1 Point estimation

1.1 Maximum Likelihood Estimators

The maximum likelihood method is the most popular way to estimate the parameter θ which specifies a probability model. The maximum likelihood estimate is the value $\hat{\theta}$ which maximize the likelihood function. That is, the maximum likelihood estimation chooses the model parameter $\hat{\theta}$ which is the **most likely to generate the observed data**.

Definition 1.1. Let $X_{1:n} \sim f_{\theta}$, where $\theta \in \Theta$. Denote the likelihood function of θ by $L(\theta) = L(\theta \mid X_{1:n}) = f_{\theta}(X_{1:n})$, and log-likelihood function by $\ell(\theta) = \log L(\theta)$. The maximum likelihood estimator (MLE) of θ is

$$\widehat{\theta} = \underset{\theta \in \Theta}{\arg\max} L(\theta) = \underset{\theta \in \Theta}{\arg\max} \ell(\theta)$$

Here we briefly review three good properties of the maximum likelihood estimation:

Theorem	Sketch of Proof
consistency (asymptotic correctness)	positivity of Kullback-Leibler divergence
asymptotic normality: $\hat{\theta} \sim \mathcal{N}\left(\bar{\theta}, \frac{1}{n}I^{-1}\right)$	central limit theorem for delta method
efficiency (minimum variance)	Cauchy-Schwarz inequality

Table 1: Theorems for maximum likelihood estimation.

To study the theoretical properties of MLEs, we need the notations below.

Definition 1.2. . Let f and g be densities with support \mathcal{X} . The Kullback-Leibler (KL) distance between f and g is

$$\mathrm{KL}(f \mid g) = \int_{x} f(x) \log \frac{f(x)}{g(x)} \mathrm{d}x = \mathsf{E}\left(\log \frac{f(X)}{g(X)}\right)$$

if we assume that $X \sim f$

Remark 1.1. The definition is motivated by concepts from information theory and relative entropy.

- <u>relative entropy</u> measures the <u>inefficiency</u> or <u>additional information required</u> when using one distribution (denoted Q) to approximate or represent another distribution (denoted P).
- The KL distance is the difference of entropy between true model and another model.

We can see that

• $\operatorname{KL}(f \mid g) \ge 0$ since

$$\mathsf{E}\left(\log\frac{f(X)}{g(X)}\right) = \mathsf{E}\left(-\log\frac{g(X)}{f(X)}\right) \ge -\log\mathsf{E}\left(\frac{g(X)}{f(X)}\right) = -\log\int_{\mathcal{X}}\frac{g(x)}{f(x)}f(x)dx = 0$$

and the equality holds iff f = g.

- $\operatorname{KL}(f \mid f) = 0$, and
- $\operatorname{KL}(f \mid g) \neq \operatorname{KL}(g \mid f)$ in general.

We consider well-specified and identifiable statistical models. Now define

$$\widehat{M}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \log \frac{f_{\theta}(X_i)}{f_{\theta_{\star}}(X_i)} \quad \text{and} \quad M(\theta) = \mathcal{E}_{\star} \left\{ \log \frac{f_{\theta}(X_1)}{f_{\theta_{\star}}(X_1)} \right\}$$

Remark 1.2. Let $M(\theta)$ represent the negative KL divergence. Our objective is to find an estimator that minimizes this divergence, i.e.,

$$\theta_{\star} = \operatorname*{arg\,max}_{\theta \in \Theta} M(\theta)$$

However, since $M(\theta)$ cannot be computed directly, we use an empirical estimate $\widehat{M}(\theta)$ as a substitute. Thus, we seek

$$\widehat{\theta} = \operatorname*{arg\,max}_{\theta \in \Theta} \widehat{M}(\theta),$$

which is equivalent to the maximum likelihood estimator (MLE). Therefore, finding the MLE is equivalent to identifying the estimator that minimizes the estimated KL divergence.

Definition 1.3. The statistical model $\mathscr{F} = \{f_{\theta} : \theta \in \Theta\}$ is said to be identifiable if

 $\forall \theta \neq \theta', \quad \mathrm{KL}\left(f_{\theta'} \mid f_{\theta}\right) > 0$

Definition 1.4. Let f_{\star} be the data generating density. The model $\mathscr{F} = \{f_{\theta} : \theta \in \Theta\}$ is said to be well-specified if

$$\forall \theta \neq \theta', \quad \operatorname{KL}\left(f_{\theta'} \mid f_{\theta}\right) > 0$$

1.1.1 Consistency

The first property is that, as the number of observations n becomes large, the estimate $\hat{\theta}$ converges to the true value θ_{\star} .

