EE6550 Machine Learning

Lecture One – Part II
The PAC Learning Framework

Chung-Chin Lu
Department of Electrical Engineering
National Tsing Hua University

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The Contents of This Lecture - Part II

- The PAC learning framework.
- Sample complexity, finite $\mathcal{H}$, consistent case.
- Sample complexity, finite $\mathcal{H}$, inconsistent case.

Fundamental Questions in Machine Learning

- What can be learned efficiently?
- What is inherently hard to learn?
- How many examples are needed to learn successfully?
- Is there a general model of learning?

What Will Be Learned? – Concept Class

- Input space $\mathscr{I}$: the population of all possible items.
  - $(\mathscr{I}, \mathcal{F}, P)$: a probability space associated with the population of all items, where the probability function P is usually unknown to the learner.
  - Example: $\mathscr{I} = \mathbb{R}^2$ is the set of all points in the plane. $\mathcal{F} = \mathcal{B}^2$ is the collection of all 2-dimensional Borel subsets of $\mathbb{R}^2$, including triangular areas, rectangular areas, disks, etc.
- Label space $\mathscr{Y}$: the set of all possible labels.
  - $(\mathscr{Y}, \mathcal{G})$: a measurable space associated with the label space $\mathscr{Y}$.
  - If $\mathscr{Y}$ is countable, $\mathcal{G}$ is commonly chosen to be $2^{\mathscr{Y}}$.
  - Example: $\mathscr{Y} = \{0, 1\}$ for binary classification and $2^{\mathscr{Y}} = \{\emptyset, \{0\}, \{1\}, \mathscr{Y}\}$.

- A concept $c : \mathscr{I} \to \mathscr{Y}$: a measurable function from the input space to the label space.
  - c is a $\mathscr{Y}$-valued random variable.
  - Example: Let R be an axis-aligned rectangular area in the plane, a member in $\mathcal{B}^2$. Define a concept

$$c(\omega) = \begin{cases} 1, & \text{if } \omega \in R, \\ 0, & \text{otherwise.} \end{cases}$$

    * c is the indicator of the rectangular area R, i.e., $c = I_R$.
    * The concept c to learn is the rectangular area R in the plane.

- Concept class $\mathcal{C}$: a set of concepts we may wish to learn.
  - Example: $\mathcal{C}$ = the set of concepts of all axis-aligned rectangular areas in the plane.

Generalization Error or Risk

- c: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $f : \mathscr{I} \to \mathscr{Y}'$: an arbitrary measurable function from the input space to the output space to approximate the concept c.
  - $(\mathscr{Y}', \mathcal{G}')$: a measurable space associated with the output space $\mathscr{Y}'$.
  - If $\mathscr{Y}'$ is countable, $\mathcal{G}'$ is commonly chosen to be $2^{\mathscr{Y}'}$.
  - f is a $\mathscr{Y}'$-valued random variable.

The generalization error (or risk) or true error of an approximation f to the concept c is defined as

$$R(f) \triangleq \underset{\omega \sim P}{E}[L(f(\omega), c(\omega))].$$

- Assume that the loss function $L : \mathscr{Y}' \times \mathscr{Y} \to \mathbb{R}$ is measurable, i.e., $L^{-1}(I) = \{(y', y) \in \mathscr{Y}' \times \mathscr{Y} \mid L(y', y) \in I\}$ is a member of the product σ-algebra $\mathcal{G}' \times \mathcal{G}$ for every interval I in $\mathbb{R}$.
- As a measurable function of r.v.s $f(\omega)$ and $c(\omega)$, $L(f(\omega), c(\omega))$ is a random variable.
- Both the probability function P and the target concept c are unknown.
- $R(f)$ is not directly accessible to the learner.
- Example: $L(y', y) = 1_{y' \neq y}$ so that

  $$R(f) = \mathop{E}_{\omega \sim P}[L(f(\omega), c(\omega))] = \mathop{E}_{\omega \sim P}[1_{f(\omega) \neq c(\omega)}] = P(f(\omega) \neq c(\omega)).$$

Bayes Error

- c: a fixed but unknown target concept in the concept class $\mathcal{C}$.

The Bayes error of learning the concept c is the least possible generalization error to learn c,

$$R^* \triangleq \inf_{f \text{ is a } \mathscr{Y}'\text{-valued r.v.}} R(f).$$

- In general, R^* is not accessible to the learner.
- If $\mathscr{Y}' = \mathscr{Y}$ and $L(y, y) = 0$ for all labels y, then $R^* = 0$.
- A hypothesis h with $R(h) = R^*$ is called a Bayes hypothesis.

Best-In-Class Hypotheses

- c: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $\mathcal{H}$: the hypothesis set chosen.
  - A hypothesis h in $\mathcal{H}$ is a $\mathscr{Y}'$-valued random variable.
- $R^*_{\mathcal{H}} \triangleq \min_{h \in \mathcal{H}} R(h)$: the least generalization error w.r.t. c achievable by some hypotheses in the hypothesis set $\mathcal{H}$.

A hypothesis h^* in $\mathcal{H}$ is called best-in-class w.r.t. c if

$$R(h^*) = R^*_{\mathcal{H}}.$$

- In general, $R^*_{\mathcal{H}}$ and h^* are not accessible to the learner.
- If $\mathcal{H} = \mathcal{C}$ and $L(y, y) = 0$ for all labels y, then $R^*_{\mathcal{H}} = R^* = 0$ and $h^* = c$ is a best-in-class hypothesis w.r.t. c.

ϵ-Best-In-Class Hypotheses

- c: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $\mathcal{H}$: the hypothesis set chosen.
  - A hypothesis h in $\mathcal{H}$ is a $\mathscr{Y}'$-valued random variable.
- $R^*_{\mathcal{H}} \triangleq \inf_{h\in\mathcal{H}} R(h)$: the least generalization error w.r.t. c asymptotically achievable by hypotheses in the hypothesis set $\mathcal{H}$.

A hypothesis h^*_ϵ in $\mathcal{H}$ is called ϵ-best-in-class w.r.t. c if

$$|R(h^*_\epsilon) - R^*_{\mathcal{H}}| \leq \epsilon.$$

- In general, $R^*_{\mathcal{H}}$ and h^*_ϵ are not accessible to the learner.

Estimation and Approximation

- c: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- R^*: the Bayes error of learning the concept c.
- $\mathcal{H}$: the hypothesis set chosen.
- h^*: a best-in-class hypothesis in $\mathcal{H}$.
- h: a hypothesis in $\mathcal{H}$.

The difference of the true error of a hypothesis h from the Bayes error R^* of learning the concept c is

$$R(h) - R^* = \underbrace{R(h) - R(h^*)}_{\text{Estimation}} + \underbrace{R(h^*) - R^*}_{\text{Approximation}}.$$

- The approximation part only depends on $\mathcal{H}$.
- The estimation part is where we can hope to bound.

