Lecture 3: Theoretical Analysis of Boosting Methods

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Algorithm 1.1

The boosting algorithm AdaBoost

Given: $(x_1, y_1), ..., (x_m, y_m)$ where $x_i \in \mathcal{X}, y_i \in \{-1, +1\}$. Initialize: $D_1(i) = 1/m$ for i = 1, ..., m. For t = 1, ..., T:

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

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

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

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

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

Output the final hypothesis:

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

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

1 Boosting Algorithm

1.1 AdaBoost

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1.2 Functional Gradient Descent

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1.3 Gradient Boost

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Algorithm 7.3

AnyBoost, a generic functional gradient descent algorithm

Goal: minimization of $\mathcal{L}(F)$.

Initialize: $F_0 \equiv 0$.

For t = 1, ..., 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: Gradient Boost Tree Algorithm [Hastie et al., 2009]

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 $R_{jm}, \ j=1,2,\ldots,J_m.$
- (c) For $j = 1, 2, \dots, J_m$ compute

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

- (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]

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**, $\mathcal{Y} = \{1, \ldots, M\}$; and for **regression task**, $\mathcal{Y} = \mathbb{R}$. A **concept** $c: \mathcal{X} \to \mathcal{Y}$ 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**, $h: \mathcal{X} \to \mathcal{Y}$. 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, <u>generalization error</u> or the <u>risk</u> or simply <u>error</u> for the classifier $h \in \mathcal{H}$ is defined as

$$L(h) \equiv L_{\mathcal{P},c}(h) = \mathcal{P}\left\{h(X) \neq c(X)\right\} \equiv \mathbb{E}_X\left[\mathbb{1}\left\{h(X) \neq c(X)\right\}\right] \tag{1}$$

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

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

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 $\underline{PAC\ learnable}$ if there exist a function $m_{\mathcal{H}}: (0,1)^2 \to \mathbb{N}$ 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 $c: \mathcal{X} \to \{0,1\}$, 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 $m_{\mathcal{H}}$: $(0,1) \to \mathbb{N}$ such that for every $\delta \in (0,1)$, for every distribution \mathcal{P} over \mathcal{X} , and for every labeling function $c: \mathcal{X} \to \{-1, +1\}$, 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 $1 - \delta$,

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

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.
- ullet 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 realizablity 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

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

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

Definition (Class of Linear Combination of Base Hypothese) Define the class of T linear combinations of base hypotheses from \mathcal{H} as

$$L(\mathcal{H}, T) := \left\{ \operatorname{sgn}\left(\sum_{t=1}^{T} \alpha_t h_t(\cdot)\right) : \alpha \in \mathbb{R}^T, h_t \in \mathcal{H}, t = 1, \dots, T \right\}$$
 (2)

• Definition Define Σ_n as the space of all linear threshold functions

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

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

• 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

$$\widehat{L}_{\mathcal{D}_1}(H) \le \prod_{t=1}^T \sqrt{1 - 4\gamma_t^2} \le \exp\left(-2\sum_{t=1}^T \gamma_t^2\right). \tag{3}$$

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 $\mathcal{D} = \{x_1, \ldots, x_m\} \subset \mathcal{X}$.

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,

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

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

ullet Definition (Shattering).

A hypothesis class \mathcal{H} <u>shatters</u> 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 <u>the growth function of</u> \mathcal{H} , denoted $\tau_{\mathcal{H}} : \mathbb{N} \to \mathcal{N}$, 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 $m \geq d + 1$,

$$\tau_{\mathcal{H}}(m) \le \sum_{i=0}^{d} {m \choose i} \le \left(\frac{em}{d}\right)^{d}.$$
(4)

• 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 $h \in \mathcal{H}$,

$$L(h) \le \widehat{L}_m(h) + \sqrt{\frac{2\log \tau_{\mathcal{H}}(m)}{m}} + \sqrt{\frac{\log(1/\delta)}{2m}}$$
 (5)

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

$$\mathcal{P}\left\{\exists h \in \mathcal{H}, \left| L(h) - \widehat{L}_m(h) \right| > \epsilon\right\} \le 4\tau_{\mathcal{H}}(2m) \exp\left(-\frac{m\epsilon^2}{8}\right)$$
 (6)

which only differs from (5) by constants.