Theorem 1.1. Assume:

$$\begin{array}{ll} (\text{Maximizer:}) & \widehat{\theta} = \operatorname*{arg\,max} \widehat{M}(\theta), \\ (\text{Uniform LLN}): & \sup_{\theta \in \Theta} |\widehat{M}(\theta) - M(\theta)| \xrightarrow{\mathrm{pr}} 0, \\ (\text{Well-separation}): & \forall \varepsilon > 0, \quad \sup_{\theta: |\theta - \theta_{\star}| > \varepsilon} M(\theta) < M(\theta_{\star}) \end{array}$$

Then $\widehat{\theta} \xrightarrow{\mathrm{pr}} \theta_{\star}$.

<u>S</u> Intuition: Since two functions $\widehat{M}(\theta)$ and $M(\theta)$ are getting closer, the points of maximum should also get closer which exactly means that $\hat{\theta} \to \theta_0$.

Proof. First, we examine the difference in the true Kullback-Leibler (KL) divergence between the true parameter θ_{\star} and the maximum likelihood estimator (MLE) $\hat{\theta}$:

$$0 \leq M(\theta_{\star}) - M(\hat{\theta}) = \left\{ M(\theta_{\star}) - \widehat{M}(\hat{\theta}) \right\} + \left\{ \widehat{M}(\hat{\theta}) - M(\hat{\theta}) \right\}$$
Add and subtract $\widehat{M}(\hat{\theta})$
$$\leq \left\{ M(\theta_{\star}) - \widehat{M}(\theta_{\star}) \right\} + \left\{ \widehat{M}(\hat{\theta}) - M(\hat{\theta}) \right\}$$
 $\hat{\theta}$ maximizes $\widehat{M}(\theta)$
$$\leq 2 \sup_{\theta \in \Theta} \left| \widehat{M}(\theta) - M(\theta) \right| \xrightarrow{\text{pr}} 0.$$
Uniform convergence

indicating that the difference converges to zero in probability. Given the strong identifiability of θ_{\star} , there exists a $\delta > 0$ such that:

$$|\theta - \theta_{\star}| \ge \varepsilon \quad \Rightarrow \quad M(\theta) < M(\theta_{\star}) - \delta$$

Note that if $A \Rightarrow B$, then $P(A) \le P(B)$. So, putting $\theta = \hat{\theta}$, we have

$$P\left(\left|\widehat{\theta} - \theta_{\star}\right| \ge \varepsilon\right) \le P\left\{M(\widehat{\theta}) < M\left(\theta_{\star}\right) - \delta\right\} \to 0$$

There are many different versions of conditions for proving consistency of MLE. Many of them <u>rely heavily</u> on the uniform LLN. We provide an alternative set of conditions.

Theorem 1.2. Let $\{f_{\theta} : \theta \in \Theta\}$ be the model, and $X_1, X_2, \ldots \stackrel{IID}{\sim} f_{\theta_{\star}}$. Assume

- 1. (Compactness.) Θ is compact;
- 2. (Uniqueness of maximizer.) θ^* is the unique maximizer of $\theta \mapsto M(\theta)$;
- 3. (Continuous.) $M(\theta)$ is continuous in θ ;
- 4. (Uniform LLN.) $\widehat{M}(\theta)$ converges uniformly in probability.

Then $\widehat{\theta} \xrightarrow{\mathrm{pr}} \theta_{\star}$.

Proof. For $\epsilon > 0$, define the ϵ -neighborhood around θ_{\star} as:

$$\Theta(\epsilon) = \{\theta : \|\theta - \theta_\star\| < \epsilon\}$$

We aim to show that

$$P_{\theta_0}\left[\hat{\theta}\in\Theta(\epsilon)\right]\to 1$$

Since $\Theta(\epsilon)$ is an open set, we know that $\Theta \cap \Theta(\epsilon)^C$ is a compact set. Since $M(\theta)$ is a continuous function, then $\sup_{\theta \in \Theta \cap \Theta(\epsilon)^C} \{M(\theta)\}$ is achieved for a θ in this compact set. Denote this value by θ_0 . Since θ_{\star} is the unique max, let $M(\theta_{\star}) - M(\theta_0) = \delta > 0$. For any θ , we distinguish between two cases.

