Theory of Generalization

FACT

△ with distribution in training data & testing data

⇒ low training error $\not\Leftrightarrow$ low testing error

Def

△ Training error :

- $E_{tr}(h) = \frac{1}{N}\sum_{n=1}^{N} e(h(x_n), f(x_n))$

  where $x_1, \ldots x_N$ sampled from D
- h is determined by $x_1 \ldots x_N$

△ Testing error :

- $E_{te}(h) = \frac{1}{N}\sum_{n=1}^{N} e(h(x_n), f(x_n))$

  where $x_1, \ldots x_N$ sampled from D
- h is independent from $x_1, \ldots x_N$

△ Generalization error

- G. error = Test error (expected performance on D)
- $E(h) = E_{x \sim D}\left[e(h(x), f(x)) \right] = E_{te}(h)$

△ summary

if $E(h) = 0$

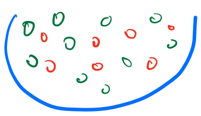
then $E(h) \approx E_{tr}(h)$ ⟶ How?

&

$E_{tr}(h) \approx 0$ ⟶ Training

Q: How do we make sure $E(h) \approx E_{tr}(h)$

FACT Hoeffding's inequality



△ $P[$ pick red ball $] = \mu$

$P[$ pick green ball $] = 1 - \mu$

→ we DO NOT know μ

△ by pick ball's independently we get fraction of ν

△ $\nu \rightarrow \mu$?

perhaps

△ Hoeffding's inequality

$$P[\,|\nu - \mu| > \epsilon\,] \le 2e^{-2\epsilon^2 N}$$

annote : ν & μ 的差距，比 ϵ 大的P，很小

多小？ → 比 $2e^{-2\epsilon^2 N}$ 还小

△ statement $\mu = \nu$ is probably approximately correct

(PAC !)

FACT

△ $P[\,|\nu - \mu| > \epsilon\,] \le 2e^{-2\epsilon^2 N}$

- valid for N
- $\epsilon > 0$
- independent from μ (real probability)

△ in learning :

- given a function h
- we randomly draw $x_1, \ldots, x_n$

independent

- generalization error

  $E(h) = E_{x \sim D}\left[h(x) \neq f(x) \right] \Leftrightarrow \mu$ unknown

  sample data error

  $E_{tr}(h) = \frac{1}{N}\sum_{n=1}^{N} [\, h(x_n) \neq y_n \,] \Leftrightarrow \nu$ known

$$P[\,|\nu - \mu| > \epsilon\,] \le 2e^{-2\epsilon^2 N}$$

FACT

△ for each h, h is a hypothesis

$$P[\,|E_{tr}(h) - E(h)| > \epsilon\,] \le 2e^{-2\epsilon^2 N}$$

△ for all h, $\mathcal{H}$ is a hypothesis set

$P[\,|E_{tr}(h_1) - E(h_1)| > \epsilon\,]$,

$P[\,|E_{tr}(h_2) - E(h_2)| > \epsilon\,]$,

⋮

$P[\,|E_{tr}(h_{|\mathcal{H}|}) - E(h_{|\mathcal{H}|})| > \epsilon\,]$

$\le P[\sup_{h \in \mathcal{H}} |E_{tr}(h) - E(h)| > \epsilon]$

$\le \sum_{m=1}^{|\mathcal{H}|} P[\,|E_{tr}(h_m) - E(h_m)|\,] \le 2|\mathcal{H}|\, e^{-2\epsilon^2 N}$

from $P(\bigcup_{i=1}^{\infty} A_i) \le \sum_{i=1}^{\infty} P(A_i)$

△ summary

$$P[\,|E_{tr}(h) - E(h)| > \epsilon\,] \le P[\sup_{h \in \mathcal{H}} |E_{tr}(h) - E(h)| > \epsilon] \le 2|\mathcal{H}| e^{-2\epsilon^2 N}$$

NOTE More on Hoeffding's inequality

	D_1	D_2	…	D_N	
h_1	Bad			Bad	P_D[BAD D for h_1] ≤ …
h_2		Bad			P_D[BAD D for h_2] ≤ …
⋮					…
h_M	Bad			Bad	P_D[BAD D for h_M] ≤ …

inforced hypothesis (假設現在我認定的模型 i.e., 不是學出來的) → 對拿到我手上的資料 $D_1, D_2 \dots D_N$, inforced 的 h on D 可能導致 "Bad" 亦即 $E_{in}(h) \neq E_{out}(h)$ → 之所以要 Hoeffding's ineq. 就是為了量化 P[Bad] 机率多高?

→ 答案是很低: bounded by $2e^{-2\epsilon^2 N}$ → 不過剛剛是1個h啊… 我algo都是在 $\mathcal{H}$ 找h… upper bound是啥?

