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CS861: Theoretical Foundations of Machine Learning

Lecture 16 - 10/11/2023

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Lecture 16: prediction problems, Stochastic Bandits

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In this lecture, we will continue our discussion on proving minimax lower bounds for prediction problems, and use it to prove a lower bound for classification in a VC class. Finally, we will briefly introduce **Stochastic Bandits**.

1 Excess risk in classification/regression (Cont'd)

Let \mathcal{Z} be a data space, \mathcal{P} be a family of distribution, and \mathcal{H} be a hypothesis space. Let $f : \mathcal{H} \times \mathcal{Z} \rightarrow \mathbb{R}$ be the instance loss, where $f(h, Z)$ is the loss of hypothesis h on instance Z . Let $F(h, P) = \mathbb{E}_{Z \sim P}[f(h, Z)]$ be the population loss of hypothesis h on distribution P , and let $L(h, P) = F(h, P) - \inf_{h \in \mathcal{H}} F(h, P)$ denote the excess population loss.

Then a dataset S drawn from some $P \in \mathcal{P}$; an estimator \hat{h} mapping the data to a hypothesis in \mathcal{H} . Thus, the risk would be

$$R(\hat{h}, P) = \mathbb{E}[L(\hat{h}, P)] = \mathbb{E}[F(\hat{h}, P)] - \inf_{h \in \mathcal{H}} F(h, P),$$

and the minimax risk is

$$R^* = \inf_{\hat{h}} \sup_{P \in \mathcal{P}} R(\hat{h}, P).$$

Example 1 (Estimation error in a hypothesis class). $\mathcal{H} \subseteq \{h : \mathcal{X} \rightarrow \mathcal{Y}\}$

Our estimator \hat{h} will choose some hypothesis in \mathcal{H} using data. We can now view $L(h, P)$ as the estimation error. Recall, that letting h^* be the Bayes' optimal classifier, we can write

$$F(h, P) - F(h^*, P) = \underbrace{F(h, P) - \inf_{h' \in \mathcal{H}} F(h', P)}_{\text{estimation error} = L(h, P)} + \underbrace{\inf_{h' \in \mathcal{H}} F(h', P) - F(h^*, P)}_{\text{approximation error}}.$$

In Homework 1, we saw that for ERM, when \mathcal{H} has VC dimension $d_{\mathcal{H}}$, we have

$$R(\hat{h}_{ERM}, P) = \underbrace{\mathbb{E}_S[F(\hat{h}_{ERM}(S), P)]}_{\mathbb{E}_S[\mathbb{E}_{X, Y \sim P}[\mathbb{1}(\hat{h}_{ERM}(S)(X) \neq Y)]]} - \inf_{h \in \mathcal{H}} F(h, P) \in \tilde{O}\left(\sqrt{\frac{d_{\mathcal{H}}}{n}}\right)$$

We will use this framework to show a corresponding lower bound

$$\inf_{\hat{h}} \sup_{P \in \mathcal{P}} \left(\mathbb{E}_{S \sim P}[F(\hat{h}(S), P)] - \inf_{h' \in \mathcal{H}} F(h', P) \right) \in \Omega\left(\sqrt{\frac{d_{\mathcal{H}}}{n}}\right)$$

To proceed, we will first define the separation of two distributions, with respect to a given hypothesis class and loss L .

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Definition 1 (Separation). For two distributions P, Q , define the separation $\Delta(P, Q)$ as



$$L(h, P) \leq \delta \Rightarrow L(h, Q) \geq \delta, \forall h \in \mathcal{H}$$

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- P, Q are δ -separated if $\Delta(P, Q) \geq \delta$. That is, a hypothesis that does well on P (i.e. $L(h, P) \leq \delta$), does poorly on Q (i.e. $L(h, Q) \geq \delta$).
- We say a collection $\{P_1, \dots, P_N\}$ are δ -separated if $\Delta(P_i, P_k) \geq \delta, \forall i \neq k$.

The following theorem is a similar technique to our previous theorem on reducing estimation to testing. You will do this in your homework.

Theorem 2 (Reduction to testing). Let $\{P_1, \dots, P_N\}$ be a δ -separated subset of \mathcal{P} . Let ψ be any test which maps the dataset to $[N]$. Then

$$R^* \geq \delta \inf_{\psi} \max_{j \in [N]} P_j(\psi \neq j)$$

We can then establish the following statements from the above result when S consists of n i.i.d data points.

