STAT 24400 Lecture 15
Section 8.5.2 Large Sample Theory for MLEs
Section 8.5.3 Confidence Intervals from MLEs

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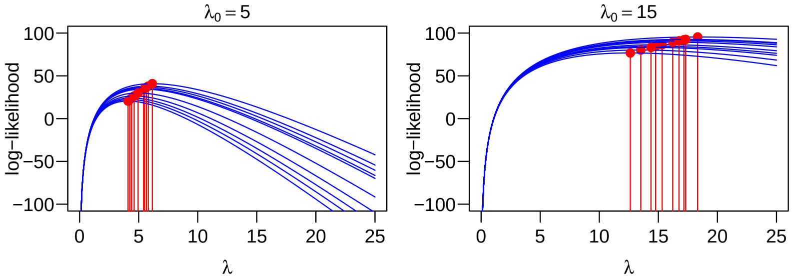
Accuracy of the MLE

Example: Suppose $X_1, \ldots, X_{50} \overset{\text{iid}}{\sim} \text{Exponential}(\lambda_0)$.

Recall the log likelihood for i.i.d. Exponential(λ) is

$$\ell(\lambda) = n \log(\lambda) - n\lambda\overline{X}$$

Here is a plot of the log likelihood function $\ell(\lambda)$, and the MLE, over 10 trials:



$\Rightarrow$ higher curvature of $\ell(\lambda)$ around the true value λ_0 leads to a more accurate estimate

Curvature of a Function (Calculus Review)

For a sufficiently smooth function $g(u)$, if u_0 is a local maximum or minimum of $g(u)$, then $g'(u_0) = 0$ and its Taylor expansion around $u = u_0$ would be

$$\begin{aligned} g(u) &\approx g(u_0) + \overbrace{g'(u_0)}^{=0}(u - u_0) + \frac{g''(u_0)}{2}(u - u_0)^2, \\ &\approx g(u_0) + \frac{g''(u_0)}{2}(u - u_0)^2, \quad \text{for } u \approx u_0. \end{aligned}$$

The curvature of $g(u)$ at a local maximum or or minimum $u = u_0$ is reflected by its second derivative at u_0,

$$g''(u_0) = \frac{d^2}{du^2} g(u) \Big|_{u=u_0}$$

- $g''(u_0) > 0$ if $g(u)$ has a upward concavity at u_0
- $g''(u_0) < 0$ if $g(u)$ has a downward concavity at u_0
- The greater the magnitude of $g''(u_0)$, the greater the curvature

Curvature of the Log Likelihood

For $X_1, \ldots, X_n \overset{\text{iid}}{\sim} f(x \mid \theta)$ for an unknown parameter θ, recall the log likelihood for θ is

$$\ell(\theta) = \sum_{i=1}^{n} \log f(X_i \mid \theta).$$

Its second derivative is

$$\frac{\partial^2}{\partial \theta^2} \ell(\theta) = \sum_{i=1}^{n} \frac{\partial^2}{\partial \theta^2} \log f(X_i \mid \theta).$$

By LLN, as $n \to \infty$,

$$\frac{1}{n} \frac{\partial^2}{\partial \theta^2} \ell(\theta) = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial^2}{\partial \theta^2} \log f(X_i \mid \theta) \longrightarrow \mathrm{E}\left[\frac{\partial^2}{\partial \theta^2} \log f(X \mid \theta) \right].$$

where the expected value is taken with respect to X.

Thus the accuracy of MLE can be reflected by $\mathrm{E}\left[\frac{\partial^2}{\partial \theta^2} \log f(X_i \mid \theta) \right]$.

Fisher Information

(From this point on, we assume there is only a single parameter θ.)

For a PDF/PMF $f(X \mid \theta)$ with a single parameter θ, the *Fisher information* for θ is defined as:

$$\mathcal{I}(\theta) = -\operatorname{E}\left[\frac{\partial^2}{\partial\theta^2}\log f(X_i \mid \theta)\right]$$

- Usually, $\frac{\partial^2}{\partial\theta^2}\log f(X_i \mid \theta) < 0$ as the log likelihood generally has a downward concavity. We add the minus sign $-$ to get rid of the sign and ensure that $\mathcal{I}(\theta) > 0$
- $\mathcal{I}(\theta)$ reflects the curvature of the log likelihood. The greater the value of $\mathcal{I}(\theta)$, the less variability of the MLE $\widehat{\theta}$.
- $\mathcal{I}(\theta)$ measures the amount of information that an observed random variable $X \sim f(X \mid \theta)$ carries about an unknown parameter θ.

