Lecture 2: Basics of Statistical Learning Theory

Week 2

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1 Elementary Probabilistic Inequalities

Theorem 1.1 (McDiarmids inequality). *Let $X_1, \cdots, X_n$ be independent random variables, where $X_i \in \mathcal{X}_i \subseteq \mathbb{R}$. Let $f : \mathcal{X}_1 \times \cdots \times \mathcal{X}_n \to \mathbb{R}$ be a function such that:*

$$|f(x_1, \cdots, x_i, \cdots, x_n) - f(x_1, \cdots, x_i', \cdots, x_n)| \leq c_i$$

for all $i = 1, 2, \cdots, n$, and all $(x_1, \cdots, x_i, \cdots, x_n), (x_1, \cdots, x_i', \cdots, x_n) \in \mathcal{X}_1 \times \cdots \times \mathcal{X}_n$. For any $t > 0$,

$$\mathbb{P}\left(|f(X_1, \cdots, X_n) - \mathbb{E}[f(X_1, \cdots, X_n)]| \geq t\right) \leq 2 \exp\left(-\frac{2t^2}{\sum_{i=1}^n c_i^2}\right).$$

If we let $f(x_1, \cdots, x_n) = \sum_{i=1}^n x_i$, the McDiarmids inequality gives the Hoeffding's inequality. The proof of McDiarmids inequality is left as homework.

2 Empirical Risk Minimization

Consider an $i.i.d.$ dataset $\{(x_i, y_i)\}_{i=1}^n$, and a hypothesis class $\mathcal{H}$. Empirical risk minimization seeks to find a classifier in $\mathcal{H}$ that solves the following optimization objective

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \mathbb{I}_{[f(x_i) \neq y_i]}. \tag{1}$$

The question is: **How good is empirical risk minimization?** More specifically, if the data points are $i.i.d.$ sampled from $\mathbb{Q}$, can we bound the true risk of a function f, which is $R_{true}(f) := \mathbb{E}_{(x,y)\sim\mathbb{Q}}\left[\mathbb{I}_{[f(x)\neq y]}\right]$, in terms of its empirical risk $R_{emp}(f) := \sum_{i=1}^n \frac{1}{n} \mathbb{I}_{[f(x_i)\neq y_i]}$ and the VC dimension of $\mathcal{H}$?

Again, this is about *generalization* and *learning*. If the model only memorizes the dataset, it cannot generalize to the true risk with respect to the true distribution.

3 Statistical Learning Theory with VC Dimension

Lemma 3.1. *Consider two* $i.i.d.$ *datasets* $\{(x_i, y_i)\}_{i=1}^n \sim \mathbb{Q}$*, and* $\{(x'_i, y'_i)\}_{i=1}^n \sim \mathbb{Q}$*. We have, for any* $f \in \mathcal{H}$ *and any* $t > 0$

$$\mathbb{P}\left(R_{emp}(f) - R'_{emp}(f) \geq t\right) \leq 2\exp\left(-\frac{nt^2}{2}\right), \tag{2}$$

where $R_{emp}(f)$ *is the empirical risk on* $\{(x_i, y_i)\}_{i=1}^n$*, and* $R'_{emp}(f)$ *is the empirical risk on* $\{(x'_i, y'_i)\}_{i=1}^n$*. The notations* $R_{emp}(f)$ *and* $R'_{emp}(f)$ *will be used henceforth.*

Proof. By definition,

$$\begin{aligned} R_{emp}(f) - R'_{emp}(f) = & \frac{1}{n}\left(\sum_{i=1}^n \left(\mathbb{I}_{[f(x_i)\neq y_i]} - \mathbb{E}_{(x_i,y_i)\sim\mathbb{Q}}\left[\mathbb{I}_{[f(x_i)\neq y_i]}\right]\right)\right) \\ & + \frac{1}{n}\left(\sum_{i=1}^n \left(\mathbb{E}_{(x'_i,y'_i)\sim\mathbb{Q}}\left[\mathbb{I}_{\left[f(x'_i)\neq y'_i\right]}\right] - \mathbb{I}_{\left[f(x'_i)\neq y'_i\right]}\right)\right). \end{aligned}$$

We can now apply the McDiarmids inequality to the above equation to conclude the proof. □

