Machine Learning

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Lecture 5: VC Theory - Generalization

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5.1 Review

As for the case where $|\mathcal{F}| = \infty$, note that we have:

$$P(\exists f \in \mathcal{F} \ P_D(Y \neq f(x)) - \frac{1}{n} \sum_{i=1}^n \mathbb{1}[Y_i \neq f(x_i)] \ge \epsilon)$$

$$\leq 2P(\exists f \in \mathcal{F} \ \frac{1}{n} \sum_{i=1}^n \mathbb{1}[Y_i \neq f(x_i)] - \frac{1}{n} \sum_{i=n+1}^{2n} \mathbb{1}[Y_i \neq f(x_i)] \ge \frac{\epsilon}{2}) \quad \text{(Double Sample Trick)}$$

$$= 2E_{x_1y_1, \dots, x_ny_n} \{ P_{\sigma \in S_{in}} (\exists f \in \mathcal{F} \ \frac{1}{n} \sum_{i=1}^n \mathbb{1}[Y_{\sigma(i)} \neq f(X_{\sigma(i)}] - \dots \ge \frac{\epsilon}{2}) \} \le N(2n)c_1 e^{-c_2n\epsilon^2} \quad \text{(Symmetrization)}$$

$$(5.1)$$

We define:

$$N^{\mathcal{F}}(x_1, y_1, \cdots, x_n, y_n) := |\{(f(x_1), f(x_2), \cdots, f(x_n)) : f \in \mathcal{F}\}|, \quad f(x_i) \in \{0, 1\}$$
(5.2)

$$N^{\Phi}(\delta_1, \cdots, \delta_n) := |\{(\phi_f(\delta_1), \cdots, \phi(\delta_n)) : \phi_f \in \Phi\}|, \text{ where } \delta_i = (x_i, y_i), \phi_f(\delta_i) = I[f(x_i) \neq y_i]$$
(5.3)

$$N^{\mathcal{F}}(n) := \max_{x_1, y_1, \dots, x_n, y_n} N^{\mathcal{F}}(x_1, y_1, \dots, x_n, y_n)$$
(5.4)

$$N^{\Phi}(n) = \max_{\delta_1, \cdots, \delta_n} N^{\Phi}(\delta_1, \dots, \delta_n)$$
(5.5)

where Φ is a set of indicator functions. (Note that these two sets are same in size) From the last lecture we have known that When n grows past some threshold (say d), the expressiveness of Φ will fall short. So we speculate that

$$N^{\Phi}(n) \begin{cases} = 2^{n}, & n \le d \\ \le \sum_{k=0}^{d} {n \choose k} = O(n^{d}), n > d \end{cases}$$
(5.6)

$$|\{(\phi(y_1) \to n_1, \dots, \phi(y_n) \to n_n) : \phi \in \Phi\}| \le \sum_{k=0}^d \binom{n}{k}$$
(5.7)

We have to proof the following inequality:

$$N^{\Phi}(n) \le \sum_{k=0}^{d} \binom{n}{k} \quad for \quad n > d$$
(5.8)

Proof for Inequality(5.8)5.2

Let's consider the special case first— From our assumption, we know that when d+1, there is a case of

$$(\phi(x_1), \phi(x_2), \dots, \phi(x_n)) \tag{5.9}$$

that cannot be obtained. In this special case, we assume that we cannot obtain d+1-zero cases. Which means that we can only have at most d zeros in this equation. There are totally

$$\sum_{k=0}^{d} \binom{n}{k} \tag{5.10}$$

possible value assignments that have less than d+1 zeros.

Special cases are limited, so consider turning general cases into special cases. We will give the complete proof next.

Proof: First, we list all the situations that cannot be obtained and consider what happen at 1-st component. There are three possibility,

0 as 1-st component, eg:

$$\begin{cases} 0, *, 1 \cdots & nbits \\ 0, 1, * \cdots & \\ \cdots & \\ 0, 0, * \cdots & \end{cases}$$
1 as 1-st component, eg:
$$\begin{cases} 1, *, 1 \cdots & \\ 1, 1, * \cdots & \\ \cdots & \\ 1, 0, * \cdots & \\ 1, 0, * \cdots & \\ &$$

1 as 1-st component, eg:

If we turn the 1 at 1-st component into 0, we will find that all possibilities are reduced.

Similarly, if we turn 1 into 0 at any component, we will find that all possibilities are reduced.

Therefore, if we turn 1 into 0 at all components, all possibilities will be reduced to a special case where only d+1 zeros cannot be obtained. So the possibilities of being able to obtain is more than that of the special case.

