**. It has been shown that *AdaBoost may converge to a margin that is significantly smaller than the maximum margin*. However, under some general assumptions, when the data is *separable* and the base learners satisfy *particular conditions*, it has been proven that *AdaBoost* can *asymptotically achieve a margin that is at least half the maximum margin*, $\rho_{\max}/2$.

- **Remark** (*Limit for Margin Theory*)

We can directly maximize the L_1 -margin by solving a *Linear Programming (LP) problem*. By definition, the solution of the LP just described admits an L_1 -margin that is larger or equal to that of the *AdaBoost* solution. However, empirical results do not show a systematic benefit for the solution of the LP. In fact, it appears that in many cases, *AdaBoost outperforms that algorithm*. *The margin theory* described *does not seem sufficient* to explain that performance.

3 Fundamental Perspectives

3.1 Game Theory

- **Definition** (*Two-Player Zero-Sum Game in Normal Form*) [Schapire and Freund, 2012, Mohri et al., 2018]

A **two-person zero-sum game** consists of a loss matrix $M \in \mathbb{R}^{m \times n}$, where m is the number of possible actions (or **pure strategies**) for the row player and n the number of possible actions for the column player. The entry $M_{i,j}$ is the **loss** for the **row player** (or equivalently the **payoff** for the **column player**) when the row player takes action i and the column player takes action j .

- **Definition** (*Mixed Strategy*) [Schapire and Freund, 2012, Mohri et al., 2018]

A **mixed strategy** for the row player is a **distribution** P over the m possible **row actions**, a **distribution** Q over the n possible **column actions** for the **column player**. The *expected loss* for the row player (expected payoff for the column player) with respect to the mixed strategies P and Q is

$$M(P, Q) := \mathbb{E}_{i \sim P} [M(i, Q)] = P^T M Q = \sum_{i=1}^m \sum_{j=1}^n P_i M_{i,j} Q_j \quad (36)$$

where the *expected loss* for row player to choose a *pure strategy* i and the column player to choose a *mixed strategy* q is

$$M(i, Q) := \sum_{j=1}^n M_{i,j} Q_j$$

- **Definition** (*Sequential Games and Minmax Strategy*) [Schapire and Freund, 2012, Mohri et al., 2018]

Suppose now that play is **sequential**. That is, suppose that the column player chooses its strategy Q after the row player has chosen and announced its strategy P . Assume further that the column player's goal is to maximize the row player's loss (that is, that the game is zero-sum). Then, given knowledge of P , such a “worst-case” or “**adversarial**” column player will **choose** Q to **maximize** $M(P, Q)$; that is, if the row player plays mixed strategy P , then its loss will be

$$\max_{Q \in \Delta_n} M(P, Q).$$

This term can be viewed as a *function of* P that specifies what the loss will be for the row player if it chooses to play that particular strategy. Knowing this, the row player should **choose** P to **minimize** this expression. Doing so will result in a loss for the row player of exactly

$$\min_{P \in \Delta_m} \max_{Q \in \Delta_n} M(P, Q). \quad (37)$$

Thus, this quantity represents the **loss** that will be suffered when the **row player plays first, followed by the column player**, and assuming both play *optimally*. Note that the order of the minmax in equation (37) matches the order of play.

A mixed strategy P^* realizing the *minimum* in equation (37) is called a **minmax strategy**, and is *optimal* in this particular setting.

If now we *reverse the order of play* so that *the column player plays first* and *the row player can choose its play with the benefit of knowing the column players chosen strategy Q* , then by a symmetric argument, the loss of the row player will be

$$\max_{Q \in \Delta_n} \min_{P \in \Delta_m} M(P, Q). \quad (38)$$

A strategy Q^* realizing the *maximum* is called a **maxmin strategy**.

- **Remark (Minmax/Maxmin Strategy is Pure Strategy)**

The minmax strategy $P^ = \operatorname{argmin}_{P \in \Delta_m} \max_{Q \in \Delta_n} M(P, Q)$ will always be realized when P is concentrated on a single row i since this is a linear optimization. That is, **the minmax strategy P^* will be a pure strategy $i^* \in [1, m]$** .*

Similarly, Q^* will always be realized when Q is concentrated on a single column j . That is, ***the maxmin strategy Q^* will be a pure strategy $j^* \in [1, n]$*** .