Lemma 3.2. *Consider two* $i.i.d.$ *datasets* $\{(x_i, y_i)\}_{i=1}^n \sim \mathbb{Q}$*, and* $\{(x'_i, y'_i)\}_{i=1}^n \sim \mathbb{Q}$*. It holds that*

$$\mathbb{P}\left(\{R_{true}(f) - R_{emp}(f) > t\}\right) \leq \frac{\mathbb{P}\left(\{R'_{emp}(f) - R_{emp}(f) > t/2\}\right)}{\mathbb{P}\left(\{R'_{emp}(f) - R_{true}(f) > -t/2\}\right)}.$$

Proof. Consider the following inclusion of events

$$\begin{aligned} & \{R_{true}(f) - R_{emp}(f) > t\} \cap \{R'_{emp}(f) - R_{true}(f) > -t/2\} \\ \Rightarrow & \{R'_{emp}(f) - R_{emp}(f) > t/2\}. \end{aligned}$$

Thus we have

$$\begin{aligned} & \mathbb{P}\left(\{R'_{emp}(f) - R_{emp}(f) > t/2\}\right) \\ \geq & \mathbb{P}\left(\{R_{true}(f) - R_{emp}(f) > t\} \cap \{R'_{emp}(f) - R_{true}(f) > -t/2\}\right) \\ = & \mathbb{P}\left(\{R_{true}(f) - R_{emp}(f) > t\}\right)\mathbb{P}\left(\{R'_{emp}(f) - R_{true}(f) > -t/2\}\right), \end{aligned}$$

where the last inequality uses independence of $\{(x_i, y_i)\}_{i=1}^n$ and $\{(x'_i, y'_i)\}_{i=1}^n$. □

Lemma 3.3 (Symmetrization)**.** *Instate the notations and assumptions in previous lemmas. . For any* n, t *satisfying* $\exp\left(-\frac{nt^2}{2}\right) \leq \frac{1}{2}$*, it holds that*

$$\mathbb{P}\left(\sup_{f\in\mathcal{H}}\left(R_{true}(f) - R_{emp}(f)\right) > t\right) \leq 2\mathbb{P}\left(\sup_{f\in\mathcal{H}}\left(R'_{emp}(f) - R_{emp}(f)\right) > t/2\right)$$

Proof. For any $f \in \mathcal{H}$, the McDiarmid's inequality gives

$$\mathbb{P}\left(\{R'_{emp}(f) - R_{true}(f) > -t/2\}\right) \geq 1 - \exp\left(-\frac{nt^2}{2}\right) \geq \frac{1}{2}.$$

Together with Lemma 3.2, the above inequality gives, for any $f \in \mathcal{H}$,

$$\mathbb{P}\left(\{R_{true}(f) - R_{emp}(f) > t\}\right) \leq 2\mathbb{P}\left(\{R'_{emp}(f) - R_{emp}(f) > t/2\}\right), \tag{3}$$

provided that $\exp\left(-\frac{nt^2}{2}\right) \leq \frac{1}{2}$.

Let $f^* \in \arg\max_{f\in\mathcal{H}}\left(R_{true}(f) - R_{emp}(f)\right)$. Note that

$$\mathbb{P}\left(R'_{emp}(f^*) - R_{emp}(f^*) > t/2\right) \leq \mathbb{P}\left(\sup_{f\in\mathcal{H}}\left(R'_{emp}(f) - R_{emp}(f)\right) > t/2\right), \tag{4}$$

since $\{R'_{emp}(f^*) - R_{emp}(f^*) > t/2\} \subseteq \{\sup_{f\in\mathcal{H}}\left(R'_{emp}(f) - R_{emp}(f) > t/2\right)\}$.

Combining (3) and (4) gives

$$\begin{aligned}\mathbb{P}\left(R_{true}(f^*) - R_{emp}(f^*) > t\right) &\leq 2\mathbb{P}\left(R'_{emp}(f^*) - R_{emp}(f^*) > t/2\right)\\ &\leq 2\mathbb{P}\left(\sup_{f\in\mathcal{H}}\left(R'_{emp}(f) - R_{emp}(f)\right) > t/2\right)\end{aligned}$$

$\square$

Lemma 3.4. *Instate the settings and notations in previous lemmas. Suppose $\mathcal{H}$ is closed. Let $f^* \in \arg\max_{f\in\mathcal{H}}\left(R'_{emp}(f) - R_{emp}(f)\right)$ with respect to fixed datasets $\{(x_i, y_i)\}_{i=1}^n$ and $\{(x'_i, y'_i)\}_{i=1}^n$. For any $t \in \mathbb{R}$, it holds that*

$$\begin{aligned}&\mathbb{P}\left(\sup_{f\in\mathcal{H}}\left(R'_{emp}(f) - R_{emp}(f)\right) \geq t/2\right)\\ \leq\ &\mathbb{P}\left(\sup_{(y_1,\cdots,y_n,y'_1\cdots,y'_n)\in\mathcal{H}_{x_1,\ldots,x_n,x'_1,\ldots,x'_n}}\left(R'_{emp}(f^*) - R_{emp}(f^*)\right) \geq t/2\right).\end{aligned}$$