In this special case, the number of 0 can be 0, 1, ..., d. So we have $N^{\Phi}(n) \leq \sum_{k=0}^{d} {n \choose k}$

$$\sum_{k=0}^{d} \binom{n}{k} \le \left(\frac{en}{d}\right)^d \tag{5.11}$$

Apply Chernoff bound and assume $d < \frac{n}{2}$

5.3 Step 3: VC Dimension

Definition 5.1 (VC Dimension) The VC Dim of a set Φ of indicator function is the maximum n, so that $N^{\Phi}(n) = 2^n$

Then, for any indicator function set Φ , if $VCD(\Phi) = d < \infty$ then

$$N^{\Phi}(n) \begin{cases} = 2^{n}, & n \le d \\ \le \sum_{k=0}^{d} {n \choose k} \le {(\frac{en}{d})^{d}}, n > d \end{cases}$$
(5.12)

5.4 Step 1,2,3

$$P(\exists f \in \mathcal{F} : P_D(Y \neq f(x)) - \frac{1}{n} \sum I[Y_i \neq f(x_i)] \ge \epsilon)$$

$$\leq N^{\Phi}(2n) \cdot c_1 e^{-c_2 n \epsilon^2}$$

$$\leq (\frac{2en}{d})^d c_1 \cdot e^{-c_2 n \epsilon^2}$$
(5.13)

Theorem 5.2 Let $\delta = (\frac{2en}{d})^d * 4e^{-\frac{1}{2}ne^2}$ then we have with prob. at $1 - \delta$ (over the random draw of the training dataset S).

$$P_D(Y \neq f(X)) \le P_S[Y \neq f(X)] + O(\sqrt{\frac{d\ln n + \ln \frac{1}{\delta}}{n}})$$
(5.14)

holds true for all $f \in \mathcal{F}$ simultanously, where d is the VC dimension of the hypothesis space \mathcal{F} , where $P_S[Y \neq f(X)] := \frac{1}{n} \sum I[Y_i \neq f(x_i)].$

Linear classifiers in \mathcal{R}^d

$$\mathcal{F} := \{ sgn(w^T x + b), w \in \mathcal{R}^d, b \in \mathcal{R} \}$$
(5.15)

then,

$$VCD(\mathcal{F}) = d + 1 \tag{5.16}$$

Proof: Let $x_1 = (1, 0, ..., 0), x_2 = (0, 1, ..., 0), x_d = (0, 0, ..., 1), x_{d+1} = (0, 0, ..., 0) \in \mathbb{R}^d$. They can represent any set in which d points are independent, cause $(x_1, ..., x_d)$ is a set of base in \mathbb{R}^d . Or we can discuss this Linear classification problem in \mathbb{R}^{d-1} . Then we have:

$$N^{\mathcal{F}}(x_1, ..., x_{d+1}) = |\{(f(x_1), ..., f(x_{d+1}) | f \in \mathcal{F}\}|$$

= |\{(sgn(w_1 + b), ..., sgn(w_d + b), sgn(b)) | w \in \mathcal{R}^d, b \in \mathcal{R}\}| (5.17)
= 2^{d+1}

Thus $VCD(\mathcal{F}) \ge d + 1$. Next we need to prove $VCD(\mathcal{F}) < d + 2$: $\forall x_1, ..., x_{d+2} \in \mathcal{R}^d, (x_1, 1), ..., (x_{d+2}, -1), \exists c_1, ..., c_{d+1}, s.t.$

$$w^{T}x_{d+2} + b = \sum_{i=1}^{d+1} c_{i}(w^{T}x_{i} + b), \forall w \in \mathcal{R}^{d}$$
(5.18)

Assuming that $(sgn(c_1), ..., sgn(c_{d+1}), -1) \in \{(f(x_1), ..., f(x_{d+2}) | f \in \mathcal{F}\}$. Then $\exists f \in \mathcal{F}$, that is $\exists w \in \mathcal{R}^d, b \in \mathcal{R}$, s.t. $sgn(c_i) = sgn(w^T x_i + b)$ and $sgn(w^T x_i + b) = -1$, which is contradict to 5.18.

Thus $(sgn(c_1), ..., sgn(c_{d+1}), -1) \notin \{(f(x_1), ..., f(x_{d+2}) | f \in \mathcal{F}\}, \forall f \in \mathcal{F}, \text{ so } VCD(\mathcal{F}) < d+2.$ So we have proved $VCD(\mathcal{F}) = d+1$

References

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 - [F76] M. L. FREDMAN, New Bounds on the Complexity of the Shortest Path Problem, SIAM Journal on Computing 5 (1976), pp. 83-89.