Machine Learning Theory (CS 6783)

Lecture 4 : MDL principle, Uniform Rate and Infinite classes

1 Recap

- 1. ERM Algorithm: $\hat{\mathbf{y}}_{\text{ERM}} = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \sum_{(x,y) \in S} \ell(f(x), y)$
- 2. For the ERM algorithm, we have

$$\mathbb{E}_{S}\left[L_{D}(\hat{\mathbf{y}}_{\text{ERM}}) - \inf_{f \in \mathcal{F}} L_{D}(f)\right] \leq \mathbb{E}_{S} \sup_{f \in \mathcal{F}} \left[\mathbb{E}_{(x,y) \sim D}[\ell(f(x), y)] - \frac{1}{n} \sum_{t=1}^{n} \ell(f(x_{t}), y_{t})\right]$$

3. For finite class,

$$\mathbb{E}_{S} \sup_{f \in \mathcal{F}} \left[\mathbb{E}_{(x,y) \sim D}[\ell(f(x), y)] - \frac{1}{n} \sum_{t=1}^{n} \ell(f(x_t), y_t) \right] \le O\left(\frac{\log(n|\mathcal{F}|)}{n}\right)$$

What about infinite \mathcal{F} ?

2 MDL bound (Occam's Razor Principle)

We saw how one can get bounds for the case when \mathcal{F} has finite cardinality. How about the case when \mathcal{F} has infinite cardinality? To start with, let us consider the case when \mathcal{F} is a countable set.

MDL Algorithm: The MDL learning rule picks the hypothesis in \mathcal{F} as follows :

$$\hat{y}_{\text{mdl}} = \operatorname*{argmin}_{f \in \mathcal{F}} \frac{1}{n} \sum_{t=1}^{n} \ell(f(x_t), y_t) + 3\sqrt{\frac{\log(n/\pi^2(f))}{n}}$$

Interpretation : minimize empirical error while also ensuring that the hypothesis we pick has a large prior π . Why is this learning rule appealing ?

We will use the below claim to provide us an intuition for why the MDL algorithm is effective.

Claim 1. For any countable set \mathcal{F} , any fixed distribution π on \mathcal{F} ,

$$\mathbb{E}_{S}\left[\sup_{f\in\mathcal{F}}\left\{\left|L_{D}(f)-\frac{1}{n}\sum_{t=1}^{n}\ell(f(x_{t}),y_{t})\right|-\sqrt{\frac{\log(n/\pi^{2}(f))}{n}}\right\}\right]\leq\frac{4}{\sqrt{n}}$$

Proof. The basic idea is to use Hoeffding bound along with union bound as before, but instead of using same ϵ for every $f \in \mathcal{F}$ in Hoeffding bound, we use f specific $\epsilon(f)$. We shall specify the exact form of $\epsilon(f)$ later. For now note that, since the losses are bounded by 1,

$$\sup_{f \in \mathcal{F}} \left\{ \left| L_D(f) - \frac{1}{n} \sum_{t=1}^n \ell(f(x_t), y_t) \right| - \epsilon(f) \right\} \le 0 + 2 \, \mathbb{1}_{\{\sup_{f \in \mathcal{F}} \left\{ \left| L_D(f) - \frac{1}{n} \sum_{t=1}^n \ell(f(x_t), y_t) \right| - \epsilon(f) > 0 \} \}}$$

Hence, taking expectation w.r.t. sample we have that

$$\mathbb{E}_{S}\left[\sup_{f\in\mathcal{F}}\left\{\left|L_{D}(f)-\frac{1}{n}\sum_{t=1}^{n}\ell(f(x_{t}),y_{t})\right|-\epsilon(f)\right\}\right] \leq 2P\left(\sup_{f\in\mathcal{F}}\left\{\left|L_{D}(f)-\frac{1}{n}\sum_{t=1}^{n}\ell(f(x_{t}),y_{t})\right|-\epsilon(f)>0\right\}\right)$$