• $\theta \in \Theta \cap \Theta(\epsilon)^C$.

Let A_n be the event that $\sup_{\theta \in \Theta \cap \Theta(\epsilon)^C} \left| M(\theta) - \widehat{M}(\theta) \right| < \delta/2$. Then

$$A_n \Rightarrow \widehat{M}(\theta) < M(\theta) + \delta/2$$

$$\leq M(\theta_0) + \delta/2$$

$$= M(\theta_{\star}) - \delta + \delta/2$$

$$= M(\theta_{\star}) - \delta/2$$

• $\theta \in \Theta(\epsilon)$.

Let B_n be the event that $\sup_{\Theta(\epsilon)} \left| M(\theta) - \widehat{M}(\theta) \right| < \delta/2$. Then

$$B_n \Rightarrow \widehat{M}(\theta) > M(\theta) - \delta/2 \text{ for all } \theta$$
$$\Rightarrow \widehat{M}(\theta) > M(\theta_\star) - \delta/2$$

We conclude that if both A_n and B_n hold then $\hat{\theta} \in \Theta(\epsilon)$. By the proof of theorem 1.1, we know that as long as $\widehat{M}(\theta)$ converges uniformly in probability, $M(\theta_*) - M(\widehat{\theta}) \xrightarrow{\text{pr}} M(\theta)$. Comparing the two cases above we have $\hat{\theta} \in \Theta(\epsilon)$.

A key element of above two proof is that converges uniformly in probability. But it is difficult to prove.

Lemma 1.3. Let $\{f_{\theta} : \theta \in \Theta\}$ be the model, and $X_1, X_2, \ldots \stackrel{IID}{\sim} f_{\theta_*}$. Θ is compact, $\log f(x; \theta)$ is continuous in θ for all $\theta \in \Theta$ and all $x \in \mathcal{X}$, and if there exists a function d(x) such that $|\log f(x; \theta)| \leq d(x)$ for all $\theta \in \Theta$ and $x \in \mathcal{X}$, and $E_{\theta_0}[d(X)] < \infty$, then

- $M(\theta)$ is continuous in θ ;
- $\sup_{\theta \in \Theta} \left| \widehat{M}(\theta) M(\theta) \right| \stackrel{\text{pr}}{\to} 0$

Proof. To establish continuity, we need to demonstrate that if $\theta_k \to \theta$, then $M(\theta_k) \to M(\theta)$. Specifically, we need to show that

$$M(\theta_k) = \mathsf{E}\left(\log\left(\frac{f_{\theta_k}}{f_{\theta_\star}}\right)\right) \to M(\theta) = \mathsf{E}\left(\log\left(\frac{f_{\theta}}{f_{\theta_\star}}\right)\right)$$

By the continuity of f_{θ} , we know that $\log f_{\theta_k} \to \log f_{\theta}$. Furthermore, since $\log f_{\theta} \leq d(X)$ and $\mathsf{E}d(X) < \infty$, we can apply the dominated convergence theorem, which ensures the desired convergence holds. Since Θ is compact, we also know that $M(\theta)$ is **uniformly continuous**.

Regarding uniform convergence, we need to establish that

$$\sup_{\theta \in \Theta} \left| \widehat{M}(\theta) - M(\theta) \right| \stackrel{\text{pr}}{\to} 0$$

We have already shown that $M(\theta)$ is uniformly continuous. Now, we consider the properties of $\widehat{M}(\theta)$. Since $\widehat{M}(\theta)$ is the average of the log-likelihood, its behavior is closely related to the properties of the likelihood function $f_{\theta}(x)$. As $f_{\theta}(x)$ is continuous in Θ and Θ is compact, it follows that $\log f_{\theta}(x)$ is also uniformly continuous. Thus, for any $\epsilon > 0$, there exists $\delta(\epsilon)$ such that if $\|\theta_1 - \theta_2\| < \delta$, we have

$$\sup_{\|\theta_1 - \theta_2\| < \delta} \left| \log f_{\theta_1}(x) - \log f_{\theta_2}(x) \right| < \epsilon$$

which implies that

$$\Delta(x,\delta) = \sup_{\|\theta_1 - \theta_2\| < \delta} \left| \log f_{\theta_1}(x) - \log f_{\theta_2}(x) \right| \to 0$$

Therefore, if $\|\theta_1 - \theta_2\| < \delta$, for all $x \in \mathcal{X}$, we obtain

$$\left|\widehat{M}(\theta_1) - \widehat{M}(\theta_2)\right| = \left|\frac{1}{n}\sum_{i=1}^n \left(\log f_{\theta_1}(x_i) - \log f_{\theta_2}(x_i)\right)\right|$$
$$\leq \frac{1}{n}\sum_{i=1}^n \left|\log f_{\theta_1}(x) - \log f_{\theta_2}(x)\right|$$
$$\leq \frac{1}{n}\sum_{i=1}^n \Delta(x,\delta) \to 0$$

So $M(\theta)$ is also uniform continuous.

