CSCI699: Theory of Machine Learning

Fall 2021

Lecture 6: VC Theorem and Rademacher Complexity

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Today

- Finish VC Theorem proof
- Introduce Rademacher complexity

Last time, we introduced the Vapnik-Chervonenkis (VC) dimension and the VC Theorem. Today, we will finish its 4-step proof and introduce Rademacher complexity.

1 VC Theorem

Theorem 1 (VC Theorem). Let \mathcal{H} be a hypothesis class with $VCdim(\mathcal{H}) = d < \infty$. Then there is an absolute constant c > 0 such that \mathcal{H} has the uniform convergence property with,

$$n_{\mathcal{H}}^{VC}(\epsilon, \delta) = c \cdot \frac{d \cdot \log(d/\epsilon) + \log(1/\epsilon)}{\epsilon^2}.$$

Corollary 2. \mathcal{H} is agnostically-PAC learnable with $\mathcal{O}\left(\frac{d \cdot \log(d/\epsilon) + \log(1/\delta)}{\epsilon^2}\right)$ samples.

Proof. Theorem 1 Proof Outline:

- 1) For any set $C \subseteq \mathcal{X}$, the effective size of the restriction of \mathcal{H} on C, denoted \mathcal{H}_C , is approximately $|C|^d$ ($|\mathcal{H}_C| \approx |C|^d$).
- 2) This small "effective size" will be good for when using the union bound to get the VC theorem result.

Definition 3 (Restriction). The <u>restriction</u> of class \mathcal{H} to a set of examples $C = \{c_1, ..., c_n\} \in \mathcal{X}$ is a subset of $\{0,1\}^{|C|}$ given by $\mathcal{H}_C = \{(h(c_1), ..., h(c_n)) : \forall h \in \mathcal{H}\}.$

Step 1: Polynomial growth of \mathcal{H}_C .

We saw this in the last lecture, so here we will just re-state the definition of the growth function and Sauer's Lemma without re-proving it.

Definition 4 (Growth function). The growth function of \mathcal{H} , $\tau_{\mathcal{H}} : \mathbb{N} \to \mathbb{N}$, is defined as

$$\tau_{\mathcal{H}} = \max_{C \subseteq \mathcal{X}, |C| = n} |\mathcal{H}_C|.$$

Lemma 5 (Sauer's Lemma). $\forall n$, $VCdim(\mathcal{H}) = d$,

$$\tau_{\mathcal{H}}(n) \le \sum_{i=0}^{d} \binom{n}{i}.$$

For n > d + 1, this implies:

$$\tau_{\mathcal{H}}(n) \le \left(\frac{n \cdot e}{d}\right)^d.$$

Step 2: Symmetrization

Lemma 6. For a class \mathcal{H} with growth function $\tau_{\mathcal{H}}$,

$$\mathbb{E}_{S \sim \mathcal{D}^n} \left[\sup_{h \in \mathcal{H}} \left| R(h) - \hat{R}_S(h) \right| \right] \le \sqrt{\frac{2 \cdot \log(2 \cdot \tau_{\mathcal{H}}(2n))}{n}}.$$

Proof. (Lemma 6): We will use the idea of symmetrization.

Let $S' = \{(x'_i, y'_i), i \in [n]\}$ be a training set sample indentically distributed as S.

Note that
$$\mathbb{E}_{S'}\left[\hat{R}_{S'}(h)\right] = R(h)$$
.

Therefore,

$$\mathbb{E}_{S} \left[\sup_{h \in \mathcal{H}} \left| R(h) - \hat{R}_{S}(h) \right| \right] = \mathbb{E}_{S} \left[\sup_{h \in \mathcal{H}} \left| \mathbb{E}_{S'} \left[\hat{R}_{S'}(h) \right] - \hat{R}_{S}(h) \right| \right]. \tag{1}$$

Now, fix S.