By Hoeffding inequality, for any fixed $f \in \mathcal{F}$

$$P\left(\left|\mathbb{E}\left[\ell(f(x), y)\right] - \frac{1}{n} \sum_{t=1}^{n} \ell(f(x_t), y_t)\right| - \epsilon(f) > 0\right) \le 2 \exp\left(-\frac{\epsilon^2(f)n}{2}\right)$$

Taking union bound we have,

$$P\left(\sup_{f\in\mathcal{F}}\left|\mathbb{E}\left[\ell(f(x),y)\right] - \frac{1}{n}\sum_{t=1}^{n}\ell(f(x_t),y_t)\right| - \epsilon(f) > 0\right) \le \sum_{f\in\mathcal{F}} 2\exp\left(-\frac{\epsilon^2(f)n}{2}\right)$$

Hence we conclude that

$$\mathbb{E}_{S}\left[\sup_{f\in\mathcal{F}}\left\{\left|L_{D}(f)-\frac{1}{n}\sum_{t=1}^{n}\ell(f(x_{t}),y_{t})\right|-\epsilon(f)\right\}\right] \leq 4\sum_{f\in\mathcal{F}}\exp\left(-\frac{\epsilon^{2}(f)n}{2}\right)$$

For the prior choice of π of distribution over set \mathcal{F} , let us use

$$\epsilon(f) = \sqrt{\frac{\log(n/\pi^2(f))}{n}}$$

Hence we can conclude that,

$$\mathbb{E}_{S}\left[\sup_{f\in\mathcal{F}}\left\{\left|L_{D}(f)-\frac{1}{n}\sum_{t=1}^{n}\ell(f(x_{t}),y_{t})\right|-\sqrt{\frac{\log(n/\pi^{2}(f))}{n}}\right\}\right] \leq 4\sum_{f\in\mathcal{F}}\exp\left(-\frac{\epsilon^{2}(f)n}{2}\right)$$
$$\leq \frac{4\sum_{f}\pi(f)}{\sqrt{n}}=\frac{4}{\sqrt{n}}$$

Let us use the claim above to analyze the learning rule.

Theorem 2. For the MDL algorithm, we have that:

$$\mathbb{E}_{S}\left[L_{D}(\hat{y}_{\mathrm{mdl}})\right] \leq \inf_{f \in \mathcal{F}} \left\{L_{D}(f) + \sqrt{\frac{\log(n/\pi^{2}(f))}{n}}\right\} + \frac{4}{\sqrt{n}}$$

Proof. Note that from the Claim 1, we have that,

$$\mathbb{E}_{S}\left[L_{D}(\hat{y}_{\mathrm{mdl}}) - \frac{1}{n}\sum_{t=1}^{n}\ell(\hat{y}_{\mathrm{mdl}}(x_{t}), y_{t}) - \sqrt{\frac{\log(n/\pi^{2}(\hat{y}_{\mathrm{mdl}}))}{n}}\right] \leq \frac{4}{\sqrt{n}}$$

By definition of \hat{y}_{mdl} we can conclude that

$$\mathbb{E}_{S}\left[L_{D}(\hat{y}_{\mathrm{mdl}}) - \inf_{f \in \mathcal{F}} \left\{\frac{1}{n} \sum_{t=1}^{n} \ell(\hat{y}_{\mathrm{mdl}}(x_{t}), y_{t}) + \sqrt{\frac{\log(n/\pi^{2}(\hat{y}_{\mathrm{mdl}}))}{n}}\right\}\right] \leq \frac{4}{\sqrt{n}}$$

In other words,

$$\mathbb{E}_{S}\left[L_{D}(\hat{y}_{\mathrm{mdl}})\right] \leq \mathbb{E}_{S}\left[\inf_{f \in \mathcal{F}} \left\{\frac{1}{n} \sum_{t=1}^{n} \ell(f(x_{t}), y_{t}) + \sqrt{\frac{\log(n/\pi^{2}(f))}{n}}\right\}\right] + \frac{4}{\sqrt{n}}$$