Formulation of Learning Problem

- c: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $\mathcal{H}$: the hypothesis set.
- $S = (\omega_1, \ldots, \omega_m)$: a sample of m items, drawn i.i.d. from the population according to P, with labels $(c(\omega_1), \ldots, c(\omega_m))$.

To learn the concept c from the labeled sample S, the learner's task is to use the labeled sample S to select a hypothesis h_S in the hypothesis set $\mathcal{H}$ that has a "small" generalization error with respect to the concept c and then is a "good" approximation to c.

- But the learner does not know how far the true error $R(h_S)$ is from the least generalization error $R^*_{\mathcal{H}}$ over $\mathcal{H}$.

Empirical Error

- c: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $S = (\omega_1, \ldots, \omega_m)$: a sample of m items, drawn i.i.d. from the population according to P, with labels $(c(\omega_1), \ldots, c(\omega_m))$.
- h: an arbitrary hypothesis in the hypothesis set $\mathcal{H}$.

The empirical error or risk of a hypothesis h w.r.t. the concept c on the labeled sample S is defined as

$$\hat{R}_S(h) \triangleq \frac{1}{m} \sum_{i=1}^{m} L(h(\omega_i), c(\omega_i)).$$

- The learner can measure the empirical error of a hypothesis w.r.t. the unknown concept on the labeled sample.

The Sample Space Ω_m of Size m

- The sample space Ω_m of size m: the set of all samples $S = (\omega_1, \ldots, \omega_m)$ of m items from the population $\mathscr{I}$.
- The σ-algebra $\mathcal{F}_m$: the product $\underbrace{\mathcal{F} \times \cdots \times \mathcal{F}}_{m \text{ times}}$ of m copies of the σ-algebra $\mathcal{F}$.
- The probability function P_m: the product $\underbrace{P \times \cdots \times P}_{m \text{ times}}$ of m copies of the probability function P, i.e.,

$$P_m(E_1 \times \cdots \times E_m) = P(E_1) \cdots P(E_m)$$

for all members $E_1, \ldots, E_m$ in $\mathcal{F}$.

Projections ϕ_i

- $\phi_i : \Omega_m \to \mathscr{I}$: the ith projection function from the sample space to the input space, defined as

$$\phi_i(S) = \phi_i((\omega_1, \ldots, \omega_m)) = \omega_i$$

  for all sample $S = (\omega_1, \ldots, \omega_m) \in \Omega_m$ and for all $1 \leq i \leq m$.

- ϕ_i is measurable and then is an $\mathscr{I}$-valued random variable.

$\phi_1, \phi_2, \ldots, \phi_m$ Are I.I.D. R.V.s

Proof. Let $E_1, \ldots, E_m$ be members in $\mathcal{F}$. Since

$$(\phi_i \in E_i) = \phi_i^{-1}(E_i) = \mathscr{I} \times \cdots \times E_i \times \cdots \times \mathscr{I},$$

the joint event $(\phi_1 \in E_1, \phi_2 \in E_2, \ldots, \phi_m \in E_m)$ is

$$\phi_1^{-1}(E_1) \cap \phi_2^{-1}(E_2) \cap \cdots \cap \phi_m^{-1}(E_m) = E_1 \times E_2 \times \cdots \times E_m$$

so that

$$\begin{aligned}
& P_m(\phi_1 \in E_1, \phi_2 \in E_2, \ldots, \phi_m \in E_m) \\
= \quad & P_m(E_1 \times E_2 \times \cdots \times E_m) \\
= \quad & P(E_1) \cdot P(E_2) \cdots P(E_m) \\
= \quad & P_m(E_1 \times \mathscr{I} \times \cdots \times \mathscr{I}) \cdot P_m(\mathscr{I} \times E_2 \times \cdots \times \mathscr{I}) \\
& \cdots P_m(\mathscr{I} \times \mathscr{I} \times \cdots \times E_m) \\
= \quad & P_m(\phi_1 \in E_1) \cdot P_m(\phi_2 \in E_2) \ldots P_m(\phi_m \in E_m).
\end{aligned}$$

Thus $\phi_1, \phi_2, \ldots, \phi_m$ are statistically independent. For any E in $\mathcal{F}$,

$$P_m(\phi_i \in E) = P_m(\mathscr{I} \times \cdots \times E \times \cdots \times \mathscr{I}) = P(E)$$

so that ϕ_i's are identically distributed. $\square$

- The probability distributions of the projections ϕ_i's are the same as P.

$\hat{R}_S(h)$ Is a Random Variable

- c: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $S = (\omega_1, \ldots, \omega_m)$: a sample of m items, drawn i.i.d. from the population according to P, with labels $(c(\omega_1), \ldots, c(\omega_m))$.
- h: an arbitrary hypothesis in the hypothesis set $\mathcal{H}$.
- $\phi_i(S) = \phi_i((\omega_1, \ldots, \omega_m)) = \omega_i$: the ith projection function.
- $h(\omega_i) \triangleq h(\phi_i(S))$, $c(\omega_i) \triangleq c(\phi_i(S))$: measurable functions from the sample space to the output space.

The empirical error of h w.r.t. c on a labeled sample S

$$\hat{R}_S(h) = \frac{1}{m} \sum_{i=1}^{m} L(h(\omega_i), c(\omega_i)) = \frac{1}{m} \sum_{i=1}^{m} L(h(\phi_i(S)), c(\phi_i(S)))$$

is a measurable function from Ω_m to $\mathbb{R}$, i.e., a random variable.

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$$\boxed{\underset{S\sim P_m}{E}[\hat{R}_S(h)] = R(h)}$$

- The expectation of empirical error of a hypothesis h w.r.t. the target concept c on a labeled sample S of size m is equal to the generalization error of h w.r.t. the target concept c.
- Observation: since r.v.'s ϕ_i have the same probability distribution P, r.v.'s $h(\phi_i(S))$ $(c(\phi_i(S)))$ have the same probability distribution as the r.v. $h(\omega)$ $(c(\omega))$.

Proof.

$$
\begin{aligned}
& \mathop{E}_{S\sim P_m}[\hat{R}_S(h)] \\
= \quad & \mathop{E}_{S\sim P_m}\left[\frac{1}{m}\sum_{i=1}^{m} L(h(\phi_i(S)), c(\phi_i(S)))\right] \\
= \quad & \frac{1}{m}\sum_{i=1}^{m} \mathop{E}_{S\sim P_m}\left[L(h(\phi_i(S)), c(\phi_i(S)))\right] \\
= \quad & \frac{1}{m}\sum_{i=1}^{m} \mathop{E}_{\omega\sim P}\left[L(h(\omega), c(\omega))\right] \\
& \text{ since } h(\phi_i(S))\text{'s } (c(\phi_i(S))\text{'s) have the same probability} \\
& \text{ distribution as } h(\omega)\ (c(\omega)) \\
= \quad & \mathop{E}_{\omega\sim P}\left[L(h(\omega), c(\omega))\right] = R(h).
\end{aligned}
$$

$\square$

Empirical Risk Minimization (ERM)

- c: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $S = (\omega_1, \ldots, \omega_m)$: a sample of m items, drawn i.i.d. from the population according to P, with labels $(c(\omega_1), \ldots, c(\omega_m))$.
- $\mathcal{H}$: the hypothesis set.