∴ P_D[BAD D]

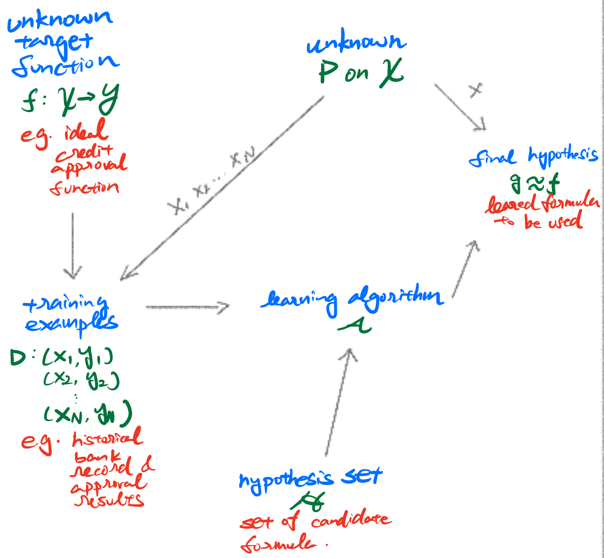
= P_D[BAD D for h_1 or BAD D for h_2 … or BAD D for h_M]

≤ P_D[BAD D for h_1] + P_D[BAD D for h_2] + … + P_D[BAD D for h_M]
(union bound)

≤ $2M e^{-2\epsilon^2 N} = 2|\mathcal{H}| e^{-2\epsilon^2 N}$

- finite-bin version of Hoeffding
- & hope… $E_{in}(g) = E_{out}(g)$ is PAC.
  → $\mathcal{A}$ will pick h_m w/ min. $E_{in}(h_m)$ as g

△ summary: statistical learning flow



& hope $E_{out}(g) \approx E_{in}(g) \approx 0$
(test) (train)

- for batch & supervised learning, $g \approx f \Leftrightarrow E_{out}(g) \approx 0$
  achieved through $E_{out}(g) \approx E_{in}(g)$ & $E_{in}(g) \approx 0$
  ① can we make sure $E_{out}(g) \approx E_{in}(g)$
  ② can we make $E_{in}(g)$ small enough

FACT $|\mathcal{H}| = \infty$

△ Question: How do we deal with it?

- small $|\mathcal{H}|$
  $P[BAD] \le 2|\mathcal{H}| e^{-2\epsilon^2 N}$
  small! great!
  but $|\mathcal{H}|$ too little
  $E_{in}(g)$ ↑
- large $|\mathcal{H}|$
  $E_{in}(g) \to 0$
  small error! great!
  but $|\mathcal{H}|$ too large
  P[BAD] ↑

FACT establish a finite quantity replace $|\mathcal{H}|$

let $|\mathcal{H}|$ replaced by $m_{\mathcal{H}}$
s.t.

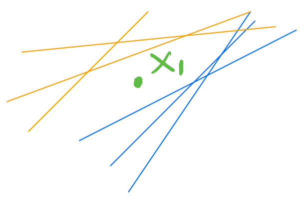
$$P[|E_{in}(g) - E_{out}(g)| > \epsilon] \le 2 m_{\mathcal{H}} e^{-2\epsilon^2 N}$$

FACT $|\mathcal{H}|$ is over-estimated for BAD events

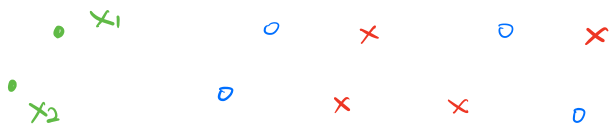
- BAD events B_m: $|E_{in}(h_m) - E_{out}(h_m)| > \epsilon$
- over-lapping for similar hypothesis $h_1 \approx h_2$
- as ① $E_{out}(h_1) \approx E_{out}(h_2)$
  ② for most D $E_{in}(h_1) \approx E_{out}(h_2)$
- should be instead of

- so: can we group similar kinds?

e.g. $\mathcal{H}$ in R^2 $|\mathcal{H}| \to \infty$



→ $|\mathcal{H}| = 2$



↓

$|\mathcal{H}| = 4$

⋮

N = 3 $|\mathcal{H}| = 8$ but if on same line, different
N = 4 $|\mathcal{H}| = 14$ but if on same line, differen

FACT observation: effective $|\mathcal{H}| \le 2^N$
perhaps can replace $|\mathcal{H}|$ by effective $|\mathcal{H}|$?
need more rigorous proof

FACT Dichotomies: mini-hypotheses

△ limited hypothesis: $\mathcal{H}(x_1, x_2 \dots x_N)$

△ $|\mathcal{H}(x_1, x_2, \dots, x_N)|$: depend on inputs $(x_1, x_2 \dots, x_N)$

△ growth function:
remove dependence by taking max of all possible $(x_1, x_2, \dots, x_N)$

$$m_{\mathcal{H}}(N) = \max_{x_1, x_2 \dots x_N \in X} |H(x_1, x_2 \dots x_n)|$$

△ finite, upper-bounded by 2^N

Q: How to calculate growth function

FACT shattered

- △ if $m_{\mathcal{H}}(N) = 2^N \Leftrightarrow$ exists N inputs that can be shattered

- △ eg. convex set

FACT summary of 4 growth function

- positive rays $N+1$
- positive intervals $C_2^{N+1}+1$
- convex sets 2^N
- 2D perceptrons $< 2^N$

polynomial good !

exponential bad !

FACT Break point ⤳ k 開始,無法被 shattered

- △ if no k inputs can be shattered by $\mathcal{H}$ call k a break point for $\mathcal{H}$

- △ $m_{\mathcal{H}}(k) < 2^k$
- △ k+1, k+2, k+3 ... are all break points
- △ study minimum break point

eg linear case break point $k=4$

note: 4 个無法被 shattered

FACT conjecture:

- △ no break point : $m_H(N) = 2^N$
- △ break point k : $m_{\mathcal{H}}(N) = O(N^{k-1})$

proof ?

FACT $m_{\mathcal{H}}(N) \leq$ maximum possible $m_{\mathcal{H}}(N)$ given k

$\leq$ poly (N)

FACT Bounding function