Let $f_D = \underset{f \in \mathcal{F}}{\operatorname{argmin}} L_D(f) + \sqrt{\frac{\log(n/\pi^2(f))}{n}}$, replacing the infimum above we conclude that

$$\mathbb{E}_{S}\left[L_{D}(\hat{y}_{\text{mdl}})\right] \leq \mathbb{E}_{S}\left[\frac{1}{n}\sum_{t=1}^{n}\ell(f_{D}(x_{t}), y_{t}) + \sqrt{\frac{\log(n/\pi^{2}(f_{D}))}{n}}\right] + \frac{4}{\sqrt{n}}$$
$$= L_{D}(f_{D}) + \sqrt{\frac{\log(n/\pi^{2}(f_{D}))}{n}} + \frac{4}{\sqrt{n}}$$
$$= \inf_{f\in\mathcal{F}}\left\{L_{D}(f) + \sqrt{\frac{\log(n/\pi^{2}(f))}{n}}\right\} + \frac{4}{\sqrt{n}}$$
(1)
(2)

Thus with the above bound, even for countably infinite \mathcal{F} we can get bounds on $\mathbb{E}_S[L_D(\hat{y})] - \min_{f \in \mathcal{F}} L_D(f)$ as

$$\mathbb{E}_S\left[L_D(\hat{y})\right] - \min_{f \in \mathcal{F}} L_D \le \sqrt{\frac{\log(n/\pi^2(f_D))}{n}} + \frac{4}{\sqrt{n}}$$

that decreases with n, however the rate depends on $\log(1/\pi(f_D))$ where $f_D = \underset{f \in \mathcal{F}}{\operatorname{argmin}} L_D(f)$.

3 Infinite Hypothesis Class : first attempt

As a first attempt, one can think of approximating the function class to desired accuracy by a finite number of representative elements. We call this a point-wise cover.

Definition 1. We say that set $\mathcal{F}_{\delta} = {\tilde{f}_1, \ldots, \tilde{f}_N}$ is an δ point-wise cover for function class \mathcal{F} if $\forall f \in \mathcal{F}$ there exists $i \in [N]$ s.t.

$$\sup_{x,y} |\ell(f(x),y) - \ell(\tilde{f}_i(x),y)| \le \delta$$

Further define $N(\delta)$ to be the smallest N such that there exists an δ cover of \mathcal{F} of cardinality at most N.

Claim 3. For any function class \mathcal{F} , we have that

$$\mathcal{V}_n^{\text{stat}}(\mathcal{F}) \le \inf_{\delta>0} \left\{ 4\delta + \sqrt{\frac{\log N(\delta)}{n}} \right\}$$

Proof. Let $\mathcal{F}_{\delta} = \{\tilde{f}_1, \ldots, \tilde{f}_{N(\delta)}\}$ be an δ cover for the function class \mathcal{F} . Further for every $f \in \mathcal{F}$, let i(f) correspond to the index of the element in \mathcal{F}_{δ} that is δ close to that f. Now note that,

$$\begin{split} \mathbb{E}_{S} \left[\sup_{f \in \mathcal{F}} \left\{ \mathbb{E} \left[\ell(f(x), y) \right] - \frac{1}{n} \sum_{t=1}^{n} \ell(f(x_{t}), y_{t}) \right\} \right] \\ & \leq \mathbb{E}_{S} \left[\max_{i \in [N_{\delta}]} \left\{ \mathbb{E} \left[\ell(\tilde{f}_{i}(x), y) \right] - \frac{1}{n} \sum_{t=1}^{n} \ell(\tilde{f}_{i}(x_{t}), y_{t}) \right\} \right] \\ & + \mathbb{E}_{S} \left[\sup_{f \in \mathcal{F}} \left| \mathbb{E} \left[\ell(f(x), y) \right] - \frac{1}{n} \sum_{t=1}^{n} \ell(f(x_{t}), y_{t}) - \mathbb{E} \left[\ell(\tilde{f}_{i(f)}(x), y) \right] + \frac{1}{n} \sum_{t=1}^{n} \ell(\tilde{f}_{i(f)}(x_{t}), y_{t}) \right| \right] \\ & \leq \sqrt{\frac{\log N(\delta)}{n}} + 4\delta \end{split}$$

where the first term in the last inequality is by using the finite class bound and the second term is by using the definition of δ cover as $\tilde{f}_{i(f)}$ is δ close to f. Since choice of δ was arbitrary we can take the infimum over choices of δ to conclude the proof.