The learner will return a hypothesis among all hypotheses in $\mathcal{H}$ which minimizes the empirical error,

$$h_S = \arg\min_{h \in \mathcal{H}} \hat{R}(h).$$

- Overfitting may occur, i.e., h_S matches to the training data sample S too well so that it may have large generalization error.
  - The hypothesis set $\mathcal{H}$ may be too complex.
  - The sample size may not be large enough.

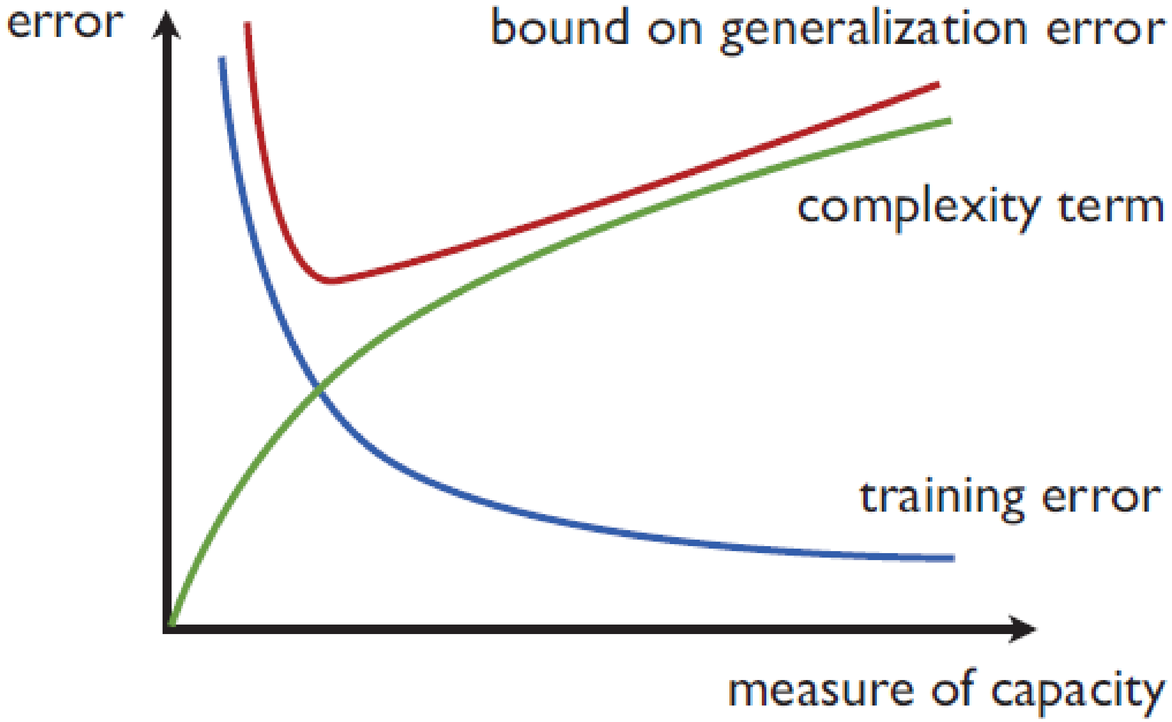
Structural Risk Minimization (SRM)

- c: a fixed but unknown target concept in the concept class $\mathcal{C}$.
- $S = (\omega_1, \ldots, \omega_m)$: a sample of m items, drawn i.i.d. from the population according to P, with labels $(c(\omega_1), \ldots, c(\omega_m))$.
- $\mathcal{H}_1 \subseteq \mathcal{H}_2 \subseteq \cdots \subseteq \mathcal{H}_n \subseteq \cdots$: an increasing sequence of hypothesis sets.

The learner will return a hypothesis among all hypotheses in $\cup_{n=1}^{\infty} \mathcal{H}_n$ which minimizes the empirical error plus a complexity measure of $\mathcal{H}_n$ and the sample size m,

$$h_S = \arg \min_{h \in \mathcal{H}_n, n \in \mathbb{N}} [\hat{R}(h) + \text{complexity}(\mathcal{H}_n, m)].$$

- Theoretical guarantees: consistency under general assumptions.
- Computational complexity: typically hard problems.



Structural risk minimization, where a bound (in red) on the generalization error is the sum of the empirical error and the complexity term as functions of the size or capacity of the hypothesis set.

Probably Approximately Correct (PAC) Learning

- Definition: A concept class $\mathcal{C}$ is PAC-learnable if there exists a learning algorithm $\mathbb{A}$, which returns $h_S \in \mathcal{H}$ to approximate an unknown target concept $c \in C$ on a labeled sample S of size m,

$$h_S = \mathbb{A}(S; c, \mathcal{H}),$$

such that for any $\epsilon > 0$, $\delta > 0$, $c \in \mathcal{C}$ and P, we have

$$P_m(R(h_S) \leq \epsilon) \geq 1 - \delta,$$

provided that the sample size m is

$$m \geq \text{poly}(1/\epsilon, 1/\delta, n, \text{size}(c))$$

for a fixed polynomial, where

  - $O(n)$: cost of computational representation of an item ω.
  - $O(\text{size}(c))$: cost of computational representation of a c.

- When such an algorithm $\mathbb{A}$ exists, it is called a PAC-learning algorithm for $\mathcal{C}$.