- **Theorem 3.1 (Von Neumann's Minimax Theorem).** [Schapire and Freund, 2012, Mohri et al., 2018]

For any two-person zero-sum game defined by matrix M ,

$$\min_{P \in \Delta_m} \max_{Q \in \Delta_n} M(P, Q) = \max_{Q \in \Delta_n} \min_{P \in \Delta_m} M(P, Q) \equiv v. \quad (39)$$

- **Remark (Value of the Game)**

The common value v in (39) is called **the value of the game**.

The theorem states that for *any two-person zero-sum game*, there exists a ***mixed strategy*** for each player such that ***the expected loss for one is the same as the expected payoff for the other***, both of which are ***equal to the value of the game***.

- **Remark (Approximate Minmax/Maxmin Strategy)**

Consider *the average strategy* over T rounds of game

$$\bar{P} := \frac{1}{T} \sum_{t=1}^T P_t, \quad \bar{Q} := \frac{1}{T} \sum_{t=1}^T Q_t.$$

The proof of minmax theorem shows that

$$\max_{Q \in \Delta_n} M(\bar{P}, Q) \leq \min_{P \in \Delta_m} \max_{Q \in \Delta_n} M(P, Q) + \Delta_T = v + \Delta_T$$

Thus, the mixed strategy \bar{P} is an **approximate minmax strategy** in the sense that for all column strategies Q , $M(\bar{P}, Q)$ does not exceed the game value v by more than Δ_T . Similarly, we have

$$\min_{P \in \Delta_m} M(P, \bar{Q}) \geq v - \Delta_T,$$

so \bar{Q} is an **approximate maxmin strategy**.

3.2 Online Prediction

- **Remark (*Excess Risk for Repeated Game*)**

To emphasize the roles of the two players, we here refer to *the row player* as *the learner*, and *the column player* as *the environment*. As before, M is a *game matrix*, possibly *unknown* to *the learner*. Assume that the game is *repeated* T rounds. At each iteration $t \in [1, T]$, the *learner* chooses *mixed strategy* P_t ; and then the *environment* chooses *mixed strategy* Q_t . Define the *total cumulative loss* as

$$\sum_{t=1}^T M(P_t, Q_t)$$

The *goal* of the learner is to *do almost as well as the best strategy* against the actual sequence of plays Q_1, \dots, Q_T which were chosen by the environment. That is, the learner's goal is to suffer cumulative loss which is “*not much worse*” than the cumulative loss of *the best (fixed) strategy in hindsight*; i.e. the learner need to minimize *the excess risk*

$$\sum_{t=1}^T M(P_t, Q_t) - \min_{P \in \Delta_m} \sum_{t=1}^T M(P, Q_t) \quad (40)$$

- **Remark (*Exponential Weighted Average Strategy*)** [Cesa-Bianchi and Lugosi, 2006, Schapire and Freund, 2012]

Consider an *exponential weighted average (EWA) strategy* for repeated games: at round t , the learner choose a new mixed strategy P_{t+1} as

$$P_{t+1}(i) := \frac{P_t(i) \exp(-\eta M(i, Q_t))}{Z_t}$$

where Z_t is a normalization factor

$$Z_t := \sum_{i=1}^m P_t(i) \exp(-\eta M(i, Q_t)); \text{ and } M(i, Q_t) := \sum_{j=1}^n M_{i,j} Q_t(j).$$

- *The EWA algorithm* has a performance guarantee in terms of excess risk:

Theorem 3.2 (*Excess Risk Bound of Exponential Weighted Average*) [Schapire and Freund, 2012]

For any matrix M with m rows and entries in $[0, 1]$, and for any sequence of mixed strategies Q_1, \dots, Q_T played by the environment, the sequence of mixed strategies P_1, \dots, P_T produced by the exponential weighted average algorithm with parameter η satisfies

$$\begin{aligned} \sum_{t=1}^T M(P_t, Q_t) &\leq \min_{P \in \Delta_m} \left[a_\eta \sum_{t=1}^T M(P, Q_t) + c_\eta \text{KL}(P \parallel P_1) \right] \\ &= a_\eta \min_{P \in \Delta_m} \sum_{t=1}^T M(P, Q_t) + c_\eta \log(m) \quad (\text{assume } P_1 \text{ uniform}) \end{aligned} \quad (41)$$

