**CS861: Theoretical Foundations of Machine Learning** University of Wisconsin–Madison, Fall 2023 Lecture 8 - 09/22/2023

Lecture 08: Introduction to Minimax Optimality

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In this lecture, we introduce Minimax Optimality and some related concepts. We will first introduce minimax optimality, then discuss some topics beyond point estimation.

## **1** Minimax Optimality

Recall that we cannot find an estimator that is uniformly better than other estimators in most cases, i.e. there is no  $\hat{\theta}$  better than any other  $\hat{\theta}'$  in the sense that

$$R(P,\widehat{\theta}) \le R(P,\widehat{\theta}'), \qquad \forall P \in \mathcal{P},$$

Therefore, we wish to find an estimator which minimizes the maximum risk,

$$\sup_{P\in\mathcal{P}} R(P,\widehat{\theta}).$$

**Definition 1.** The minimax risk  $R^*$  of a point estimation problem is defined as follows,

$$R^* = \inf_{\widehat{\theta}} \sup_{P \in \mathcal{P}} R(P, \widehat{\theta}) = \inf_{\widehat{\theta}} \sup_{P \in \mathcal{P}} \mathbb{E}_{S \sim P} \left[ \ell(\theta(P), \widehat{\theta}(S)) \right]$$

Note that  $R^*$  depends on  $\mathcal{P}$ , loss function  $\ell$ , and the size of S. An estimator  $\hat{\theta}^*$  which achieves the minimax risk, i.e.  $\sup_{P \in \mathcal{P}} R(P, \hat{\theta}^*) = R^*$  is said to be **minimax-optimal**.

How do you compute the minimax risk? Classically, this was done via a concept called the "least favorable prior", which involved finding a Bayes' estimator with constant (frequentist) risk.

In this class, we will follow the following recipe for computing the minimax risk, which we will also apply to general estimation problems.

1. Design a "good estimator"  $\hat{\theta}$ , and upper bound its risk by  $U_n$ , then

$$R^* \le \sup_{P \in \mathcal{P}} R(P, \widehat{\theta}) \le U_n$$

2. Design a "good prior"  $\Lambda$  on  $\mathcal{P}$  and lower bound the Bayes' risk, say by  $L_n$ .

Recall that for any estimator  $\hat{\theta}$ ,

$$\sup_{P \in \mathcal{P}} R(P, \widehat{\theta}) \ge \mathbb{E}_{P \sim \Lambda} \left[ R(P, \widehat{\theta}) \right] \ge \mathbb{E}_{P \sim \Lambda} \left[ R(P, \widehat{\theta}_{\Lambda}) \right] \ge L_n.$$

where  $\hat{\theta}_{\Lambda}$  is the Bayes' estimator. the first inequality holds since "sup  $\geq$  average" and the second inequality holds since the Bayes' estimator minimizes the Bayes' risk. By taking the infimum over all estimators, we have  $R^* \geq L_n$ .

3. Sometimes, we may need to restrict to a sub-class  $\mathcal{P}' \subset \mathcal{P}$ , and construct our prior  $\Lambda$  on  $\mathcal{P}'$ . We have,

$$\sup_{P \in \mathcal{P}} R(P, \widehat{\theta}) \ge \sup_{P \in \mathcal{P}'} R(P, \widehat{\theta}).$$

- 4. If  $U_n = L_n$ , then  $U_n$  is the **minimax risk** and  $\hat{\theta}$  is **minimax-optimal**.
- 5. It is not always possible to achieve exact equality. However, if  $U_n > L_n$ , but  $U_n \in O(L_n)$ , then  $U_n$  is the minimax rate and  $\hat{\theta}$  is rate-optimal.

**Example 1.** Let  $S = \{X_1, ..., X_n\}$  drawn i.i.d. from  $\mathcal{N}(\mu, \sigma^2)$ ,  $\mathcal{P} = \{\mathcal{N}(\mu, \sigma^2); \mu \in \mathbb{R}\}$ , we will show that  $\widehat{\theta}_{SM}(S) = \frac{1}{n} \sum_{i=1}^{n} X_i$  is minimax-optimal. **Proof** First, we find the upper bound

$$\sup_{P \in \mathcal{P}} R(P, \widehat{\theta}) \stackrel{def}{=} \sup_{\mu \in \mathbb{R}} \mathbb{E}_{S \sim \mathcal{N}(\mu, \sigma^2)} \left[ (\mu - \widehat{\theta}(S))^2 \right] = \sup_{\mu \in \mathbb{R}} \frac{\sigma^2}{n} = \frac{\sigma^2}{n} \implies R^* \le \frac{\sigma^2}{n}$$

Then we find the lower bound via Bayes' risk. Consider the prior  $\Lambda = \mathcal{N}(0, \tau^2)$ , from our example in the last lecture,

$$R^* \ge L_n = \left(\frac{1}{\tau^2} + \frac{1}{\sigma^2/n}\right)^{-1} \quad \text{holds for every } \tau^2,$$
$$\Longrightarrow R^* \ge \sup_{\tau^2 > 0} \left(\frac{1}{\tau^2} + \frac{1}{\sigma^2/n}\right)^{-1} = \frac{\sigma^2}{n}.$$

Combining two bounds together, we can conclude that  $\hat{\theta}_{SM}$  is minimax-optimal and  $\frac{\sigma^2}{n}$  is the minimax risk.