Efficient PAC Learning

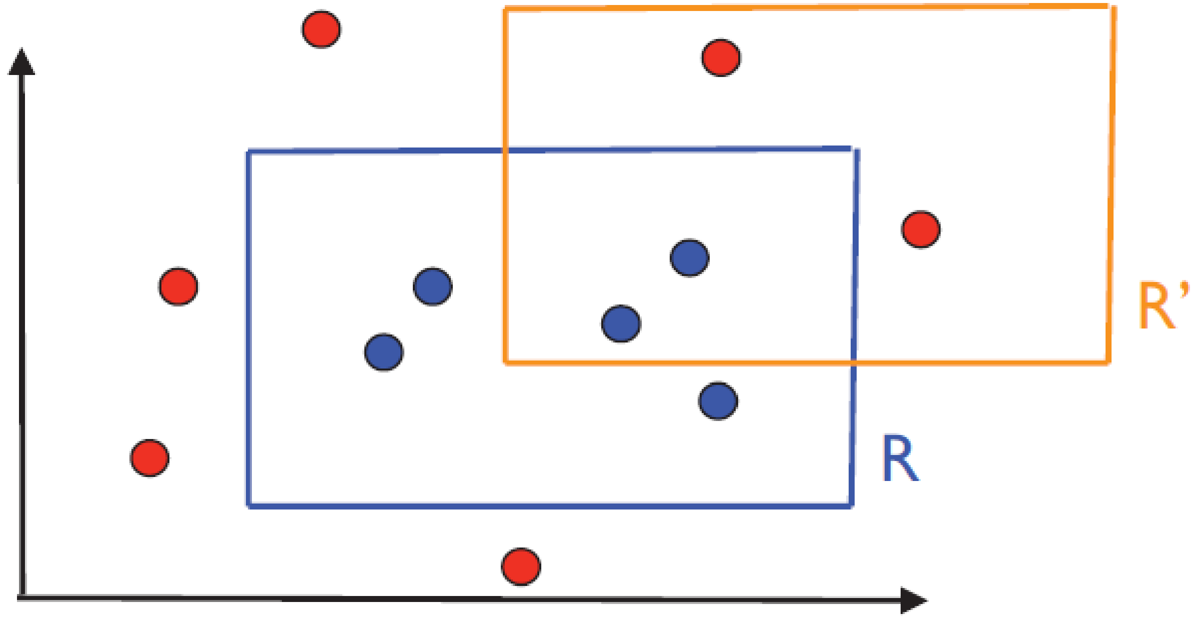
- Definition: A concept class $\mathcal{C}$ is efficiently PAC-learnable if
  - $\mathcal{C}$ is PAC-learnable by a learning algorithm $\mathbb{A}$,
  - $\mathbb{A}$ further runs in $\text{poly}(1/\epsilon, 1/\delta, n, \text{size}(c))$.
- When such an algorithm $\mathbb{A}$ exists, it is called an efficient PAC-learning algorithm for $\mathcal{C}$.

Remarks

- Concept class $\mathcal{C}$ is known to the algorithm $\mathbb{A}$.
- But a specific target concept $c \in \mathcal{C}$ is unknown to $\mathbb{A}$.
- Hypothesis set $\mathcal{H}$ is built in the algorithm $\mathbb{A}$.
- Distribution-free model: no assumption on the probability function P.
- Both training and test samples are drawn i.i.d. from the population according to P, which is unknown to $\mathbb{A}$.
- The mapping $S \mapsto R(h_S)$ is measurable so that $R(h_S)$ is a random variable.
- High probable: at least $1 - \delta$.
- Approximately correct: true error at most ϵ.

Example 2.1: Learning Axis-Aligned Rectangular Areas

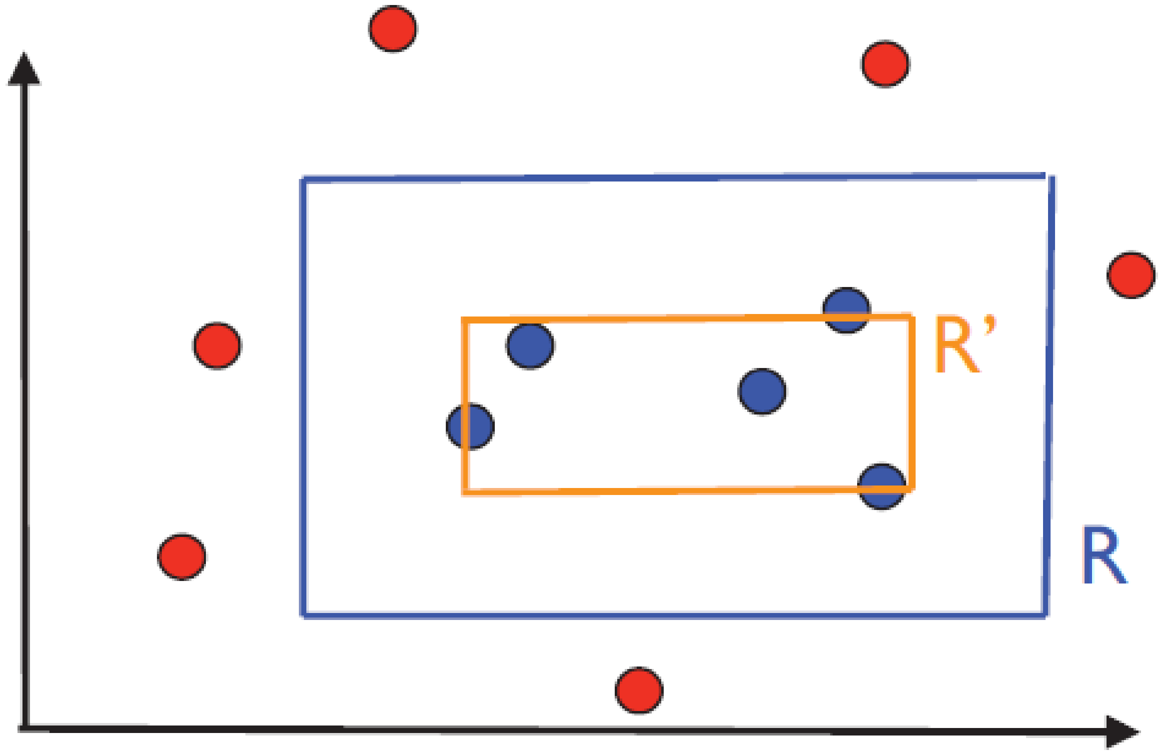
- Problem: learn with small error an unknown axis-aligned rectangular area R using as small a labeled training sample as possible.
- Input space $\mathscr{I} = \mathbb{R}^2$, the plane.
- Label space $\mathscr{Y} = \{0, 1\}$.
- Concept class $\mathcal{C}$ = the set of all axis-aligned rectangular area in the plane.
- We will show that this concept class $\mathcal{C}$ is PAC-learnable.



The target "unknown" concept R and a possible hypothesis R'.

Example 2.1: A Learning Algorithm $\mathbb{A}$

- $R \in \mathcal{C}$: an unknown target axis-aligned rectangular area to learn.
- $S = (\omega_1, \ldots, \omega_m)$: a labeled sample of size m.
- The hypothesis set is $\mathcal{H} = \mathcal{C} =$ the set of all axis-aligned rectangular area.
- $R'_S = \mathbb{A}(S; R, \mathcal{H}) =$ the tightest axis-aligned rectangular area containing the points in the sample S labeled with 1.



The hypothesis $R' = R'_S$ returned by the algorithm.