Theorem 3 (Le Cam & Fano Method). 1. **Le Cam:** If $\{P_0, P_1\}$ are δ -separated,

$$R^* \geq \frac{\delta}{2} \|P_0 \wedge P_1\| \geq \frac{\delta}{4} e^{-\text{KL}(P_0, P_1)}$$

Hence, for i.i.d. data $S \sim P^n$, if $\text{KL}(P_0, P_1) \leq \frac{\log(2)}{n}$, then $R^* \geq \frac{\delta}{8}$

2. **Local Fano Method:** If $\{P_1, \dots, P_N\}$ are δ -separated, then

$$R^* \geq \delta \left(1 - \frac{\sum_{j,k} \text{KL}(P_j, P_k) + \log(2)}{N^2 \log(N)} \right)$$

Hence, for i.i.d. data $S \sim P^n$, if $\text{KL}(P_j, P_k) \leq \frac{\log(N)}{4n}$, and $N \geq 16$, then $R^* \geq \frac{\delta}{8}$

Remark While our focus is on prediction problems, this framework and theorems apply to any problem for which

$$\inf_{h \in \mathcal{H}} L(h, P) = 0 \quad \forall P \in \mathcal{P}.$$

2 Application: Classification in a VC class

We will now use the above results to prove a lower bound for classification in a VC class.

Theorem 4. Let \mathcal{P} be the set of all distributions supported on $\mathcal{X} \times \{0, 1\}$. Let $\mathcal{H} \subseteq \{h : \mathcal{X} \rightarrow \mathcal{Y}\}$ be a hypothesis class with VC dimension $d \geq 8$. Let $S = \{(X_1, Y_1), \dots, (X_n, Y_n)\} \sim_{iid} P$, where $P \in \mathcal{P}$. Then, for any estimator \hat{h} which maps the data set S to a hypothesis in \mathcal{H} ,

$$R^* = \inf_{\hat{h}} \sup_{P \in \mathcal{P}} \left(\mathbb{E}[F(\hat{h}, P)] - \inf_{h' \in \mathcal{H}} F(h', P) \right) \geq C_1 \sqrt{\frac{d}{n}}$$

for some global constant C_1 .

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Proof Our proof will follow the usual four step recipe when applying Fano/Le Cam methods.

Step 1: Construct alternatives.

Let $\mathcal{X}_d = \{x_1, \dots, x_d\}$ be a d -lettered alphabet by \mathcal{H} . Let $\gamma \leq 1/4$ be a value which will be specified later. Define

$$\mathcal{P}' = \{P_\omega : P_\omega(X = x_i) = \frac{1}{d}, P_\omega(Y = 1|X = x_i) = \frac{1}{2} + (2\omega_i - 1)\gamma, \omega \in \Omega_d\},$$

where Ω_d is the VG-primitive set of size d .

Remark To illustrate the proof, consider the class of two-sided threshold classifiers with $d = 2$, i.e. $\mathcal{X}_2 = \{x_1, x_2\}$ with $P_\omega(X = x_1) = P_\omega(X = x_2) = 1/2$. Then the conditional distribution of Y should be

$$P_\omega(Y = 1|X = x_1) = \frac{1}{2} - \gamma, \quad P_\omega(Y = 1|X = x_2) = \frac{1}{2} + \gamma$$

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Step 2: Lower bound the separation $\min_{\omega, \omega'} \Delta(P_\omega, P_{\omega'})$.

We have the following claim: For any $P_\omega, P_{\omega'} \in \mathcal{P}'$, the separation satisfies

$$\Delta(P_\omega, P_{\omega'}) \geq \frac{\gamma}{d} H(\omega, \omega')$$

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We will prove this claim in homework. Then by the Varshamov-Gilbert lemma, we have

$$\min_{\omega, \omega'} \Delta(P_\omega, P_{\omega'}) \geq \frac{\gamma}{d} \delta \triangleq \delta$$