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

Lemma 2.4 |Schapire and Freund, 2012|

The space Σ_n of linear threshold functions over \mathbb{R}^n has VC-dimension n.

• Lemma 2.5 (Growth Number of Combined 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:

$$|L(\mathcal{H},T)| \le \tau_{L(\mathcal{H},T)}(m) \le \left(\frac{em}{T}\right)^T |\mathcal{H}|^T.$$
 (7)

• Theorem 2.6 (Generalization Bound for AdaBoost, Finite Hypothesis) [Schapire and Freund, 2012]

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

$$L_{\mathcal{P},c}(H) \le \widehat{L}_m(H) + \sqrt{\frac{2T\left(\log|\mathcal{H}| + \log(em/T)\right)}{m}} + \sqrt{\frac{\log(1/\delta)}{2m}}$$
(8)

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

$$L_{\mathcal{P},c}(H) \le \frac{2T\left(\log|\mathcal{H}| + \log(2em/T)\right) + 2\log(2/\delta)}{m}.$$
(9)

2.4 Generalization Error Bounds via VC Dimension

• Lemma 2.7 (Growth Number of Combined 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:

$$|L(\mathcal{H},T)| \le \tau_{L(\mathcal{H},T)}(m) \le \left(\frac{em}{T}\right)^T \left(\frac{em}{d}\right)^{dT}.$$
 (10)

Lemma 2.8 (VC-Dimension of Combined Hypothesis Class, VC Class). [Schapire and Freund, 2012, Shalev-Shwartz and Ben-David, 2014]
 Assume H has finite VC-dimension ν(H) = d and min {T, d} ≥ 3. Then the VC dimension of combined hypothesis class is bounded by

$$\nu(L(\mathcal{H}, T)) \le T(d+1) (3\log(T(d+1)) + 2) = \mathcal{O}(Td\log(Td)). \tag{11}$$

• 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 $T \geq 1$,

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

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

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

$$L_{\mathcal{P},c}(H) \le \widehat{L}_m(H) + \sqrt{\frac{2T \left(d \log(em/d) + \log(em/T)\right)}{m}} + \sqrt{\frac{\log(1/\delta)}{2m}}$$
(12)

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

$$L_{\mathcal{P},c}(H) \le \frac{2T \left(d \log(2em/d) + \log(2em/T)\right) + 2\log(2/\delta)}{m}.$$
(13)

• 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

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

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

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

• Remark Ignoring the log factor, the generalization error bound (12) can be summarized as

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

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

• Theorem 2.11 (Strong Learnable = Weak Learnable) [Schapire and Freund, 2012]
A target class H is (efficiently) weakly PAC learnable if and only if it is (efficiently) strongly PAC learnable.

2.5 Generalization Error Bounds via Large Margin Theory

- 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. 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.
- **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

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

$$\tag{14}$$

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

$$\rho := \min_{i=1,...,m} y_i \frac{\langle \alpha, h(x_i) \rangle}{\|\alpha\|_1} = \min_{i=1,...,m} \frac{\sum_{t=1}^T \alpha_t y_i h_t(x_i)}{\|\alpha\|_1}$$
(15)

- 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 $conv(\mathcal{H})$, is defined as

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

• 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 $\mathcal{D} = (z_1,\ldots,z_n)$ 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:

$$\widehat{\mathfrak{R}}_{\mathcal{D}}(\mathcal{G}) = \mathbb{E}_{\sigma} \left[\sup_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \sigma_{i} g(z_{i}) \right]$$
(16)

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

• 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

$$\widehat{\mathfrak{R}}_{\mathcal{D}}(conv(\mathcal{H})) = \widehat{\mathfrak{R}}_{\mathcal{D}}(\mathcal{H}) \tag{17}$$

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

- 3 Fundamental Perspectives
- 3.1 Game Theory
- 3.2 Online Learning
- 3.3 Maximum Entropy Estimation
- 3.4 Iterative Projection Algorithms and Convergence Analysis

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