Proof. For any $f \in \mathcal{H}$, it holds that

$$R_{emp}(f) = \frac{1}{n}\sum_{i=1}^n \mathbb{I}_{[f(x_i)\neq y_i]} \leq \sup_{(y_1,\cdots,y_n)\in\mathcal{H}_{x_1,\ldots,x_n}} \frac{1}{n}\sum_{i=1}^n \mathbb{I}_{[f'(x_i)\neq y_i]},$$

and also,

$$R_{emp}(f) \geq \inf_{(y_1,\cdots,y_n)\in\mathcal{H}_{x_1,\ldots,x_n}} \frac{1}{n}\sum_{i=1}^n \mathbb{I}_{[f(x_i)\neq y_i]}.$$

We use the above observations and we arrive at the following argument. Let

$$f^* \in \arg\max_{f\in\mathcal{H}} \left(R'_{emp}(f) - R_{emp}(f)\right)$$

for a fixed realization of datasets. We have

$$\begin{aligned}\sup_{f\in\mathcal{H}} \left(R'_{emp}(f) - R_{emp}(f)\right) &\le R'_{emp}(f^*) - R_{emp}(f^*)\\ &\le \sup_{(y_1,\cdots,y_n,y'_1\cdots,y'_n)\in\mathcal{H}_{x_1,\ldots,x_n,x'_1,\ldots,x'_n}} \left(R'_{emp}(f^*) - R_{emp}(f^*)\right),\end{aligned}$$

which finishes the proof. □

Note 1. By taking a supremum over all possible data configurations, the randomness in f is effectively removed.

Note 2. Lemma 3.4 converts a supremum over a possibly infinite set $\mathcal{H}$ to a maximum over a finite set $\mathcal{H}_{x_1,\ldots,x_n,x'_1,\ldots,x'_n}$. This will be helpful when we later apply a union bound.

Theorem 3.5. *Instate the assumptions and notations in previous lemmas. Then it holds that*

$$\mathbb{P}\left(R_{true}(f) \le R_{emp}(f) + O\left(\sqrt{\frac{\log(S_{\mathcal{H}}(2n)/\delta)}{n}}\right), \quad \forall f\in\mathcal{H}\right) \ge 1-\delta, \quad \forall\delta\in(0,1).$$

Proof. We gathers results from previous lemmas to give a proof. By Lemma 3.3, it holds that

$$\begin{aligned}&\mathbb{P}\left(R_{true}(f) \ge R_{emp}(f) + t, \quad \exists f\in\mathcal{H}\right)\\ &= \mathbb{P}\left(\sup_{f\in\mathcal{H}}\left(R_{true}(f) - R_{emp}(f)\right) \ge t\right) \le 2\mathbb{P}\left(\sup_{f\in\mathcal{H}}\left(R'_{emp}(f) - R_{emp}(f)\right) \ge t\right).\end{aligned}$$

Also, we have

$$\begin{aligned}&\mathbb{P}\left(\sup_{f\in\mathcal{H}}\left(R'_{emp}(f) - R_{emp}(f)\right) \ge t/2\right)\\ &\le \mathbb{P}\left(\sup_{(y_1,\cdots,y_n,y'_1\cdots,y'_n)\in\mathcal{H}_{x_1,\ldots,x_n,x'_1,\ldots,x'_n}} \left(R'_{emp}(f^*) - R_{emp}(f^*)\right) \ge t/2\right) && \text{(by Lemma 3.4)}\\ &\le \sum_{(y_1,\cdots,y_n,y'_1\cdots,y'_n)\in\mathcal{H}_{x_1,\ldots,x_n,x'_1,\ldots,x'_n}} \mathbb{P}\left(\left(R'_{emp}(f^*) - R_{emp}(f^*)\right) \ge t/2\right) && \text{(by union bound)}\\ &\le S_{\mathcal{H}}(2n)e^{-nt^2/8}.\end{aligned}$$

We then let $\delta = S_{\mathcal{H}}(2n)e^{-nt^2/8}$ and rearrange the terms to finish the proof. □