Example 2.1: Error Analysis (1)

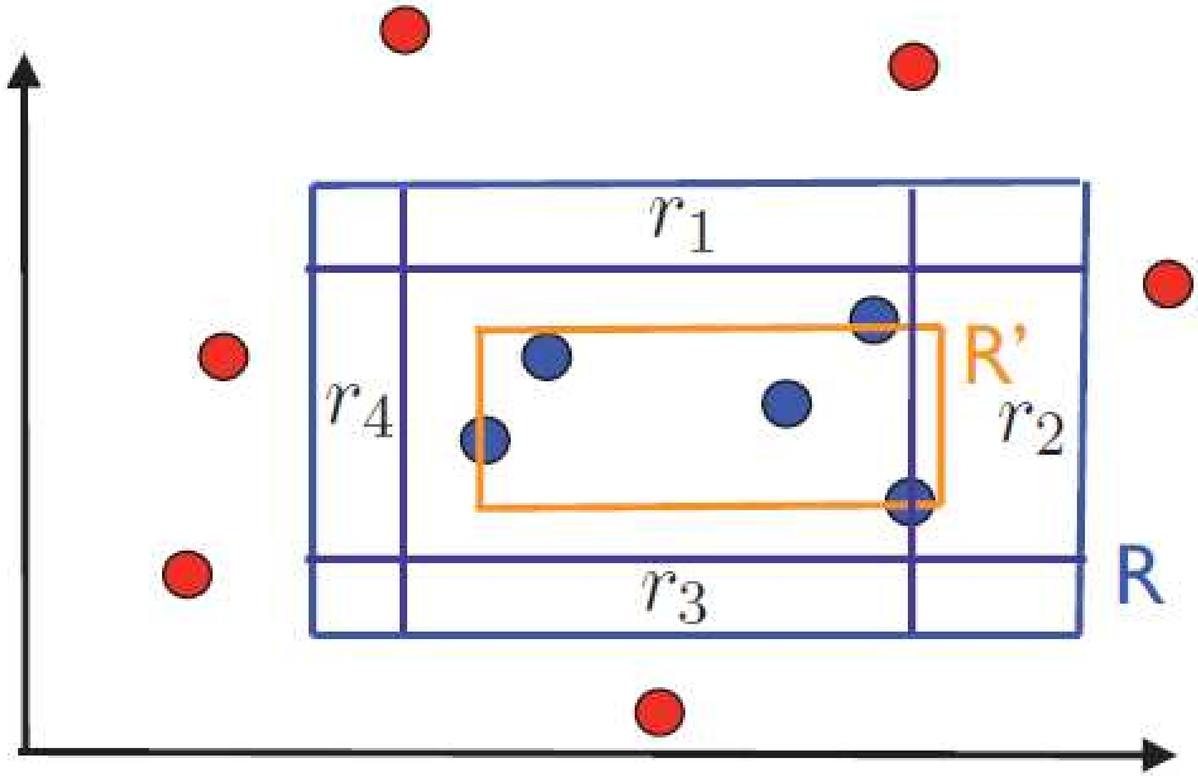
- The loss function is $L(y', y) = 1_{(y' \neq y)}, \ \forall\, y', y \in \{0, 1\}$.
- The generalization error of a hypothesis R' w.r.t. a concept R is

$$R(R') = \underset{\omega \sim P}{E}[1_{(1_{R'}(\omega) \neq 1_R(\omega))}] = \underset{\omega \sim P}{E}[1_{R' \Delta R}(\omega)] = P(R' \Delta R),$$

  - $R' \Delta R \triangleq (R' \setminus R) \cup (R \setminus R')$: the symmetric difference of two events R' and R.
  - A point $\omega \in R' \setminus R$ will make a false positive.
  - A point $\omega \in R \setminus R'$ will make a false negative.
- Since $R'_S \subseteq R$, the error region $R'_S \Delta R = R \setminus R'_S$ is included in R and R'_S does not produce any false positive.
- $R(R'_S) = P(R'_S \Delta R) = P(R \setminus R'_S) = P(R) - P(R'_S)$.

Example 2.1: Error Analysis (2)

- The self-empirical error is $\hat{R}_S(R'_S) = \frac{1}{m}\sum_{i=1}^{m} 1_{1_{R'_S}(\omega_i) \neq 1_R(\omega_i)} = 0.$
- With zero self-empirical error for all labeled sample S, both the hypothesis R'_S and the learning algorithm $\mathbb{A}$ are called consistent.
- If $P(R) \le \epsilon$, then the generalization error $R(R'_S) = P(R) - P(R'_S) \le P(R) \le \epsilon$ for all labeled sample S.
- Assume $P(R) > \epsilon$. Let r_1, r_2, r_3, r_4 be the four smallest sub-rectangular areas of R along the four sides of R such that $P(r_i) = \frac{\epsilon}{4}$.
- That the event $(R(R'_S) > \epsilon) = (P(R) - P(R'_S) > \epsilon)$ occurs implies that R'_S misses at least one of four r_i's.



The regions r_1, r_2, r_3, r_4 in the target "unknown" concept R.

Example 2.1: Error Analysis (3)

- Thus we have

$$\begin{aligned}
P_m(R(R'_S) > \epsilon) &\leq P_m(\cup_{i=1}^{4}(R'_S \cap r_i = \emptyset)) \\
&\leq \sum_{i=1}^{4} P_m(R'_S \cap r_i = \emptyset) \text{ by the union bound} \\
&\leq 4(1-\epsilon/4)^m \\
&< 4e^{-m\epsilon/4} \text{ by } 1-x < e^{-x} \text{ for all } x \in \mathbb{R} \setminus \{0\}
\end{aligned}$$

- Set $4e^{-m\epsilon/4} \leq \delta$ if and only if set $m \geq \frac{4}{\epsilon} \ln \frac{4}{\delta}$.
- For any $\epsilon > 0$, $\delta > 0$, $R \in \mathcal{C}$ and P, if $m \geq \frac{4}{\epsilon} \ln \frac{4}{\delta}$, we have

$$P_m(R(R'_S) > \epsilon) < \delta.$$

Example 2.1: PAC-Learnability

- The concept class $\mathcal{C}$ of axis-aligned rectangular areas is PAC-learnable.
- $\mathbb{A}$ is a PAC-learning algprithm.
- The sample complexity of PAC-learning axis-aligned rectangular areas is in $O(\frac{4}{\epsilon} \ln \frac{4}{\delta})$.
- An equivalent statement: with probability at least $1 - \delta$ and a sample size m, the generalization error of the PAC-learning algorithm is upper bounded as:

$$R(R'_S) \leq \frac{4}{m} \ln \frac{4}{\delta}$$

by setting $\delta = 4e^{-m\epsilon/4}$ and solving ϵ.

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Learning Bound for Finite $\mathcal{H}$ - Consistent Case

Theorem 2.1: Let

- $\mathscr{I}$: input space, which is general.
- $\mathscr{Y} = \{0, 1\}$: label space with loss function $L(y', y) = 1_{y' \neq y}$.
- $\mathcal{H} = \mathcal{C}$: finite hypothesis set and concept class.
- $\mathbb{A}$: consistent learning algorithm.
  - $h_S = \mathbb{A}(S; c, \mathcal{H})$ is consistent for any i.i.d. sample S of size m and any target concept c, i.e., $\hat{R}_S(h_S) = 0$.