Claim 7.
$$\sup_{h \in \mathcal{H}} \left| \mathbb{E}_{S'} \left[\hat{R}_{S'}(h) \right] \right| \leq \mathbb{E}_{S'} \sup_{h \in \mathcal{H}} \left| \hat{R}_{S'}(h) \right|.$$

Proof. (Claim 7):

This follows from the fact that $|\cdot|$ is a convex function, and \sup / \max of convex functions is convex.

Therefore, $\sup_{h\in\mathcal{H}}\left|\mathbb{E}_{S'}\left[\hat{R}_{S'}(h)\right]\right|$ is a convex function of $\hat{R}_{S'}(h)$.

By applying Jensen's inequality $(f(\mathbb{E}(X)) \leq \mathbb{E}(f(x)))$ if f convex), the claim follows.

Using Claim 7 and combining with Eq. 1 and pulling the expectation out, we have

$$\mathbb{E}_{S} \left[\sup_{h \in \mathcal{H}} \left| R(h) - \hat{R}_{S}(h) \right| \right] \leq \mathbb{E}_{S,S'} \left[\sup_{h \in \mathcal{H}} \left| \hat{R}_{S'}(h) - \hat{R}_{S}(h) \right| \right]$$

$$= \mathbb{E}_{S,S'} \left[\sup_{h \in \mathcal{H}} \left| \frac{1}{n} \sum_{i=1}^{n} \left(\mathbb{I} \{ h(x'_{i}) \neq y'_{i} \} - \mathbb{I} \{ h(x_{i}) \neq y_{i} \} \right) \right| \right].$$

Now, let $\sigma_{1:n} = \{\sigma_1, ..., \sigma_n\}$ be independent Rademacher random variables, i.e. $\sim \text{Unif}(\{\pm 1\})$. Since $(x_i, y_i), (x_i', y_i')$ are i.i.d.,

$$\mathbb{1}\{h(x_i') \neq y_i'\} - \mathbb{1}\{h(x_i) \neq y_i\} \sim \mathbb{1}\{h(x_i) \neq y_i\} - \mathbb{1}\{h(x_i') \neq y_i'\}.$$

Therefore,

$$\mathbb{E}_{S}\left[\sup_{h\in\mathcal{H}}\left|R(h)-\hat{R}_{S}(h)\right|\right] \leq \mathbb{E}_{\sigma_{1:n}}\mathbb{E}_{S,S'}\sup_{h\in\mathcal{H}}\left|\frac{1}{n}\sum_{i=1}^{n}\sigma_{i}\left(\mathbb{1}\{h(x'_{i})\neq y'_{i}\}-\mathbb{1}\{h(x_{i})\neq y_{i}\}\right)\right|$$

$$=\mathbb{E}_{S,S'}\mathbb{E}_{\sigma_{1:n}}\sup_{h\in\mathcal{H}}\left|\frac{1}{n}\sum_{i=1}^{n}\sigma_{i}\left(\mathbb{1}\{h(x'_{i})\neq y'_{i}\}-\mathbb{1}\{h(x_{i})\neq y_{i}\}\right)\right|.$$

Now fix both S, S' and let C be the set of examples appearing in $S \cup S'$ (both of them). Note that $|C| \leq 2n$ as there can be some overlap between S, S'.

The key idea here is that we can replace the supremem over the (possibly infinite) set \mathcal{H} by the maximum over the discrete restriction \mathcal{H}_C , as all possible labelings for all training examples from both S, S' are included in \mathcal{H}_C . Thus,

$$\mathbb{E}_{S} \left[\sup_{h \in \mathcal{H}} \left| R(h) - \hat{R}_{S}(h) \right| \right] \leq \mathbb{E}_{S,S'} \mathbb{E}_{\sigma_{1:n}} \sup_{h \in \mathcal{H}} \left| \frac{1}{n} \sum_{i=1}^{n} \sigma_{i} \left(\mathbb{1} \left\{ h(x'_{i}) \neq y'_{i} \right\} - \mathbb{1} \left\{ h(x_{i}) \neq y_{i} \right\} \right) \right|$$

$$= \mathbb{E}_{S,S'} \mathbb{E}_{\sigma_{1:n}} \max_{h \in \mathcal{H}_{C}} \left| \frac{1}{n} \sum_{i=1}^{n} \sigma_{i} \left(\mathbb{1} \left\{ h(x'_{i}) \neq y'_{i} \right\} - \mathbb{1} \left\{ h(x_{i}) \neq y_{i} \right\} \right) \right|.$$