Corollary 3.6. *Instate the assumptions and notations from previous lemmas. Let $f_{\min}$ be a function in $\mathcal{H}$ such that $f_{\min} \in \arg\min_{f\in\mathcal{H}} R_{true}(f)$. Let $f_n \in \arg\min_{f\in\mathcal{H}} R_{emp}(f)$. Then it holds that*

$$\mathbb{P}\left(R_{true}(f_{\min}) \leq R_{emp}(f_n) + O\left(\sqrt{\frac{\log(S_{\mathcal{H}}(2n)/\delta)}{n}}\right)\right) \geq 1-\delta, \quad \forall \delta \in (0,1).$$

Proof. Since $R_{true}(f_{\min}) \leq R_{true}(f_n)$, this corollary follows from the Theorem 3.5. Note that $R_{true}(f)$ does not depend on the realization of the datasets. □

4 Back to Growth Function

First of all, note that VC dimension of a hypothesis class $\mathcal{H}$ can be equivalently defined as

$$\text{VC-dim}(\mathcal{H}) = \max\{n : S_{\mathcal{H}}(n) = 2^n\}.$$

This can be verified by checking the definition of shattering.

Lemma 4.1. *Let $\mathcal{H}$ be a class of functions with finite VC dimension d. Then for all positive integers n,*

$$S_{\mathcal{H}}(n) \leq \sum_{i=0}^{d} \binom{n}{i},$$

where $d :=$ VC-dim$(\mathcal{H})$, (and $n \gg d$).

Proof. For any $X = \{x_1, \cdots, x_n\}$, consider a table containing values of $\mathcal{H}_X$. Recall the definition of $\mathcal{H}_X$ in the previous notes.

$h(x_1)$	$h(x_2)$	$h(x_3)$	$\cdots$	$h(x_n)$
-	+	-	$\cdots$	+
+	-	-	$\cdots$	+
-	+	+	$\cdots$	-
+	+	+	$\cdots$	+
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Table 1: The evaluation table.

Obviously the number of unique rows in the evaluation table T is the same as the cardinality of $\mathcal{H}_X$. Let $d :=$ VC-dim$(\mathcal{H})$. If one row has i "+"s in it, it must be one of the $\binom{n}{i}$ patterns. Summing over i from 0 to d, we know that the number of unique rows in T is upper bounded by $\sum_{i=0}^{d} \binom{n}{i}$, which means

$$\sup_{X,|X|=n} |\mathcal{H}_X| \leq \sum_{i=0}^{d} \binom{n}{i}.$$

Note that there is no need to sum over $i = d+1, d+2, \cdots, n$. The reason is that $\mathcal{H}$ cannot correctly classify points of size $d+1$ and above.

$\square$

Lemma 4.2. *Let $\mathcal{H}$ be a hypothesis class with VC-dim$(\mathcal{H}) = d$. Then for all $m \geq d$,*

$$S_{\mathcal{H}}(n) \leq \left(\frac{en}{d}\right)^d \leq O(n^d).$$

Proof.

$$\begin{aligned}
S_{\mathcal{H}}(n) &\leq \sum_{i=0}^{d} \binom{n}{i} && \text{(by Lemma 4.1)} \\
&\leq \sum_{i=0}^{n} \binom{n}{i} \left(\frac{n}{d}\right)^{d-i} \\
&= \left(\frac{n}{d}\right)^d \sum_{i=0}^{n} \binom{n}{i} \left(\frac{d}{n}\right)^i \\
&= \left(\frac{n}{d}\right)^d \left(1 + \frac{d}{n}\right)^n && \text{(by the binomial theorem)} \\
&\leq \left(\frac{n}{d}\right)^d e^d && \text{(since } \left(1+\tfrac{d}{n}\right)^n \text{ converges to } e^d \text{ from below.)}
\end{aligned}$$

$\square$

Theorem 4.3. *Instate the assumptions and notations from previous lemmas. Let $f_{\min}$ be a function in $\mathcal{H}$ such that $f_{\min} \in \arg\min_{f \in \mathcal{H}} R_{true}(f)$. Let $f_n \in \arg\min_{f \in \mathcal{H}} R_{emp}(f)$. Then it holds that*

$$\mathbb{P}\left(R_{true}(f_{\min}) \leq R_{emp}(f_n) + O\left(\sqrt{\frac{\textit{VC-dim}(\mathcal{H}) \log(n/\delta)}{n}}\right)\right) \geq 1 - \delta, \quad \forall \delta \in (0,1).$$

Proof. This theorem is a consequence of Lemma 4.2 and Corollary 3.6. $\square$

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