Then for any $\epsilon > 0, \delta > 0$, we have

$$P_m(R(h_S) \leq \epsilon) \geq 1 - \delta,$$

provided that

$$m \geq \frac{1}{\epsilon}\left(\ln|\mathcal{H}| + \ln\frac{1}{\delta}\right).$$

Proof. Since $\hat{R}_S(h_S) = 0$ for every returned hypothesis h_S, the event $(R(h_S) > \epsilon) = (R(h_S) > \epsilon, \hat{R}_S(h_S) = 0)$ implies the event that there exists a hypothesis $h \in \mathcal{H}$ with $R(h) > \epsilon$ such that $\hat{R}_S(h) = 0$, i.e., $\cup_{h\in\mathcal{H} \text{ with } R(h)>\epsilon}(\hat{R}_S(h) = 0)$. By union bound, we have

$$
\begin{aligned}
& P_m(R(h_S) > \epsilon) \\
\leq\ & P_m(\cup_{h \in \mathcal{H} \text{ with } R(h) > \epsilon}(\hat{R}_S(h) = 0)) \\
\leq\ & \sum_{h \in \mathcal{H} \text{ with } P(h(\omega) \neq c(\omega)) > \epsilon} P_m\left(\frac{1}{m}\sum_{i=1}^{m} 1_{h(\omega_i) \neq c(\omega_i)} = 0\right) \\
=\ & \sum_{h \in \mathcal{H} \text{ with } P(h(\omega) \neq c(\omega)) > \epsilon} P_m(\cap_{i=1}^{m}(h(\phi_i(S)) = c(\phi_i(S)))) \\
=\ & \sum_{h \in \mathcal{H} \text{ with } P(h(\omega) \neq c(\omega)) > \epsilon} \prod_{i=1}^{m} P_m(h(\phi_i(S)) = c(\phi_i(S))) \\
& \text{ since } \phi_i\text{'s are statistically independent} \\
=\ & \sum_{h \in \mathcal{H} \text{ with } P(h(\omega) \neq c(\omega)) > \epsilon} \prod_{i=1}^{m} P(h(\omega) = c(\omega)) \\
& \text{ since } \phi_i(S)\text{'s are identically distributed with } \omega \\
<\ & |\mathcal{H}|(1-\epsilon)^m \leq |\mathcal{H}|e^{-m\epsilon}.
\end{aligned}
$$

By setting

$$\delta \geq |\mathcal{H}| e^{-m\epsilon},$$

we have

$$m \geq \frac{1}{\epsilon}\left(\ln|\mathcal{H}| + \ln\frac{1}{\delta}\right).$$

$\square$

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Remarks

- The theorem shows that when the hypothesis set $\mathcal{H}$ is finite, a consistent algorithm $\mathbb{A}$ is a PAC-learning algorithm.
- Equivalently, with probability at least $1-\delta$ and sample size m, the true error of the returned hypothesis h_S is upper bounded as:
$$R(h_S) \leq \frac{1}{m}\left(\ln|\mathcal{H}| + \ln\frac{1}{\delta}\right).$$
- True error bound is linear in $1/m$ and only logarithmic in $1/\delta$.
- The price to pay for coming up with a consistent algorithm is the use of a larger hypothesis set H containing target concepts.
- $\log_2|\mathcal{H}|$ is the number of bits used for the representation of $\mathcal{H}$.
- Bound is loose for large $\mathcal{H}$.

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Markov Inequality

- X: a nonnegative r.v. with $E[X] < \infty$;
- $a > 0$.

Then we have

$$P(X \geq a) \leq \frac{E[X]}{a}.$$

Proof. Since $X \geq 0$, we have $a \cdot 1_{(X \geq a)} \leq X$ so that

$$\begin{aligned} & E[a \cdot 1_{(X \geq a)}] \leq E[X] \\ \Rightarrow \quad & a \cdot E[1_{(X \geq a)}] \leq E[X] \\ \Rightarrow \quad & a \cdot P(X \geq a) \leq E[X] \\ \Rightarrow \quad & P(X \geq a) \leq \frac{E[X]}{a}. \end{aligned}$$

$\square$

Moment Generating Function

- X: a r.v.
- $M_X(t) = E[e^{tX}]$: moment generating function of the r.v. X for all t such that the expectation exists.
  - e^{tX} is a nonnegative r.v. for each $t \in \mathbb{R}$.

Chernoff Bounds

- X: a r.v. with moment generating function $M_X(t)$.

Then we have, for all $a \in \mathbb{R}$,

$$\begin{aligned} P(X \geq a) &\leq e^{-ta} M_X(t) \quad \forall\, t > 0, \\ P(X \leq a) &\leq e^{-ta} M_X(t) \quad \forall\, t < 0. \end{aligned}$$

Proof. For $t > 0$, e^{tx} is an increasing function of x so that

$$P(X \geq a) = P(e^{tX} \geq e^{ta}) \leq \frac{E[e^{tX}]}{e^{ta}} = e^{-ta} M_X(t)$$

since $e^{tX} \geq 0$ and by Markov inequality. For $t < 0$, e^{tx} is a decreasing function of x so that

$$P(X \leq a) = P(e^{tX} \geq e^{ta}) \leq \frac{E[e^{tX}]}{e^{ta}} = e^{-ta} M_X(t)$$

since $e^{tX} \geq 0$. $\square$

Azuma-Hoeffding Lemma

- X: a r.v. with $E[X] = 0$ and $a \le X \le b$.

Then for any $t \in \mathbb{R}$,

$$E[e^{tX}] \le e^{t^2(b-a)^2/8}.$$

Proof. It is clear that $a \le 0 \le b$. If $a = b$, then $X = 0$ and $E[e^{tX}] = 1 = e^{t^2(b-a)^2/8}$ for all $t \in \mathbb{R}$. Assume that $a < b$. Fix a $t \in \mathbb{R}$. Since e^{tx} is a convex function of x on $\mathbb{R}$ and each $x \in [a, b]$ is a convex combination of a and b, $x = \frac{b-x}{b-a}a + \frac{x-a}{b-a}b$, we have

$$e^{tx} \le \frac{b-x}{b-a}e^{ta} + \frac{x-a}{b-a}e^{tb}$$

which implies that

$$E\left[e^{tX}\right] \le E\left[\frac{b-x}{b-a}\right]e^{ta} + E\left[\frac{x-a}{b-a}\right]e^{tb} = \frac{b}{b-a}e^{ta} + \frac{-a}{b-a}e^{tb} = e^{\phi(t)},$$

where

$$\phi(t) \triangleq \ln\left(\frac{b}{b-a}e^{ta} + \frac{-a}{b-a}e^{tb}\right) = ta + \ln\left(\frac{b}{b-a} - \frac{a}{b-a}e^{t(b-a)}\right)$$