Now denote $\theta_h = \frac{1}{n} \sum_{i=1}^n \sigma_i \left(\mathbb{1}\{h(x_i') \neq y_i'\} - \mathbb{1}\{h(x_i) \neq y_i\} \right)$. We shorten the above to

$$\mathbb{E}_{S} \sup_{h \in \mathcal{H}} \left| R(h) - \hat{R}_{S}(h) \right| \leq \mathbb{E}_{S,S'} \mathbb{E}_{\sigma_{1:n}} \max_{h \in \mathcal{H}_{C}} |\theta_{h}|. \tag{2}$$

Now we want to bound $\mathbb{E}_{\sigma_{1:n}} \max_{h \in \mathcal{H}_C} |\theta_h|$ in Eq. 2. To do this, we will prove a bound regarding the max of sub-Gaussian variables and also show that θ_h is sub-Gaussian.

Lemma 8 (Max of sub-Gaussians). If $(x_1, ..., x_m)$ are mean 0 σ -sub-Gaussians (not necessarily independent), then

 $\mathbb{E}\max_{i} x_i \le \sigma \sqrt{2\log(m)}.$

Proof. (Lemma 8):

$$\mathbb{E} \max_{i} x_{i} = \frac{1}{\lambda} \log \exp \left(\lambda \mathbb{E} \left[\max_{i} x_{i} \right] \right) \quad \forall \lambda$$

$$\leq \frac{1}{\lambda} \log \mathbb{E} \left[\exp(\lambda \max_{i} x_{i}) \right] \quad \text{(Jensen's)}$$

$$\leq \frac{1}{\lambda} \log \mathbb{E} \left[\sum_{i=1}^{m} \exp(\lambda x_{i}) \right]$$

$$= \frac{1}{\lambda} \log \left(\sum_{i=1}^{m} \mathbb{E} \left[\exp(\lambda x_{i}) \right] \right)$$

$$\leq \frac{1}{\lambda} \log \left(\sum_{i=1}^{m} \exp(\frac{\lambda^{2} \sigma^{2}}{2}) \right) \quad \text{(sub-Gaussian definition)}$$

$$\leq \frac{\sigma}{\sqrt{2 \log(m)}} \log \left(\sum_{i=1}^{m} \exp(\log m) \right) \quad \text{by setting } \lambda = \frac{\sqrt{2 \log(m)}}{\sigma}$$

$$= \sigma \sqrt{2 \log m}.$$

Claim 9. θ_h is sub-Gaussian with parameter $\frac{1}{\sqrt{n}}$, $\mathbb{E}[\theta_h] = 0$.

Proof. (Claim 9):

Remember that
$$\theta_h = \sum_{i=1}^n \frac{\sigma_i}{n} \left(\mathbb{1}\{h(x_i') \neq y_i'\} - \mathbb{1}\{h(x_i) \neq y_i\} \right)$$
. Thus,

$$\mathbb{E}\left[\theta_h\right] = \sum_{i=1}^n \frac{\mathbb{E}\left[\sigma_i\right]}{n} \left(\mathbb{1}\left\{h(x_i') \neq y_i'\right\} - \mathbb{1}\left\{h(x_i) \neq y_i\right\}\right) = 0 \quad \text{as } \mathbb{E}\left[\sigma_i\right] = 0.$$

Now we show that θ_h is sub-Gaussian:

$$\theta_h = \sum_{i=1}^n \underbrace{\frac{\sigma_i}{n} \left(\mathbb{1}\{h(x_i') \neq y_i'\} - \mathbb{1}\{h(x_i) \neq y_i\} \right)}_{\text{each term is sub-Gaussian with parameter } \frac{1}{n}.$$

The above is due to how Rademacher RV's are sub-Gaussian with parameter 1, and each σ_i is being further multiplied by ± 1 which does not change its sub-Gaussianaeity.