Example : linear predictor, absolute loss, 1 dimension

$$f(x) = f \cdot x, \quad \mathcal{F} = \mathcal{X} = [-1, 1], \quad \mathcal{Y} = [-1, 1], \quad \ell(y', y) = |y - y'|$$

 $N_{\delta} = \frac{2}{\delta}, \text{ Cover given by } f_1 = -1, f_2 = -1 + \delta, \dots, f_{N_{\delta}-1} = 1 - \delta, f_{N_{\delta}} = 1$
 $V_n^{\text{stat}}(\mathcal{F}) \leq \sqrt{\frac{\log n}{n}}$

Example : linear predictor/loss, d dimensions $f(x) = \mathbf{f}^{\top} \mathbf{x}$. $\mathcal{F} = \mathcal{X} = \{ \mathbf{v} \in \mathbb{R}^d : \|\mathbf{v}\|_2 \leq 1 \}$. $\mathcal{Y} = [-1, 1]$. $\ell(y', y) = y \cdot y'$ $N_{\delta} = \Theta\left(\frac{2}{\delta}\right)^d$ $V_n^{\text{stat}}(\mathcal{F}) \le \sqrt{\frac{d\log n}{n}}$

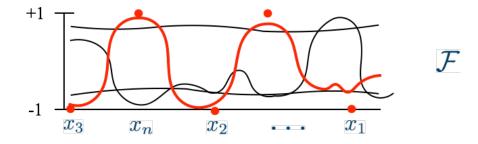
Example : thresholds $f(x) = \operatorname{sign}(f - x), \quad \mathcal{F} = \mathcal{X} = [-1, 1], \quad \mathcal{Y} = \{-1, 1\}, \quad \ell(y', y) = \mathbb{1}_{\{y \neq y'\}}, \quad N_{\delta} = \infty \text{ for any } \delta < 1.$

4 Symmetrization and Rademacher Complexity

$$\begin{split} \mathbb{E}_{S}\left[L_{D}(\hat{y}_{\text{erm}})\right] &- \inf_{f \in \mathcal{F}} L_{D}(f) \\ &\leq \mathbb{E}_{S}\left[\sup_{f \in \mathcal{F}} \left\{\mathbb{E}\left[\ell(f(x), y)\right] - \frac{1}{n} \sum_{t=1}^{n} \ell(f(x_{t}), y_{t})\right\}\right] \\ &\leq \mathbb{E}_{S,S'}\left[\sup_{f \in \mathcal{F}} \left\{\frac{1}{n} \sum_{t=1}^{n} \ell(f(x'_{t}), y'_{t}) - \frac{1}{n} \sum_{t=1}^{n} \ell(f(x_{t}), y_{t})\right\}\right] \\ &= \mathbb{E}_{S,S'}\mathbb{E}_{\epsilon}\left[\sup_{f \in \mathcal{F}} \left\{\frac{1}{n} \sum_{t=1}^{n} \epsilon_{t}(\ell(f(x'_{t}), y'_{t}) - \ell(f(x_{t}), y_{t}))\right\}\right] \\ &\leq 2\mathbb{E}_{S}\mathbb{E}_{\epsilon}\left[\sup_{f \in \mathcal{F}} \left\{\frac{1}{n} \sum_{t=1}^{n} \epsilon_{t}\ell(f(x_{t}), y_{t})\right\}\right] \\ &=: \mathcal{R}_{n}(\ell \circ \mathcal{F}) \end{split}$$

Where in the above each ϵ_t is a Rademacher random variable that is +1 with probability 1/2 and -1 with probability 1/2. The above is called Rademacher complexity of the loss class $\ell \circ \mathcal{F}$. In general Rademacher complexity of a function class measures how well the function class correlates with random signs. The more it can correlate with random signs the more complex the class is.

Example : $\mathcal{X} = [0, 1], \ \mathcal{Y} = [-1, 1]$



How does this help?