where

$$a_\eta = \frac{\eta}{1 - e^{-\eta}}, \quad c_\eta = \frac{1}{1 - e^{-\eta}}.$$

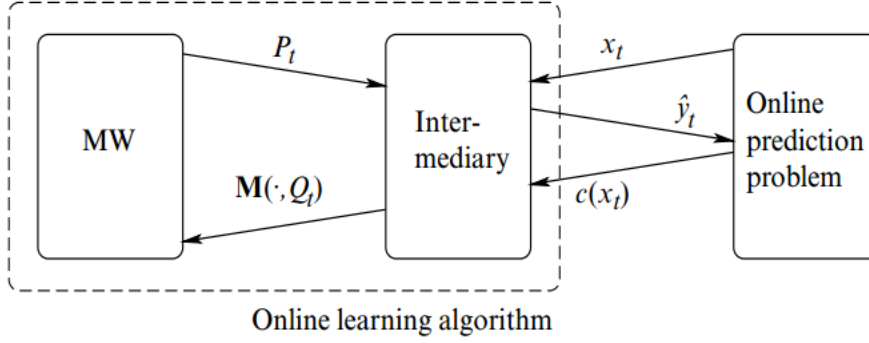


Figure 6.1

A schematic diagram of the reduction showing how MW can be used in the context of online prediction.

Figure 7: A generic online prediction algorithm [Schapire and Freund, 2012]

• **Corollary 3.3** [Schapire and Freund, 2012]

Under the same condition above, and set

$$\eta = \log \left(1 + \sqrt{\frac{2 \log m}{T}} \right),$$

the excess risk bound becomes

$$\sum_{t=1}^T M(P_t, Q_t) \leq \min_{P \in \Delta_m} \sum_{t=1}^T M(P, Q_t) + \Delta_T \quad (42)$$

where

$$\Delta_T := \sqrt{\frac{2 \log m}{T}} + \frac{\log m}{T} = \mathcal{O} \left(\sqrt{\frac{\log m}{T}} \right).$$

• **Algorithm (Online Learning via Exponential Weighted Average)** [Cesa-Bianchi and Lugosi, 2006, Schapire and Freund, 2012, Mohri et al., 2018]

Based on EWA, we can develop a general framework to solve the **online prediction** problem. Define the loss matrix $M \in \mathbb{R}^{|\mathcal{H}| \times |\mathcal{X}|}$ as the *mistake matrix*

$$M_{i,j} := M(h_i, x_j) := 1 - y_j h_i(x_j) = \begin{cases} 1 & \text{if } h_i(x_j) \neq y_j \\ 0 & \text{otherwise} \end{cases},$$

where *the environment's choice* of a **column** will correspond to *the choice of an instance* $x \in \mathcal{X}$ that is presented to the learner on a given iteration, while *the learner's choice* of a **row** will correspond to *choosing a specific hypothesis* $h \in \mathcal{H}$ which is then used to predict the label $h(x)$.

On round $t = 1, \dots, T$:

1. the **environment** chooses an instance $x_t \in \mathcal{X}$;
2. the **learner** chooses a new base hypothesis h_t according to the distribution P_t on \mathcal{H} ;

3. the hypothesis **predict** $\hat{y}_t = h_t(x_t)$; and **receive feedback** (true label $y_t = c(x_t)$)
4. Let Q_t be a **pure strategy** concentrated on x_t for **environment**

$$M(h, Q_t) := \mathbb{1} \{h(x_t) \neq y_t\}, \quad \forall h \in \mathcal{H}$$

5. the **learner** computes distribution P_{t+1} using *exponential weighted average algorithm*; this reduces to the following **update rule** for all $h \in \mathcal{H}$:

$$P_{t+1}(h) = \frac{P_t(h)}{Z_t} \times \begin{cases} e^{-\eta} & \text{if } h(x_t) \neq y_t \\ 1 & \text{o.w.} \end{cases}$$

where Z_t is the normalization factor.