Now we can maginify the target inequality and use the properties of uniformly continuous.

To begin, we first cut off our set Θ by considering an open ball of radius δ around each $\theta \in \Theta$, i.e., $B(\theta, \delta) = \{\tilde{\theta} : \|\tilde{\theta} - \theta\| < \delta\}$. The union of these balls forms an open cover of Θ . By compactness, we can find a finite subcover, denoted as $\{B(\theta_j, \delta), j = 1, \ldots, J\}$. For each $\theta \in \Theta$, there exists a θ_j such that $\theta \in B(\theta_j, \delta)$. Therefore, for any $\theta \in \Theta$, we have

$$|\widehat{M}(\theta) - M(\theta)| \le |\widehat{M}(\theta) - \widehat{M}(\theta_j)| + |\widehat{M}(\theta_j) - M(\theta_j)| + |M(\theta_j) - M(\theta)|$$

Since $M(\theta)$ and $M(\theta)$ are uniformly continuous, we can choose δ small enough such that both $|M(\theta) - M(\theta_j)|$ and $|M(\theta_j) - M(\theta)|$ can be bounded by $\epsilon/3$. So

$$|\widehat{M}(\theta) - M(\theta)| \le \epsilon/3 + \max_{j=1,2,\cdots,J} |\widehat{M}(\theta_j) - M(\theta_j)| + \epsilon/3$$

which implies that

$$\sup_{\theta \in \Theta} |\widehat{M}(\theta) - M(\theta)| \le 2\epsilon/3 + \max_{j=1,2,\cdots,J} |\widehat{M}(\theta_j) - M(\theta_j)|$$

Further, we have

$$\sup_{\theta \in \Theta} |\widehat{M}(\theta) - M(\theta)| > \epsilon \implies \max_{j=1,2,\cdots,J} |\widehat{M}(\theta_j) - M(\theta_j)| > \epsilon/3$$

We now show that

$$\mathsf{P}\left(\max_{j=1,2,\cdots,J}|\widehat{M}(\theta_j) - M(\theta_j)| > \epsilon/3\right) \xrightarrow{\mathrm{pr}} 0.$$

It is easy since

$$\mathsf{P}\left(\max_{j=1,2,\cdots,J}|\widehat{M}(\theta_{j}) - M(\theta_{j})| > \epsilon/3\right) = \mathsf{P}\left(\bigcup_{j=1,2,\cdots,J}\left\{|\widehat{M}(\theta_{j}) - M(\theta_{j})| > \epsilon/3\right\}\right) \\
\leq \sum_{j=1,2,\cdots,J}\mathsf{P}\left(\left\{|\widehat{M}(\theta_{j}) - M(\theta_{j})| > \epsilon/3\right\}\right)$$

then by WLLN, we know that for each θ_j and for any $\epsilon > 0, \eta > 0$ there exists $N(\epsilon, \eta)$ so that for all $n > N_j(\epsilon, \eta)$

$$\mathsf{P}\left(\left\{|\widehat{M}(\theta_j) - M(\theta_j)| > \epsilon/3\right\}\right) < \eta/J$$

Let $N = \max N_j$ we have that

$$\sum_{j=1,2,\cdots,J} \mathsf{P}\left(\left\{ |\widehat{M}(\theta_j) - M(\theta_j)| > \epsilon/3 \right\} \right) < \eta$$

Finally,

$$\mathsf{P}\left(\sup_{\theta\in\Theta}\left|\widehat{M}(\theta) - M(\theta)\right| > \epsilon\right) \le \mathsf{P}\left(\max_{j=1,2,\cdots,J}\left|\widehat{M}(\theta_j) - M(\theta_j)\right| > \epsilon/3\right) \xrightarrow{\mathrm{pr}} 0$$

which completes the proof.