Therefore using the sub-Gaussian sum corrolary in lecture 4, θ_h is sub-Gaussian with

parameter
$$\left(\sum_{i=1}^{n} \frac{1}{n^2}\right)^{\frac{1}{2}} = \frac{1}{\sqrt{n}}$$
.

Now we can finally bound $\mathbb{E}_{\sigma_{1:n}} \max_{h \in \mathcal{H}_C} |\theta_h|$ in Eq. 2.

Claim 10.
$$\mathbb{E}_{\sigma_{1:n}} \max_{h \in \mathcal{H}_C} |\theta_h| \leq \frac{1}{\sqrt{n}} \sqrt{2 \log(2|\mathcal{H}_C|)}$$

Proof. (Claim 10):

$$\mathbb{E}_{\sigma_{1:n}} \max_{h \in \mathcal{H}_C} |\theta_h| = \mathbb{E}_{\sigma_{1:n}} \max_{h \in \mathcal{H}_C} \max\{\theta_h, -\theta_h\}.$$

Recall that if θ_h is sub-Gaussian then $-\theta_h$ is also sub-Gaussian. Thus we have the max over $2|\mathcal{H}_C|$ sub-Gaussian variables with the same parameter. Thus,

$$\mathbb{E}_{\sigma_{1:n}} \max_{h \in \mathcal{H}_C} |\theta_h| \le \frac{1}{\sqrt{n}} \sqrt{2 \log(2|\mathcal{H}_C|)},$$

by combining Claim 9 and Lemma 8.

In summary, we have now shown that the right hand side of Eq. 2, $\mathbb{E}_{S,S'}[\mathbb{E}_{\sigma_{1:n}} \max |\theta_h|]$ is bounded by $\sqrt{\frac{2 \cdot \log(2|\mathcal{H}_C|)}{n}}$. Thus, by plugging into Eq. 2,

$$\mathbb{E}_{S} \sup_{h \in \mathcal{H}} \left| R(h) - \hat{R}_{S}(h) \right| \le \sqrt{\frac{2 \cdot \log(2|\mathcal{H}_{C}|)}{n}}.$$
 (3)

Note that $|\mathcal{H}_C| \leq \tau_{\mathcal{H}}(2n)$ since $|C| \leq 2n$ and we can finally finish the proof of Lemma 6 by plugging in $\tau_{\mathcal{H}}(2n)$ for $|\mathcal{H}_C|$.

Step 3: McDiarmid's Inequality

Define

$$f(S) = \sup_{h \in \mathcal{H}} \left| R(h) - \hat{R}_S(h) \right|.$$

Observe that f(S) satisfies the bounded differences property with constant $\frac{1}{n}$ (changing (x_i, y_i) can only change $\hat{R}_S(h)$ by $\frac{1}{n}$ for any $h \in \mathcal{H} \to \text{the max also changes by at most } \frac{1}{n}$).

Using McDiarmid's, we get that

$$P[f(S) - \mathbb{E}[f(S)] > t] \le 2\exp(-2nt^2).$$

If we choose $t = \sqrt{\frac{\log(2/\delta)}{2n}}$ to get the failure probability δ , then with probability $1 - \delta$,

$$f(S) < \mathbb{E}[f(S)] + \sqrt{\frac{\log(2/\delta)}{2n}}.$$

Now plug in Lemma 1 to replace $\mathbb{E}[f(S)]$, replace f(S), and we get that

$$\sup_{h \in \mathcal{H}} \left| R(h) - \hat{R}_S(h) \right| < \sqrt{\frac{2\log\left(2\tau_H(2n)\right)}{n}} + \sqrt{\frac{\log\left(2/\delta\right)}{2n}}.$$
 (4)

Step 4: Finish the VC theorem proof

Using Sauer's lemma, for n > d + 1, $\tau_{\mathcal{H}}(n) \leq \left(\frac{ne}{d}\right)^d$.