Note that

$$M(P_t, x_t) = \sum_{h \in \mathcal{H}} P_t(h) \mathbb{1} \{h(x_t) \neq y_t\} = \mathcal{P}_{h \sim P_t} \{h(x_t) \neq y_t\} = \mathcal{P} \{h_t(x_t) \neq y_t\}$$

The excess risk is

$$\sum_{t=1}^T M(P_t, x_t) - \min_{h \in \mathcal{H}} \sum_{t=1}^T M(h, x_t). \quad (43)$$

The excess risk bound (41) gives us

$$\mathbb{E} \left[\frac{1}{T} \sum_{t=1}^T \mathbb{1} \{h_t(x_t) \neq y_t\} \right] \leq \min_{h \in \mathcal{H}} \frac{1}{T} \sum_{t=1}^T \mathbb{1} \{h(x_t) \neq y_t\} + \mathcal{O} \left(\sqrt{\frac{\log |\mathcal{H}|}{T}} \right).$$

• **Remark (Minmax Analysis for Online Prediction with Weak Learner)**

We assume the availability of a **weak learning algorithm** such that, for some $\gamma > 0$, and for any distribution \mathcal{D} over the set \mathcal{X} , the algorithm is able to find a hypothesis $h \in \mathcal{H}$ with error at most $1/2 - \gamma$ with respect to the distribution \mathcal{D} ; this is **the empirical γ -weak learning assumption**. By *min-max theorem*,

$$\begin{aligned} \min_P \max_{x \in \mathcal{X}} M(P, x) &= \min_P \max_Q M(P, Q) = v \\ &= \max_Q \min_P M(P, Q) \\ &= \max_Q \min_{h \in \mathcal{H}} M(h, Q). \end{aligned} \quad (44)$$

– In the right-hand side of (44),

$$M(h, Q) = \mathbb{E}_{X \sim Q} [\mathbb{1} \{h(X) \neq Y\}] := \mathbb{E}_{X \sim Q} [\mathbb{1} \{h(X) \neq c(X)\}].$$

Therefore, the right-hand part of equation (44) says that there exists a distribution Q^* on \mathcal{X} such that for every hypothesis h ,

$$M(h, Q^*) = \mathbb{E}_{X \sim Q^*} [\mathbb{1} \{h(X) \neq c(X)\}] \geq v.$$

However, because we assume γ -weak learnability, there must exist a hypothesis h such that

$$M(h, Q^*) = \mathbb{E}_{X \sim Q^*} [\mathbb{1} \{h(X) \neq c(X)\}] \leq \frac{1}{2} - \gamma.$$

Combining these facts gives that $v \leq 1/2 - \gamma$.

- On the other hand, the left part of equation (44) implies that there exists a distribution P^* over the hypothesis space \mathcal{H} such that for every $x \in \mathcal{X}$,

$$\mathbb{E}_{h \in P^*} [\mathbb{1} \{h(x) \neq c(x)\}] = M(P^*, x) \leq v \leq \frac{1}{2} - \gamma < \frac{1}{2}$$

In words, this says that every instance x is misclassified by less than $1/2$ of the hypotheses, as weighted by P^* .

Therefore, a **weighted majority vote** for all $h \in \mathcal{H}$ with optimal distribution P^* **will correctly classify all of instances**. That is, for all $x \in \mathcal{X}$, the true concept is

$$c(x) = \text{sgn} \left(\sum_{h \in \mathcal{H}} P^*(h) h(x) \right).$$

This reasoning tells us something even stronger about the **margins** for this weighted majority vote. Recall that the margin of an example is the **difference** between *the weighted fraction of hypotheses voting for the correct label* and the weighted fraction voting for *an incorrect label*. Thus the bound above tells us that difference will be at least

$$\left(\frac{1}{2} + \gamma \right) - \left(\frac{1}{2} - \gamma \right) = 2\gamma$$

In other word, the empirical γ -weak learnability is equivalent to linear separability with margin 2γ .

3.3 AdaBoost as Repeated Zero-Sum Game

- **Algorithm (AdaBoost as Dual Problem of Online Prediction)** [Schapire and Freund, 2012, Mohri et al., 2018]

AdaBoost is a **dual** problem to *the online learning algorithm* above. In particular, define the loss matrix $M \in \mathbb{R}^{|\mathcal{X}| \times |\mathcal{H}|}$ as *the accuracy matrix*

$$M_{i,j} := M(x_i, h_j) := y_i h_j(x_i) = \begin{cases} 1 & \text{if } h_j(x_i) = y_i \\ 0 & \text{otherwise} \end{cases},$$

See that $M_{\text{boost}} = 1 - M_{\text{online}}^T$. In this game, **the booster (environment)** is *the row player* and *the (weak) learner is the column player*.