**Example 2.** Let  $S = \{X_1, ..., X_n\}$  drawn i.i.d. from  $Bernoulli(\theta)$ , where  $\theta = \mathbb{E}_{X \sim P}[X]$ . Let  $\mathcal{P} = \{Bernoulli(\theta); \theta \in [0, 1]\}$ . Let us consider  $\hat{\theta}(S) = \frac{1}{n} \sum_{i=1}^{n} X_i$ .

First, the upper bound is found as follows,

$$R(P,\hat{\theta}) = \mathbb{E}_{S \sim P} \left[ (\theta - \hat{\theta}(S))^2 \right] = \frac{\text{Variance}}{n} = \frac{\theta(1-\theta)}{n},$$
$$\sup_{P \in \mathcal{P}} R(P,\hat{\theta}) = \sup_{\theta \in [0,1]} \frac{\theta(1-\theta)}{n} = \frac{1}{4n} \implies R^* \le \frac{1}{4n}.$$

To find the lower bound, we use  $\Lambda = \text{Beta}(a, b)$  as the prior, then we have the following Bayes' risk,

$$\frac{1}{(n+a+b)^2} \left[ \left( n - (a+b)^2 \right) \mathbb{E}_{\theta} \left[ \theta^2 \right] + \left( n - 2a(a+b) \right) \mathbb{E}_{\theta} \left[ \theta \right] + a^2 \right].$$

By choosing  $a = b = \frac{\sqrt{n}}{2}$ , we get

$$L_n = \frac{a^2}{(n+a+b)^2} = \frac{n/4}{(n+a+b)^2} = \frac{1}{4(\sqrt{n}+1)^2} = \frac{1}{4n+8\sqrt{n}+4}$$

We have  $U_n > L_n$ , but  $U_n \in O(L_n) \Longrightarrow \widehat{\theta}_{SM}$  is rate-optimal and  $\frac{1}{n}$  is the minimax-rate. As a side note, it can be shown that

$$\hat{\theta}^* = \frac{\sqrt{n}}{1+\sqrt{n}} \left(\frac{1}{n} \sum_{i=1}^n X_i\right) + \frac{1}{2} \left(\frac{1}{1+\sqrt{n}}\right)$$

is minimax-optimal and  $\frac{1}{4(\sqrt{n}+1)^2}$  is the minimax risk.

**Example 3.**  $S = \{X_1, ..., X_n\}$  drawn i.i.d. from  $P \in \mathcal{P}$ .  $\mathcal{P} = \{$  all distribution with variance bounded by  $B^2\}$ . We will show that  $\hat{\theta}_{SM}(S) = \frac{1}{n} \sum_{i=1}^n X_i$  is minimax-optimal. **Proof** For the upper bound,

$$\sup_{P \in \mathcal{P}} R(P, \widehat{\theta}) = \sup_{P \in \mathcal{P}} \mathbb{E}_{S \sim P} \left[ (\widehat{\theta}(S) - \theta)^2 \right] = \sup_{P \in \mathcal{P}} \frac{\text{variance}}{n} = \frac{B^2}{n} \implies R^* \le \frac{B^2}{n}$$

The lower bound can be found by choosing a sub-class  $\mathcal{P}' = \{\mathcal{N}(\mu, B^2); \mu \in \mathbb{R}\},\$ 

$$R^* = \inf_{\widehat{\theta}} \sup_{P \in \mathcal{P}} R(P, \widehat{\theta}) \ge \inf_{\widehat{\theta}} \sup_{P \in \mathcal{P}'} R(P, \widehat{\theta}) = \frac{B^2}{n}$$

Combining two bounds together, we know that  $\frac{B^2}{n}$  is the minimax risk and  $\hat{\theta}_{SM}$  is minimax-optimal.  $\Box$ 

We will now study minimaxi optimality for general estimation problems. The following lessons from point estimation will be useful going forward.

- 1) Often, the easiest way to lower bound the maximum risk is to lower bound it via the average risk, by using the fact that the maximum is larger than the average.
- 2) We should be careful in how we choose a subset  $\mathcal{P}$  and prior  $\Lambda$ , so that the lower bound is tight.
- 3) We still need to design a good estimator to establish the upper bound.