Plugging this into Eq. 4, with probability $(1 - \delta)$,

$$\sup_{h \in \mathcal{H}} \left| R(h) - \hat{R}_S(h) \right| \le \sqrt{\frac{2 \cdot d \log \left(2ne/d\right)}{n}} + \sqrt{\frac{\log \left(2/\delta\right)}{2n}}.$$
 (5)

Therefore, for $n \geq \mathcal{O}\left(\frac{d \log (d/\epsilon) + \log (1/\delta)}{\epsilon^2}\right)$, the right hand side $\leq \epsilon$, implying the uniform convergence property for hypothesis classes \mathcal{H} with finite $VCdim(\mathcal{H}) = d$.

Exercise: Show this explicity from Eq. 5.

2 Rademacher Complexity

Let us recall the proof of the VC theorem. We wanted to bound

$$\mathbb{E}_{S} \sup_{h \in \mathcal{H}} \left| R(h) - \hat{R}_{S}(h) \right|.$$

This quantity is called an "empirical process." Empirical process theory studies such quantities. Let's use symmetrization to bound this empirical process (without the absolute values):

$$\mathbb{E}_{S} \sup_{h \in \mathcal{H}} \left(R(h) - \hat{R}_{S}(h) \right) \leq \mathbb{E}_{S,S'} \sup_{h \in \mathcal{H}} \left(\hat{R}_{S'}(h) - \hat{R}_{S}(h) \right)$$

$$= \mathbb{E}_{S,S'} \sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \left(\mathbb{I}\{h(x'_{i}) \neq y'_{i}\} - \mathbb{I}\{h(x_{i}) \neq y_{i}\} \right)$$

$$= \mathbb{E}_{\sigma_{1:n}} \mathbb{E}_{S,S'} \sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \sigma_{i} \left(\mathbb{I}\{h(x'_{i}) \neq y'_{i}\} - \mathbb{I}\{h(x_{i}) \neq y_{i}\} \right)$$

$$\leq \mathbb{E}_{S'} \mathbb{E}_{\sigma_{1:n}} \sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \sigma_{i} \left(\mathbb{I}\{h(x'_{i}) \neq y'_{i}\} \right) +$$

$$\mathbb{E}_{S} \mathbb{E}_{\sigma_{1:n}} \sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \left(-\sigma_{i} \right) \left(\mathbb{I}\{h(x_{i}) \neq y_{i}\} \right)$$

$$\leq 2\mathbb{E}_{S} \mathbb{E}_{\sigma_{1:n}} \sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \sigma_{i} \left(\mathbb{I}\{h(x_{i}) \neq y_{i}\} \right) \quad \text{(i.i.d.)}.$$
Rademacher Complexity

As we will now see, we can bound the expected maximum error between training time and testing time of our hypothesis class by the "Rademacher Complexity."

Definition 11 (Rademacher Complexity). Let \mathcal{F} be a family of real-valued functions $f: \mathcal{Z} \to \mathbb{R}$ where $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$. Then the Rademacher Complexity $R(\mathcal{F})$ is defined as:

$$R(\mathcal{F}) = \frac{1}{n} \mathbb{E}_{\sigma \sim \{\pm 1\}^n} \left[\sup_{f \in \mathcal{F}} \sum_{i=1}^n \sigma_i f(z_i) \right].$$

More generally, given a (possibly infinite) set of vectors $A \subseteq \mathbb{R}^n$, the Rademacher Complexity R(A) is defined as:

$$R(A) = \frac{1}{n} \mathbb{E}_{\sigma \sim \{\pm 1\}^n} \left[\sup_{a \in A} \sum_{i=1}^n \sigma_i a_i \right].$$

<u>Intuition</u>: $R(\mathcal{F})$ captures how well the function class \mathcal{F} can fit random noise as we're essentially measuring correlation between $f \in \mathcal{F}$ and a random vector $\sigma_{1:n}$. If \mathcal{F} can fit random noise, then \mathcal{F} will probably overfit on our training data, incurring high generalization error.

Next class we will see more of Rademacher Complexity and how to use it to bound such generalization errors.