On round $t = 1, \dots, T$:

1. *the booster (environment)* constructs a distribution $\mathcal{D}_t := P_t$ on \mathcal{X} which is passed to the weak learner;
2. The **weak learner** produces a hypothesis $h_t \in \mathcal{H}$ with error *at most* $1/2 - \gamma$.

$$\mathbb{E}_{X \sim \mathcal{D}_t} [\mathbb{1} \{h_t(X) = c(X)\}] \geq \frac{1}{2} + \gamma$$

3. Let Q_t be the **pure strategy** concentrated on h_t , and computes

$$M(x, Q_t) = M(x, h_t) := \mathbb{E}_{X \sim \mathcal{D}_t} [\mathbb{1} \{h_t(x) = c(x)\}], \quad \forall x \in \mathcal{X}$$

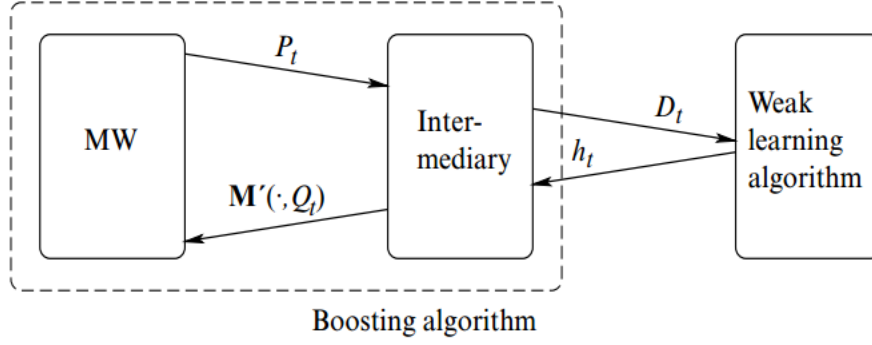


Figure 6.2

A schematic diagram of the reduction showing how MW can be used to derive a boosting algorithm.

Figure 8: AdaBoost as the dual algorithm to online prediction [Schapire and Freund, 2012]

4. the **booster (environment)** computes distribution P_{t+1} using *exponential weighted average algorithm*; this reduces to the following **update rule** for all $x \in \mathcal{X}$:

$$P_{t+1}(x) = \frac{P_t(x)}{Z_t} \times \begin{cases} e^{-\eta} & \text{if } h_t(x) = c(x) \\ 1 & \text{o.w.} \end{cases}$$

where $Z_t = \sum_{i=1}^m P_t(x_i) \exp(-\eta y_i h_t(x_i))$ is the normalization factor.

The excess risk is defined as

$$\sum_{t=1}^T M(P_t, h_t) - \min_{x \in \mathcal{X}} \sum_{t=1}^T M(x, h_t).$$

- **Remark (Adversarial Learning)**

Note that the goal of learner is to **maximize the weighted accuracy** of the weak hypotheses

$$M(x, h_t) := \mathbb{E}_{X \sim \mathcal{D}_t} [\mathbb{1} \{h_t(x) = c(x)\}],$$

but in this game-theoretic setting, the goal of the **booster** is exactly the **opposite**, namely, to **choose distributions \mathcal{D}_t** which make it **as hard as possible** for the weak learner to find an accurate hypothesis.

- **Remark (Approximate Maxmin Strategy for AdaBoost)**

Similar to the analysis for online learning, we see that the target concept $c(x)$ can be obtained by **weighted majority vote based on the maxmin strategy** of M . In particular, the average

$$\bar{Q} := \frac{1}{T} \sum_{t=1}^T Q_t$$

is seen as **the approximate maxmin strategy**. Since each Q_t is a pure strategy concentrated on h_t , the **approximate maxmin strategy** corresponds to the hypothesis

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

- **Remark** (*Minmax Analysis for AdaBoost*) [Schapire and Freund, 2012]
The minmax theorem states that

$$\begin{aligned}
\min_P \max_{h \in \mathcal{H}} M(P, h) &= \min_P \max_Q M(P, Q) = v \\
&= \max_Q \min_P M(P, Q) \\
&= \max_Q \min_{x \in \mathcal{X}} M(x, Q).
\end{aligned} \tag{45}$$

