## Machine Learning

## Lecture 5: VC Theory - Generalization

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### 5.1 Review

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

$$
\begin{align*}
& P\left(\exists f \in \mathcal{F} \quad P_{D}(Y \neq f(x))-\frac{1}{n} \Sigma_{i=1}^{n} 1\left[Y_{i} \neq f\left(x_{i}\right)\right] \geq \epsilon\right) \\
\leq & 2 P\left(\exists f \in \mathcal{F} \quad \frac{1}{n} \sum_{i=1}^{n} 1\left[Y_{i} \neq f\left(x_{i}\right)\right]-\frac{1}{n} \Sigma_{i=n+1}^{2 n} 1\left[Y_{i} \neq f\left(x_{i}\right)\right] \geq \frac{\epsilon}{2}\right) \quad \text { (Double Sample Trick) } \\
= & 2 E_{x_{1} y_{1}, \cdots, x_{n} y_{n}}\left\{P_{\sigma \in S_{i n}}\left(\exists f \in \mathcal{F} \quad \frac{1}{n} \Sigma_{i=1}^{n} 1\left[Y_{\sigma(i)} \neq f\left(X_{\sigma(i)}\right]-\cdots \geq \frac{\epsilon}{2}\right)\right\} \leq N(2 n) c_{1} e^{-c_{2} n \epsilon^{2}}\right. \tag{Symmetrization}
\end{align*}
$$

We define:

$$
\begin{gather*}
N^{\mathcal{F}}\left(x_{1}, y_{1}, \cdots, x_{n}, y_{n}\right):=\left|\left\{\left(f\left(x_{1}\right), f\left(x_{2}\right), \cdots, f\left(x_{n}\right)\right): f \in \mathcal{F}\right\}\right|, \quad f\left(x_{i}\right) \in\{0,1\}  \tag{5.2}\\
N^{\Phi}\left(\delta_{1}, \cdots, \delta_{n}\right):=\left|\left\{\left(\phi_{f}\left(\delta_{1}\right), \cdots, \phi\left(\delta_{n}\right)\right): \phi_{f} \in \Phi\right\}\right|, \text { where } \delta_{i}=\left(x_{i}, y_{i}\right), \phi_{f}\left(\delta_{i}\right)=I\left[f\left(x_{i}\right) \neq y_{i}\right]  \tag{5.3}\\
N^{\mathcal{F}}(n):=\max _{x_{1}, y_{1}, \ldots, x_{n}, y_{n}} N^{\mathcal{F}}\left(x_{1}, y_{1}, \ldots, x_{n}, y_{n}\right)  \tag{5.4}\\
N^{\Phi}(n)=\max _{\delta_{1}, \cdots, \delta_{n}} N^{\Phi}\left(\delta_{1}, \ldots, \delta_{n}\right) \tag{5.5}
\end{gather*}
$$

where $\Phi$ 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 $\Phi$ will fall short. So we speculate that

$$
\begin{gather*}
N^{\Phi}(n)\left\{\begin{array}{cc}
=2^{n}, & n \leq d \\
\leq \sum_{k=0}^{d}\binom{n}{k}=O\left(n^{d}\right), & n>d
\end{array}\right.  \tag{5.6}\\
\left|\left\{\left(\phi\left(y_{1}\right) \rightarrow n_{1}, \ldots, \phi\left(y_{n}\right) \rightarrow n_{n}\right): \phi \in \Phi\right\}\right| \leq \sum_{k=0}^{d}\binom{n}{k} \tag{5.7}
\end{gather*}
$$

We have to proof the following inequality:

$$
\begin{equation*}
N^{\Phi}(n) \leq \sum_{k=0}^{d}\binom{n}{k} \quad \text { for } \quad n>d \tag{5.8}
\end{equation*}
$$

### 5.2 Proof for Inequality(5.8)

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

$$
\begin{equation*}
\left(\phi\left(x_{1}\right), \phi\left(x_{2}\right), \ldots, \phi\left(x_{n}\right)\right) \tag{5.9}
\end{equation*}
$$

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

$$
\begin{equation*}
\sum_{k=0}^{d}\binom{n}{k} \tag{5.10}
\end{equation*}
$$

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:

$$
\left\{\begin{array}{l}
0, *, 1 \cdots \\
0,1, * \cdots \\
\cdots \\
0,0, * \cdots
\end{array}\right.
$$

1 as 1-st component, eg:

$$
\left\{\begin{array}{l}
1, *, 1 \cdots \\
1,1, * \cdots \\
\cdots \\
1,0, * \cdots
\end{array}\right.
$$

no restriction as 1-st component, eg:

$$
\left\{\begin{array}{l}
*, *, 1 \cdots \\
*, 1, * \cdots \\
\cdots \\
*, 0, * \cdots
\end{array}\right.
$$

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 $0,1, \cdots$, d. So we have $N^{\Phi}(n) \leq \sum_{k=0}^{d}\binom{n}{k}$

$$
\begin{equation*}
\sum_{k=0}^{d}\binom{n}{k} \leq\left(\frac{e n}{d}\right)^{d} \tag{5.11}
\end{equation*}
$$