is a function of t on $\mathbb{R}$ and has

$$\begin{aligned}
\phi'(t) &= a - \frac{ae^{t(b-a)}}{\frac{b}{b-a} - \frac{a}{b-a}e^{t(b-a)}} = a - \frac{a}{\frac{b}{b-a}e^{-t(b-a)} - \frac{a}{b-a}} \\
\phi''(t) &= \frac{-abe^{-t(b-a)}}{\left(\frac{b}{b-a}e^{-t(b-a)} - \frac{a}{b-a}\right)^2} \\
&= \frac{\alpha(1-\alpha)e^{-t(b-a)}(b-a)^2}{\left((1-\alpha)e^{-t(b-a)} + \alpha\right)^2}, \ \alpha \triangleq \frac{-a}{b-a} > 0 \\
&= \frac{\alpha}{(1-\alpha)e^{-t(b-a)} + \alpha} \ \frac{(1-\alpha)e^{-t(b-a)}}{(1-\alpha)e^{-t(b-a)} + \alpha} \ (b-a)^2 \\
&\le \frac{(b-a)^2}{4} \ \forall \ t \in \mathbb{R},
\end{aligned}$$

since $u(1-u) \leq \frac{1}{4}$ for any $u \in [0,1]$. By Taylor's formula, we have

$$\phi(t) = \phi(0) + t\phi'(0) + \frac{t^2}{2}\phi''(\theta) \leq \frac{t^2(b-a)^2}{8},$$

where θ is between 0 and t and since $\phi(0) = \phi'(0) = 0$. $\square$

Hoeffding's Inequality

- $X_1, X_2, \ldots, X_m$: independent r.v.s with $a_i \leq X_i \leq b_i \ \forall \ i$.
- $S_m = \sum_{i=1}^{m} X_i$.

For any $\epsilon > 0$,

$$\begin{aligned} P(S_m - E[S_m] \geq \epsilon) &\leq e^{-\frac{2\epsilon^2}{\sum_{i=1}^{m}(b_i - a_i)^2}}, \\ P(S_m - E[S_m] \leq -\epsilon) &\leq e^{-\frac{2\epsilon^2}{\sum_{i=1}^{m}(b_i - a_i)^2}}. \end{aligned}$$

Proof. For any $t > 0$,

$$
\begin{aligned}
& P(S_m - E[S_m] \geq \epsilon) \\
\leq \quad & e^{-t\epsilon} E\left[e^{t(S_m - E[S_m])}\right] \text{ by Chernoff bound} \\
= \quad & e^{-t\epsilon} \prod_{i=1}^{m} E\left[e^{t(X_i - E[X_i])}\right] \text{ since } X_i\text{'s are independent} \\
\leq \quad & e^{-t\epsilon} \prod_{i=1}^{m} e^{t^2((b_i - E[X_i]) - (a_i - E[X_i]))^2/8} \text{ by Azuma-Hoeffding lemma} \\
= \quad & e^{-t\epsilon} e^{t^2 \sum_{i=1}^{m} (b_i - a_i)^2/8}.
\end{aligned}
$$

Since the function $e^{-t\epsilon} e^{t^2 \sum_{i=1}^{m} (b_i - a_i)^2/8}$ of $t > 0$ has the minimum value $-\frac{2\epsilon^2}{\sum_{i=1}^{m}(b_i - a_i)^2}$ at $t = 4\epsilon / \sum_{i=1}^{m}(b_i - a_i)^2$, we have

$$
P(S_m - E[S_m] \geq \epsilon) \leq e^{-\frac{2\epsilon^2}{\sum_{i=1}^{m}(b_i - a_i)^2}}.
$$

The other inequality can be obtained by a similar argument. $\square$

A Relation Between True Error And Empirical Error

Corollary 2.1: Let

- $c : \mathscr{I} \to \{0, 1\}$: a fixed but unknown target concept.
- $h : \mathscr{I} \to \{0, 1\}$: an arbitrary hypothesis.
- $S = (\omega_1, \ldots, \omega_m)$: a sample drawn i.i.d. from the population $\mathscr{I}$.

For any $\epsilon > 0$,

$$\begin{aligned} P_m(\hat{R}_S(h) - R(h) > \epsilon) &< e^{-2m\epsilon^2}, \\ P_m(\hat{R}_S(h) - R(h) < -\epsilon) &< e^{-2m\epsilon^2}. \end{aligned}$$

And by union bound,

$$P_m(|\hat{R}_S(h) - R(h)| > \epsilon) < 2e^{-2m\epsilon^2}.$$

Proof. Since the empirical error of h is

$$\hat{R}_S(h) = \frac{1}{m}\sum_{i=1}^{m} L(h(\omega_i), c(\omega_i)),$$

$m\hat{R}_S(h)$ is a sum of m i.i.d. r.v.s $L(h(\omega_i), c(\omega_i))$ with $E[m\hat{R}_S(h)] = mR(h)$. and $0 \le L(h(\omega_i), c(\omega_i)) \le 1$, $1 \le i \le m$. For any $\epsilon > 0$,

$$\begin{aligned} P_m(m\hat{R}_S(h) - mR(h) > m\epsilon) &< e^{-2(m\epsilon)^2/\sum_{i=1}^{m}(1-0)^2} = e^{-2m\epsilon^2}, \\ P_m(m\hat{R}_S(h) - mR(h) < -m\epsilon) &< e^{-2(m\epsilon)^2/\sum_{i=1}^{m}(1-0)^2} = e^{-2m\epsilon^2}, \end{aligned}$$

which are the first two inequalities. Also

$$\begin{aligned} & P_m(|\hat{R}_S(h) - R(h)| > \epsilon) \\ = \; & P_m((\hat{R}_S(h) - R(h) > \epsilon) \cup (\hat{R}_S(h) - R(h) < -\epsilon)) \\ \le \; & P_m(\hat{R}_S(h) - R(h) > \epsilon) + P_m(\hat{R}_S(h) - R(h) < -\epsilon) < 2e^{-2m\epsilon^2} \end{aligned}$$

by union bound. $\square$

Generalization Bound - Single Hypothesis

Corollary 2.2: Let

- $c : \mathscr{I} \to \{0, 1\}$: a fixed but unknown target concept.
- $h : \mathscr{I} \to \{0, 1\}$: an arbitrary hypothesis.
- $S = (\omega_1, \ldots, \omega_m)$: a sample of size m drawn i.i.d. from the population $\mathscr{I}$.

For any $\delta > 0$, with probability at leat $1 - \delta$,

$$R(h) \leq \hat{R}_S(h) + \sqrt{\frac{\ln \frac{2}{\delta}}{2m}}.$$

Proof. Setting $\delta = 2e^{-2m\epsilon^2}$ and solving $\epsilon = \sqrt{\frac{\ln\frac{2}{\delta}}{2m}}$ in Corollary 2.1, we have

$$P_m\left(|R(h) - \hat{R}_S(h)| > \sqrt{\frac{\ln\frac{2}{\delta}}{2m}}\right) < \delta.$$

Thus with probability at least $1 - \delta$,

$$|R(h) - \hat{R}_S(h)| \le \sqrt{\frac{\ln\frac{2}{\delta}}{2m}},$$

which implies

$$R(h) \le \hat{R}_S(h) + \sqrt{\frac{\ln\frac{2}{\delta}}{2m}}.$$

$\square$

Applicable to Learning Algorithm?