## 2 Beyond Point Estimation

We will now extend the ideas beyond point estimation. Our estimation problem will have the following components:

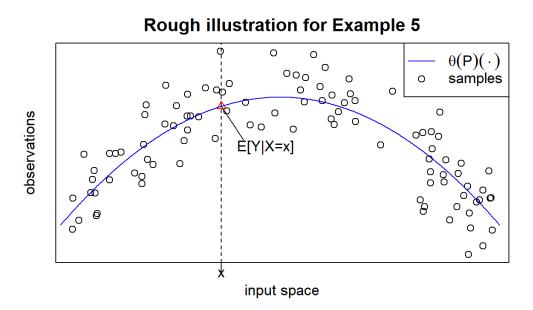
- 1. A family of distributions  $\mathcal{P}$
- 2. A dataset S of n i.i.d points drawn from  $P \in \mathcal{P}$
- 3. A function(parameter)  $\theta : \mathcal{P} \to \Theta$ . We wish to estimate  $\theta(P)$  from S.
- 4. An estimator  $\hat{\theta} = \hat{\theta}(S) \in \Theta$
- 5. A loss function  $\ell$ ,  $\ell = \Phi \circ \rho$ , satisfies the following conditions:
  - $\rho: \Theta \times \Theta \to \mathbb{R}_+$  satisfies the following properties for all  $\theta_1, \theta_2, \theta_3 \in \Theta$ ,
    - (i)  $\rho(\theta_1, \theta_1) = 0$ ,
    - (ii)  $\rho(\theta_1, \theta_2) = \rho(\theta_2, \theta_1),$
    - (iii)  $\rho(\theta_1, \theta_2) \le \rho(\theta_1, \theta_3) + \rho(\theta_3, \theta_2).$
  - $\Phi : \mathbb{R}_+ \to \mathbb{R}_+$  is non-decreasing.

When we estimate  $\theta(P)$  with  $\hat{\theta}$ , the loss is  $\ell(\theta(P), \hat{\theta}) = \Phi(\rho(\theta(P), \hat{\theta}))$ .

6. The risk of an estimato r  $\hat{\theta}$  is,

$$R(P,\hat{\theta}) = \mathbb{E}_{S \sim P} \left[ \Phi \circ \rho(\theta(P), \hat{\theta}(S)) \right] = \mathbb{E}_S \left[ \Phi \circ \rho(\theta, \hat{\theta}) \right].$$

Note that, as before we have overloaded notation so that  $\theta$  denotes the parameter  $\theta \in \Theta$  and the function  $\theta : \mathcal{P} \to \Theta$ . Similarly,  $\hat{\theta}$  denotes the estimate  $\hat{\theta} \in \Theta$  and the estimator, which maps the data to  $\Theta$ .



**Figure 1:** Figure to explain  $\theta(P)(\cdot)$ . Black dots are the observed data, blue curve is the regression function  $\theta(P)(\cdot)$ , For every *x*, the point of intersection, which is marked in red, is the regression result  $\mathbb{E}[Y|X = x]$ .

**Definition 2.** We can now define the minimax risk  $R^*$  as follows,

$$R^* = \inf_{\widehat{\theta}} \sup_{P \in \mathcal{P}} \mathbb{E}_S \left[ \Phi \circ \rho \left( \theta(P), \widehat{\theta}(S) \right) \right].$$

**Example 4.** Normal mean estimation Let  $S = \{X_1, ..., X_n\}$  drawn i.i.d. from  $\mathcal{N}(\mu, \sigma^2)$ , where  $\sigma^2$  is known. Here,  $\mathcal{P} = \{\mathcal{N}(\mu, \sigma^2); \mu \in \mathbb{R}\}$ . We wish to estimate  $\theta(P) = \mathbb{E}_{X \sim P}[X]$ , therefore  $\Theta = \mathbb{R}$ . If we use the squared loss  $\ell(\theta_1, \theta_2) = (\theta_1 - \theta_2)^2$ , then  $\rho = |\theta_1 - \theta_2|$  and  $\Phi(t) = t^2$ .

**Example 5.** (Regression) Here,  $\mathcal{P}$  is the set of all distributions with support on  $\mathcal{X} \times \mathbb{R}$ , where is the input space. = The parameter space  $\Theta = \{h : \mathcal{X} \to \mathbb{R}\}$ , is the class of functions mapping  $\mathcal{X}$  to . We wish to estimate the regression function, which is given by

$$\theta(P)(\cdot) = \underbrace{\mathbb{E}[Y|X=\cdot]}_{\text{regression function: see Fig 1}} = \int y dP(y|X=x)$$

We have illustrated this in Figure 1. If we use the  $L_2$  loss,  $\ell(\theta_1, \theta_2) = \int_{\mathcal{X}} (\theta_1(x) - \theta_2(x))^2 dx$ , then, we have

$$\rho(\theta_1, \theta_2) = \sqrt{\int_{\mathcal{X}} (\theta_1(x) - \theta_2(x))^2 dx} \stackrel{\Delta}{=} \|\theta_1 - \theta_2\|_2, \text{ and } \Phi(t) = t^2$$