Note that for all t , by γ -weak learnability

$$M(P_t, h_t) := \mathbb{E}_{X \sim \mathcal{D}_t} [\mathbb{1} \{h_t(X) = c(X)\}] \geq \frac{1}{2} + \gamma$$

From the excess risk bound (42), for an appropriate choice of η , this implies that

$$\frac{1}{2} + \gamma \leq \frac{1}{T} \sum_{t=1}^T M(P_t, h_t) \leq \min_{x \in \mathcal{X}} \frac{1}{T} \sum_{t=1}^T M(x, h_t) + \Delta_T \tag{46}$$

where $\Delta_T = \mathcal{O}(\sqrt{\frac{\log(|\mathcal{X}|)}{T}})$ and so, for all x ,

$$\frac{1}{T} \sum_{t=1}^T M(x, h_t) \geq \frac{1}{2} + \gamma - \Delta_T > \frac{1}{2} \tag{47}$$

where the last inequality holds for sufficiently large T (esp. when $\Delta_T < \gamma$).

Note that by definition of M , $\frac{1}{T} \sum_{t=1}^T M(x, h_t)$ is exactly *the number of hypotheses h_t which agree with c on instance x* . Therefore, in words, equation (47) says that *more than half the hypotheses h_t are correct on x* . This means, by definition of H , that

$$c(x) = H(x) = \text{sgn} \left(\sum_{t=1}^T h_t \right), \quad \forall x \in \mathcal{X}.$$

For the above to hold, we need only that $\Delta_T < \gamma$, which will be the case for

$$T = \Omega \left(\frac{\log |\mathcal{X}|}{\gamma^2} \right).$$

Moreover, we see that *every x will have margin at least $2(\gamma - \Delta_T)$* . Thus, as T gets large and Δ_T approaches zero, *a minimum margin of at least 2γ is obtained asymptotically.*

3.4 Maximum Entropy Learning and Bregman Iterative Projection

- **Remark** We focus now on the learning of distribution \mathcal{D} in AdaBoost. By construction of \mathcal{D}_{t+1} , the following equation holds

$$\begin{aligned}
\sum_{i=1}^m \mathcal{D}_{t+1}(i) y_i h_j(x_i) &= \frac{1}{Z_t} \sum_{i=1}^m \mathcal{D}_t(i) e^{-\alpha_t y_i h_j(x_i)} y_i h_j(x_i) \\
&= -\frac{1}{Z_t} \frac{dZ_t}{d\alpha_t} = 0
\end{aligned}$$

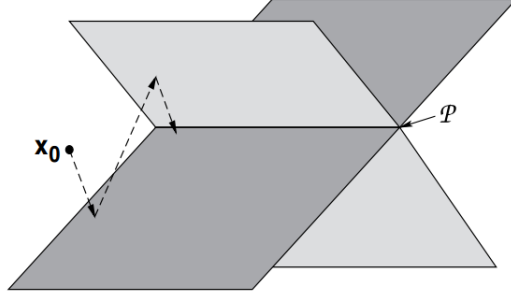


Figure 8.1

An example in \mathbb{R}^3 of the input to an iterative projection algorithm. Here, the problem is to find the point at the intersection of the two planes that is closest to the reference point \mathbf{x}_0 . The dashed arrows depict the first three steps of the algorithm.

Figure 9: An illustration of the iterative projection algorithm [Schapire and Freund, 2012]

In other word, the booster aims at find a distribution \mathcal{D} in region

$$\mathcal{R} = \left\{ D \in \Delta_m : \sum_{i=1}^m \mathcal{D}(i) y_i h(x_i) = 0, \quad \forall h \in \mathcal{H} \right\} \quad (48)$$

that is, a distribution \mathcal{D} that is so **hard** that **no weak classifier** $h_j \in \mathcal{H}$ is at all **correlated** under \mathcal{D} **with the labels** y_i . For \mathcal{D} , the feasible region \mathcal{R} is a **linear**.