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Step 3: Upper bound the KL divergence $\max_{\omega, \omega'} KL(P_\omega, P_{\omega'})$. We have,

$$\begin{aligned} KL(P_\omega, P_{\omega'}) &= \sum_{x, Y} P_\omega(x, Y) \log \frac{P_\omega(x, Y)}{P_{\omega'}(x, Y)} \\ &= \sum_{i=1}^d P_\omega(x_i) \sum_{y \in \{0,1\}} P_\omega(y|x_i) \log \frac{P_\omega(y|x_i)}{P_{\omega'}(y|x_i)} \quad (\text{as } P_\omega(x) = P_{\omega'}(x)) \\ &= \sum_{i=1}^d \frac{1}{d} \mathbb{1}_{\{\omega \neq \omega'\}} \underbrace{\left[(1/2 + \gamma) \log \frac{1/2 + \gamma}{1/2 - \gamma} + (1/2 - \gamma) \log \frac{1/2 - \gamma}{1/2 + \gamma} \right]}_{=O(\gamma^2)} \\ &\leq C_2 \frac{\gamma^2}{d} H(\omega, \omega'). \end{aligned}$$

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Therefore, with $H(\omega, \omega') \leq d$, we have

$$\max_{\omega, \omega'} KL(P_\omega, P_{\omega'}) \leq C_2 \gamma^2.$$

Step 4: To conclude the proof, we will choose $\gamma = C_3 \sqrt{d/n}$. Then we have

$$\max_{\omega, \omega'} KL(P_\omega, P_{\omega'}) \leq C_4 \frac{d}{n} \leq \frac{\log(2^{d/8})}{4n} \leq \frac{\log(|\mathcal{P}'|)}{4n},$$

where the last inequality is by the Varshamov-Gilbert lemma. Then, by the local Fano method, we have

$$R^* \geq \frac{\delta}{2} \geq C_5 \sqrt{\frac{d}{n}}.$$

□

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3 Stochastic Bandits

In the next series of lectures, we will consider solving sequential/adaptive decision making problems in which there exists a sequence of possible actions. Specifically, on round t , the learner chooses an action A_t from a set of possible actions. Then the environment reveals an observation O_t . In return, the learner receives a reward $X_t = X_t(O_t, A_t)$. The learner's goal is to maximize the sum of rewards $\sum_{t=1}^T X_t$. Sequential/adaptive decision making problems are typical examples of stochastic bandits and online learning.



We will first focus on stochastic bandits. A stochastic bandit problem consists of the following components:

- Let $\nu = \{\nu_a, a \in \mathcal{A}\}$ be a family of probability distributions indexed by actions in \mathcal{A} . ν is called a bandit model and is a subset of some family \mathcal{P} .
- On round t , the learner chooses $A_t \in \mathcal{A}$ and observes a reward X_t sampled from ν_{A_t} .
- The learner is characterized by a policy $\Pi = (\Pi_t)_{t \in \mathbb{N}}$, where Π_t maps the history $\{(A_s, X_s)\}_{s=1}^{t-1}$ to an action in \mathcal{A} .
- If Π is a randomized policy, Π_t maps the history to a probability distribution on \mathcal{A} , and then an action is sampled from this distribution. It can also be a deterministic policy.
- $\mu_a = \mathbb{E}_{X \sim \nu_a}[X]$ is defined to be the expected reward of the action a . Let $a^* \in \arg \max_{a \in \mathcal{A}} \mu_a$ be an optimal action, and let $\mu_* = \mu_{a^*}$ be the corresponding optimal value of the expected reward.
- Finally, we define the regret after T rounds of interaction as

$$R_T = R_T(\pi, \nu) = T\mu_* - \mathbb{E}\left[\sum_{t=1}^T X_t\right]$$

where \mathbb{E} is with respect to the distribution of the action-reward sequence $A_1, X_1, A_2, X_2, \dots, A_T, X_T$ induced by the interaction between the policy π and bandit model ν . Here, μ_a , a^* , and μ_* should be viewed as functions of the bandit model ν and can be written as $\mu_a(\nu)$, $a^*(\nu)$, and $\mu_*(\nu)$.

When designing an algorithm for bandits, at the bare minimum, we will require $R_T \in \mathcal{O}(T)$, i.e. $\lim_{T \rightarrow \infty} \frac{R_T}{T} = 0$. This implies that over time, a learner is able to eventually learn the optimal arm.