- Can we apply that bound to the hypothesis h_S returned by a learning algorithm when training on an i.i.d. sample S ?
- No, because h_S is a random hypothesis, depending on the training sample S.
- Note also that the generalization error $R(h_S)$ of the returned hypothesis h_S is a random variable.
- We need a bound that holds simultaneously for all hypotheses, a uniform generalization bound.

Uniform Generalization Bound - Finite Hypothesis Set

Theorem 2.2: Let

- $c : \mathscr{I} \to \{0, 1\}$: a fixed but unknown target concept.
- $\mathcal{H}$: the hypothesis set, consisting of finitely many hypotheses $h : \mathscr{I} \to \{0, 1\}$.
- $S = (\omega_1, \ldots, \omega_m)$: a sample of size m drawn i.i.d. from the population $\mathscr{I}$.

For any $\delta > 0$, with probability at leat $1 - \delta$,

$$\forall\ h \in \mathcal{H}, \quad R(h) \leq \hat{R}_S(h) + \sqrt{\frac{\ln |\mathcal{H}| + \ln \frac{2}{\delta}}{2m}}.$$

Proof. For any $\epsilon > 0$,

$$\begin{aligned} & P_m(\max_{h \in \mathcal{H}} |R(h) - \hat{R}_S(h)| > \epsilon) \\ = \quad & P_m(\cup_{h \in \mathcal{H}} (|R(h) - \hat{R}_S(h)| > \epsilon)) \\ \leq \quad & \sum_{h \in \mathcal{H}} P_m(|R(h) - \hat{R}_S(h)| > \epsilon) \text{ by union bound} \\ < \quad & 2|\mathcal{H}|e^{-2m\epsilon^2} \text{ by Corollary 2.1.} \end{aligned}$$

Setting $\delta = 2|\mathcal{H}|e^{-2m\epsilon^2}$ and solving $\epsilon = \sqrt{\frac{\ln|\mathcal{H}| + \ln\frac{2}{\delta}}{2m}}$, we have

$$P_m\left(\max_{h \in \mathcal{H}} |R(h) - \hat{R}_S(h)| > \sqrt{\frac{\ln|\mathcal{H}| + \ln\frac{2}{\delta}}{2m}}\right) < \delta.$$

Thus with probability at least $1 - \delta$,

$$\forall\ h \in \mathcal{H}, \ \ |R(h) - \hat{R}_S(h)| \leq \sqrt{\frac{\ln|\mathcal{H}| + \ln\frac{2}{\delta}}{2m}},$$

which implies

$$\forall\ h \in \mathcal{H}, \quad R(h) \leq \hat{R}_S(h) + \sqrt{\frac{\ln |\mathcal{H}| + \ln \frac{2}{\delta}}{2m}}.$$

$\square$

Remarks

- Equivalently, for any $\epsilon > 0, \delta > 0$,

$$P_m(\max_{h \in \mathcal{H}} |R(h) - \hat{R}_S(h)| \leq \epsilon) \geq 1 - \delta,$$

provided that the sample size $m \geq \frac{1}{2\epsilon^2}\left(\ln|\mathcal{H}| + \ln \frac{2}{\delta}\right)$.

- The uniform generalization bound $\hat{R}_S(h) + \sqrt{\frac{\ln|\mathcal{H}| + \ln\frac{2}{\delta}}{2m}}$ suggests seeking a trade-off between reducing the empirical error versus controlling the size of the hypothesis set.
  - A larger hypothesis set is penalized by the second term but could help reduce the empirical error, that is the first term.
  - Occam's Razor principle (law of parsimony): the simplest explanation is best. Thus if all other things being equal (a similar empirical error), a simpler (smaller) hypothesis set is better.

- The uniform generalization bound is in $O(\sqrt{\frac{\ln|\mathcal{H}|}{m}})$, not in $O(\frac{\ln|\mathcal{H}|}{m})$.

Agnostic PAC-Learning

- Definition: A concept class $\mathcal{C}$ is agnostically PAC-learnable if there exists a learning algorithm $\mathbb{A}$, which returns $h_S \in \mathcal{H}$ to approximate an unknown target concept $c \in C$ on a labeled sample S of size m,

$$h_S = \mathbb{A}(S; c, \mathcal{H}),$$

such that for any $\epsilon > 0$, $\delta > 0$, $c \in \mathcal{C}$ and P, we have

$$P_m(R(h_S) - R_H^* \leq \epsilon) \geq 1 - \delta,$$

provided that the sample size m is

$$m \geq \text{poly}(1/\epsilon, 1/\delta, n, \text{size}(c))$$

for a fixed polynomial, where

  - $O(n)$: cost of computational representation of an item ω.

- $O(\text{size}(c))$: cost of computational representation of a c.

- When such an algorithm $\mathbb{A}$ exists, it is called an agnostic PAC-learning algorithm for $\mathcal{C}$.

Efficient Agnostic PAC-Learning

- Definition: A concept class $\mathcal{C}$ is efficiently agnostically PAC-learnable if
  - $\mathcal{C}$ is agnostically PAC-learnable by a learning algorithm $\mathbb{A}$,
  - $\mathbb{A}$ further runs in $\mathrm{poly}(1/\epsilon, 1/\delta, n, \mathrm{size}(c))$.
- When such an algorithm $\mathbb{A}$ exists, it is called an efficient agnostic PAC-learning algorithm for $\mathcal{C}$.

The Empirical Risk Minimization Algorithm $\mathbb{A}^{ERM}$

- $h_S^{ERM} = \mathbb{A}^{ERM}(S; c, \mathcal{H}) = \arg\min_{h\in\mathcal{H}} \hat{R}_S(h)$.
- The estimation error is

$$\begin{aligned} R(h_S^{ERM}) - R_H^* &= R(h_S^{ERM}) - \hat{R}_S(h_S^{ERM}) + \hat{R}_S(h_S^{ERM}) - R_H^* \\ &\leq R(h_S^{ERM}) - \hat{R}_S(h_S^{ERM}) + \hat{R}_S(h^*) - R(h^*) \\ &\leq 2 \sup_{h\in\mathcal{H}} |R(h) - \hat{R}_S(h)|. \end{aligned}$$

- Application of the uniform generalization bound in Theorem 2.2.
- The ERM algorithm $\mathbb{A}^{ERM}$ with a finite hypothesis set $\mathcal{H}$ is an agnostic PAC-learning algorithm for any concept class $\mathcal{C}$.