- **Remark (Maximum Entropy Learning)**

From **booster perspective**, the goal is to **find the distribution** in \mathcal{D} that is **closest to uniform** U in terms of relative entropy. That is, we reach the following **optimization program**:

$$\min_{\mathcal{D}} \text{KL}(\mathcal{D} \parallel U) \quad (49)$$

$$\begin{aligned} \text{s.t. } & \sum_{i=1}^m \mathcal{D}(i) y_i h_j(x_i) = 0, \quad j = 1, \dots, N; \quad (\text{i.e. } \mathcal{D} \in \mathcal{R}) \\ & \mathcal{D}(i) \geq 0, \quad i = 1, \dots, m \\ & \sum_{i=1}^m \mathcal{D}(i) = 1. \end{aligned} \quad (50)$$

This formulation is called **the maximum entropy learning** where the goal is to minimize the “relative distance” between distribution \mathcal{D} to a reference distribution U . Note that the condition (50) corresponds to $N = |\mathcal{H}|$ linear constraints since it is satisfied by all $h \in \mathcal{H}$

- **Remark (AdaBoost as Bregman Iterative Projection Algorithm)**

When N is large, solving the **maximum entropy problem** with N linear constraints can be complex. One way to solve (49) is to construct a **trajectory** towards the **optimal solution** by **iteratively projecting onto one individual constraint**. This trajectory will eventually **enter the feasible region \mathcal{R} if it is not empty**. Then we have the optimal solution. Figure 9 illustrates the idea of iterative projection.

Specifically, **AdaBoost** can be seen to be an **iterative projection algorithm** that operates in **the space of probability distributions** over **training examples**. For $t = 1, \dots, T$, the

Algorithm 8.2

An iterative projection algorithm corresponding to AdaBoost

Given: $(x_1, y_1), \dots, (x_m, y_m)$ where $x_i \in \mathcal{X}$, $y_i \in \{-1, +1\}$
 finite, binary hypothesis space \mathcal{H} .
 Goal: find sequence D_1, D_2, \dots converging to the solution of program (8.11).
 Initialize: $D_1 = U$.
 For $t = 1, 2, \dots$

- Choose $h_t \in \mathcal{H}$ defining one of the constraints.
- Let $D_{t+1} = \arg \min_{D: \sum_{i=1}^m D(i)y_i h_t(x_i) = 0} \text{RE}(D \parallel D_t)$.
- Greedy constraint selection: Choose $h_t \in \mathcal{H}$ so that $\text{RE}(D_{t+1} \parallel D_t)$ is maximized.

Figure 10: An iterative projection algorithm corresponding to AdaBoost [Schapire and Freund, 2012]

booster find \mathcal{D}_{t+1} by minimizing the relative entropy with respect to \mathcal{D}_t

$$\begin{aligned}
 & \min_{\mathcal{D}} \text{KL}(\mathcal{D} \parallel \mathcal{D}_t) \\
 \text{s.t. } & \sum_{i=1}^m \mathcal{D}(i) y_i h_t(x_i) = 0, \\
 & \mathcal{D}(i) \geq 0, \quad i = 1, \dots, m \\
 & \sum_{i=1}^m \mathcal{D}(i) = 1.
 \end{aligned}$$

Note that this problem is simpler than (49) since the feasible region only involves *one* hypothesis h_t instead of *all* $h \in \mathcal{H}$. This algorithm is called ***the Bregman iterative projection algorithm***. Figure 10 describe the steps of the algorithm, which corresponds to the AdaBoost.

- **Remark (γ -Weak Learnability \Rightarrow Empty Feasible Region)**

It turns out that the γ -weak learnability leads to ***empty feasible region*** \mathcal{R} ; that is,

$$\mathbb{E}_{X \sim \mathcal{D}_t} [\mathbb{1} \{h_t(X) = Y\}] \geq \frac{1}{2} + \gamma \Rightarrow \sum_{i=1}^m \mathcal{D}(i) y_i h_t(x_i) \geq 2\gamma > 0.$$

In fact, as we know above, both conditions are equivalent to data being 2γ ***linearly separable***.

- **Theorem 3.4 [Schapire and Freund, 2012]**

The feasible set \mathcal{R} defined in equation (48) is ***empty if and only if the data is empirically γ -weakly learnable for some $\gamma > 0$*** .