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 $\Phi$ of indicator function is the maximum n, so that $N^{\Phi}(n)=2^{n}$

Then, for any indicator function set $\Phi$, if $V C D(\Phi)=d<\infty$ then

$$
N^{\Phi}(n)\left\{\begin{array}{cr}
=2^{n}, & n \leq d  \tag{5.12}\\
\leq \sum_{k=0}^{d}\binom{n}{k} \leq\left(\frac{e n}{d}\right)^{d}, & n>d
\end{array}\right.
$$

### 5.4 Step 1,2,3

$$
\begin{align*}
P\left(\exists f \in \mathcal{F}: P_{D}(Y \neq f(x))-\frac{1}{n}\right. & \left.\sum I\left[Y_{i} \neq f\left(x_{i}\right)\right] \geq \epsilon\right) \\
\leq & N^{\Phi}(2 n) \cdot c_{1} e^{-c_{2} n \epsilon^{2}}  \tag{5.13}\\
\leq & \left(\frac{2 e n}{d}\right)^{d} c_{1} \cdot e^{-c_{2} n \epsilon^{2}}
\end{align*}
$$

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

$$
\begin{equation*}
P_{D}(Y \neq f(X)) \leq P_{S}[Y \neq f(X)]+O\left(\sqrt{\frac{d \ln n+\ln \frac{1}{\delta}}{n}}\right) \tag{5.14}
\end{equation*}
$$

holds true for all $f \in \mathcal{F}$ simultanously, where $d$ is the $V C$ dimension of the hypothesis space $\mathcal{F}$, where $P_{S}[Y \neq f(X)]:=\frac{1}{n} \sum I\left[Y_{i} \neq f\left(x_{i}\right)\right]$.

Linear classifiers in $\mathcal{R}^{d}$

$$
\begin{equation*}
\mathcal{F}:=\left\{\operatorname{sgn}\left(w^{T} x+b\right), w \in \mathcal{R}^{d}, b \in \mathcal{R}\right\} \tag{5.15}
\end{equation*}
$$

then,

$$
\begin{equation*}
V C D(\mathcal{F})=d+1 \tag{5.16}
\end{equation*}
$$

Proof: Let $x_{1}=(1,0, \ldots, 0), x_{2}=(0,1, \ldots, 0), x_{d}=(0,0, \ldots, 1), x_{d+1}=(0,0, \ldots, 0) \in \mathcal{R}^{d}$. They can represent any set in which $d$ points are independent, cause $\left(x_{1}, \ldots, x_{d}\right)$ is a set of base in $\mathcal{R}^{d}$. Or we can discuss this Linear classification problem in $\mathcal{R}^{d-1}$. Then we have:

$$
\begin{align*}
N^{\mathcal{F}}\left(x_{1}, \ldots, x_{d+1}\right) & =\mid\left\{\left(f\left(x_{1}\right), \ldots, f\left(x_{d+1}\right) \mid f \in \mathcal{F}\right\} \mid\right. \\
& =\left|\left\{\left(\operatorname{sgn}\left(w_{1}+b\right), \ldots, \operatorname{sgn}\left(w_{d}+b\right), \operatorname{sgn}(b)\right) \mid w \in \mathcal{R}^{d}, b \in \mathcal{R}\right\}\right|  \tag{5.17}\\
& =2^{d+1}
\end{align*}
$$

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

$$
\begin{equation*}
w^{T} x_{d+2}+b=\sum_{i=1}^{d+1} c_{i}\left(w^{T} x_{i}+b\right), \forall w \in \mathcal{R}^{d} \tag{5.18}
\end{equation*}
$$

Assuming that $\left(\operatorname{sgn}\left(c_{1}\right), \ldots, \operatorname{sgn}\left(c_{d+1}\right),-1\right) \in\left\{\left(f\left(x_{1}\right), \ldots, f\left(x_{d+2}\right) \mid f \in \mathcal{F}\right\}\right.$. Then $\exists f \in \mathcal{F}$, that is $\exists w \in \mathcal{R}^{d}, b \in$ $\mathcal{R}$, s.t. $\operatorname{sgn}\left(c_{i}\right)=\operatorname{sgn}\left(w^{T} x_{i}+b\right)$ and $\operatorname{sgn}\left(w^{T} x_{i}+b\right)=-1$, which is contradict to 5.18 .

Thus $\left(\operatorname{sgn}\left(c_{1}\right), \ldots, \operatorname{sgn}\left(c_{d+1}\right),-1\right) \notin\left\{\left(f\left(x_{1}\right), \ldots, f\left(x_{d+2}\right) \mid f \in \mathcal{F}\right\}, \forall f \in \mathcal{F}\right.$, so $\operatorname{VCD}(\mathcal{F})<d+2$. So we have proved $V C D(\mathcal{F})=d+1$

## References

[AGM97] N. Alon, Z. Galil and O. Margalit, On the Exponent of the All Pairs Shortest Path Problem, Journal of Computer and System Sciences 54 (1997), pp. 255-262.
[F76] M. L. Fredman, New Bounds on the Complexity of the Shortest Path Problem, SIAM Journal on Computing 5 (1976), pp. 83-89.