- **Remark (γ -Weak Learnability \Rightarrow Non-convergence of Maximum Entropy Problem)**

Based on AdaBoost, the optimal value of maximum entropy problem at each iteration t is

$$\begin{aligned}\text{KL}(\mathcal{D}_{t+1} \parallel \mathcal{D}_t) &= \sum_{i=1}^m \mathcal{D}_{t+1}(i) (-\alpha_t y_i h_t(x_i) - \log Z_t) \\ &= -\log Z_t - \alpha_t \left(\sum_{i=1}^m \mathcal{D}_{t+1}(i) y_i h_t(x_i) \right) \\ &= -\log Z_t.\end{aligned}$$

Under the γ -*weak learnability* assumption,

$$\begin{aligned}\text{KL}(\mathcal{D}_{t+1} \parallel \mathcal{D}_t) &= -\log Z_t \\ &= -\frac{1}{2} \log(1 - 4\gamma_t^2) \\ &\geq -\frac{1}{2} \log(1 - 4\gamma^2) > 0,\end{aligned}$$

In other word, if the data is *weakly learnable*, then *the distributions computed by AdaBoost can never converge to a single distribution* since, in this case, the distance between \mathcal{D}_t and \mathcal{D}_{t+1} must be *lower bounded by a constant*.

- **Remark (*Unnormalized Maximum Entropy Problem*)**

One way to mitigate this issue is to *drop the normalization constration*. That is, we iteratively solve the following optimization problem

$$\begin{aligned}\min_d \text{KL}(d \parallel d_t) + \sum_{i=1}^m (d_t(i) - d(i)) \\ \text{s.t. } \sum_{i=1}^m d(i) y_i h_t(x_i) = 0, \quad (\text{i.e. } d \in \mathcal{R}') \\ d(i) \geq 0, \quad i = 1, \dots, m.\end{aligned}\tag{51}$$

Earlier, we faced the problem that there might be no distributions satisfying all the constraints. Now that difficulty is entirely erased: The set \mathcal{R}' cannot be empty since all the constraints are trivially satisfied when $d = 0$, the all 0's vector.

We can compute the optimal value at iteration t for AdaBoost algorithm:

$$\begin{aligned}\text{KL}(d_{t+1} \parallel d_t) + \sum_{i=1}^m (d_t(i) - d_{t+1}(i)) &= -\alpha_t \left(\sum_{i=1}^m d_{t+1}(i) y_i h_t(x_i) \right) + \sum_{i=1}^m (d_t(i) - d_{t+1}(i)) \\ &= \left(\sum_{i=1}^m d_t(i) \right) (1 - Z_t).\end{aligned}$$

Moreover, since this problem is a *convex optimization* with *linear constraint*, this problem has a *unique solution*

$$d(i) := \exp \left(- \sum_{t=1}^T \lambda_t y_i h_t(x_i) \right),\tag{52}$$

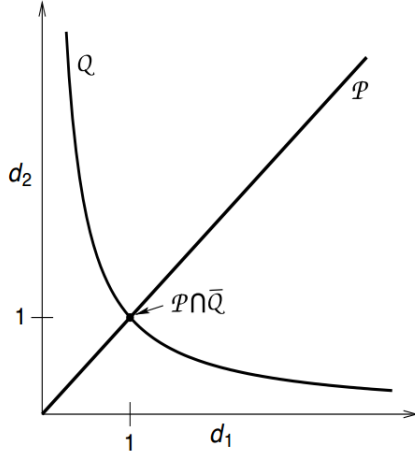


Figure 8.4

A plot of the sets \mathcal{P} and \mathcal{Q} for a tiny dataset consisting of two examples, both positive, and a single base hypothesis with $h_1(x_1) = +1$ and $h_1(x_2) = -1$.

Figure 11: The unique solution of unnormalized maximum entropy problem is determined by intersection of the objective function and the trajectory in iterative projection. [Schapire and Freund, 2012]

where the parameter $(\lambda_1, \dots, \lambda_T) \in \mathbb{R}^T$ can be obtained by solving

$$(\lambda_1, \dots, \lambda_T) = \arg \min_{\lambda \in \mathbb{R}^T} \sum_{i=1}^m \exp \left(- \sum_{t=1}^T \lambda_t y_i h_t(x_i) \right). \quad (53)$$

- **Remark (*Duality*)**

It turns out that finding the optimal distribution $d \in \mathcal{R}'$ in (51) and finding the optimal weight $\lambda \in \mathbb{R}^T$ in (53) are **dual problems** to each other. This is a classical result in maximum entropy optimization, where the objective function in (53) is *the log-partition function*.

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