Examples: Fisher Information $\mathcal{I}(\theta) = \mathrm{E}\left(-\frac{\partial^2}{\partial\theta^2}\log f(X \mid \theta)\right)$

Ex1: Exponential(λ):

- PDF $f(x \mid \lambda) = \lambda e^{-\lambda x}$
- $\log f(X \mid \lambda) = \log(\lambda) - \lambda X$
- $\frac{\partial}{\partial\lambda}\log f(X \mid \lambda) = \dfrac{1}{\lambda} - X$
- $\frac{\partial^2}{\partial\lambda^2}\log f(X \mid \lambda) = -1/\lambda^2$
- $\mathcal{I}(\lambda) = \mathrm{E}\left(-\frac{\partial^2}{\partial\lambda^2}\log f(X \mid \lambda)\right) = \mathrm{E}(1/\lambda^2) = 1/\lambda^2$

Ex2: $\mathrm{N}(\mu, \sigma^2)$ with σ^2 known:

- PDF: $f(x \mid \mu) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(X-\mu)^2/2\sigma^2}$
- $\log f(X \mid \mu) = -\frac{1}{2}\log(2\pi\sigma^2) - \frac{(X-\mu)^2}{2\sigma^2}$
- $\frac{\partial}{\partial\mu}\log f(X \mid \mu) = (X-\mu)/\sigma^2$
- $\frac{\partial^2}{\partial\mu^2}\log f(X \mid \mu) = -1/\sigma^2$
- $\mathcal{I}(\mu) = -\mathrm{E}\left(\frac{\partial^2}{\partial\mu^2}\log f(X \mid \mu)\right) = 1/\sigma^2$

Examples: Fisher Information

Ex3: Bernoulli(p):

- PMF: $f(x \mid p) = p^X (1-p)^{1-X}$
- $\log f(X \mid p) = X \log(p) + (1-X)\log(1-p)$
- $\frac{\partial}{\partial p} \log f(X \mid p) = \frac{X}{p} - \frac{1-X}{1-p}$
- $\frac{\partial^2}{\partial p^2} \log f(X \mid p) = -\frac{X}{p^2} - \frac{1-X}{(1-p)^2}$
- $\mathcal{I}(p) = -\operatorname{E}\left(\frac{\partial^2}{\partial p^2} \log f(X \mid p)\right) = \frac{\operatorname{E}(X)}{p^2} + \frac{1-\operatorname{E}(X)}{(1-p)^2} = \frac{1}{p(1-p)}$

Asymptotic (Large Sample) Distribution of the MLE

Fisher information determines the (approx) variance of the MLE.

Informally: if $X_1, \ldots, X_n \overset{\text{iid}}{\sim} f(x \mid \theta_0)$ and $\widehat{\theta}$ is the MLE,

$$\text{the distribution of } \widehat{\theta} \text{ is approx. } N\left(\theta_0,\ \frac{1}{n\mathcal{I}(\theta_0)}\right)$$

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More formally: under some regularity conditions ($f(x \mid \theta)$ is a smooth function of θ),

$$\sqrt{n\mathcal{I}(\theta_0)} \cdot (\widehat{\theta} - \theta_0) \quad \text{converge in distribution to} \quad \mathrm{N}(0, 1)$$

This means that the CDF converges — i.e., for all fixed x,

$$\mathrm{P}\left(\sqrt{n\mathcal{I}(\theta_0)} \cdot (\widehat{\theta} - \theta_0) \leq x\right) \to \Phi(x) \quad \text{as } n \to \infty.$$

The same holds with $\mathcal{I}(\widehat{\theta})$ in place of $\mathcal{I}(\theta_0)$:

$$\sqrt{n\mathcal{I}(\widehat{\theta})} \cdot (\widehat{\theta} - \theta_0) \quad \text{converge in distribution to} \quad \mathrm{N}(0, 1)$$

Asymptotic Distribution of the MLE — Examples

- Exponential(λ): $\widehat{\lambda} = 1/\overline{X}$ and $\mathcal{I}(\lambda) = 1/\lambda^2$, so:

$$\widehat{\lambda} \approx \mathsf{N}\big(\lambda_0, \tfrac{\lambda_0^2}{n}\big) \text{ or } \approx \mathsf{N}\big(\lambda_0, \tfrac{\widehat{\lambda}^2}{n}\big)$$

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- $\mathsf{N}(\mu, \sigma^2)$ with σ^2 known: $\widehat{\mu} = \overline{X}$ and $\mathcal{I}(\mu) = 1/\sigma^2$ so:

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- Bernoulli(p): $\widehat{p} = \overline{X}$ and $\mathcal{I}(p) = \frac{1}{p(1-p)}$, so:

$$\widehat{p} \approx \mathrm{N}\big(p_0, \tfrac{p_0(1-p_0)}{n}\big) \text{ or } \approx \mathrm{N}\big(p_0, \tfrac{\widehat{p}(1-\widehat{p})}{n}\big)$$

A Counter Example: Asymptotic Distribution of the MLE

For Uniform$[0, \theta]$:

- PDF $f(x \mid \theta) = \frac{1}{\theta}$, $0 \leq x \leq \theta$
- In this case the regularity conditions do not hold. $\log(f(X \mid \theta))$ is not a smooth function of θ,

$$\log(f(X \mid \theta)) = \begin{cases} -\log\theta & \text{if } \theta > X \\ \log(0) = -\infty & \text{if } \theta < X \end{cases}$$

- Recall in L14, we showed that $\widehat{\theta}_{\text{MLE}} = X_{(n)}$ and calculated

$$\text{Var}(\widehat{\theta}) = \frac{n\theta^2}{(n+1)^2(n+2)} = \mathcal{O}(\frac{1}{n^2})$$

while asymptotic normality of the MLE would yield $\text{Var}(\widehat{\theta}) = \mathcal{O}(\frac{1}{n})$

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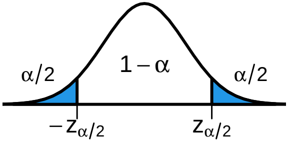
In fact, no approximation is needed here, since we actually know the <u>exact</u> distribution of the MLE in this case (via order statistics)

Confidence Intervals Based on MLE

We can use asymptotic normality of the MLE to construct a *confidence interval for θ_0*, where θ_0 is the true value of θ.

Let $z_{\alpha/2}$ be the value so that

$$\mathrm{P}(|Z| \le z_{\alpha/2}) = 1 - \alpha \text{ for } Z \sim N(0,1).$$



$$\sqrt{n\mathcal{I}(\widehat{\theta})} \cdot (\widehat{\theta} - \theta_0) \to \mathrm{N}(0,1)$$

$$\Rightarrow \quad \mathrm{P}\left(\left|\sqrt{n\mathcal{I}(\widehat{\theta})} \cdot (\widehat{\theta} - \theta_0)\right| < z_{\alpha/2}\right) \approx 1 - \alpha$$

$$\Rightarrow \quad \mathrm{P}\left(\widehat{\theta} - z_{\alpha/2} \cdot \frac{1}{\sqrt{n\mathcal{I}(\widehat{\theta})}} < \theta_0 < \widehat{\theta} + z_{\alpha/2} \cdot \frac{1}{\sqrt{n\mathcal{I}(\widehat{\theta})}}\right) \approx 1 - \alpha$$

So, after observing the data and calculating the interval

$$\widehat{\theta} \pm z_{\alpha/2} \cdot \frac{1}{\sqrt{n\mathcal{I}(\widehat{\theta})}}$$

we have approximately $(1 - \alpha)$ confidence that θ_0 lies in this interval.

Example — Confidence Interval for Normal Mean

$X_1, \ldots, X_n \overset{\text{iid}}{\sim} \mathsf{N}(\mu, \sigma^2)$ for unknown $\mu \in \mathbb{R}$ (σ^2 is known)

- The MLE is $\widehat{\mu} = \overline{X}$
- The Fisher information is $\mathcal{I}(\mu) = \frac{1}{\sigma^2}$
- Therefore, $\widehat{\mu} \approx \mathsf{N}\big(\mu_0, \frac{\sigma^2}{n}\big)$ and an approx $(1-\alpha)$ conf. int. is:

$$\overline{X} \pm z_{\alpha/2} \cdot \frac{\sigma}{\sqrt{n}}$$

- In fact, we know this distribution and conf. int. are exact for this case

Examples — Confidence Interval for Exponential

$X_1, \ldots, X_n \stackrel{\text{iid}}{\sim} \text{Exponential}(\lambda)$ for unknown $\lambda > 0$

- The MLE is $\widehat{\lambda} = \frac{1}{\overline{X}}$
- The Fisher information is $\mathcal{I}(\lambda) = \frac{1}{\lambda^2}$
- Therefore, $\widehat{\lambda} \approx \text{N}(\lambda_0, \frac{\lambda_0^2}{n})$ and an approx. $(1-\alpha)$ conf. int. is:

$$\widehat{\lambda} \pm z_{\alpha/2} \cdot \frac{\widehat{\lambda}}{\sqrt{n}} = \left(\widehat{\lambda} - z_{\alpha/2} \cdot \frac{\widehat{\lambda}}{\sqrt{n}}, \widehat{\lambda} + z_{\alpha/2} \cdot \frac{\widehat{\lambda}}{\sqrt{n}}\right)$$

Example — Bernoulli p

$X_1, \ldots, X_n \overset{\text{iid}}{\sim} \text{Bernoulli}(p)$ for unknown $p \in (0, 1)$

- The MLE is $\widehat{p} = \overline{X}$
- The Fisher information is $\mathcal{I}(p) = \frac{1}{p(1-p)}$
- Therefore, $\widehat{p} \approx \text{N}\big(p_0, \frac{p_0(1-p_0)}{n}\big) \approx \text{N}\big(p_0, \frac{\widehat{p}(1-\widehat{p})}{n}\big)$ and an approx. $(1-\alpha)$ conf. int. is:

$$\widehat{p} \pm z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}} = \left(\widehat{p} - z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}, \widehat{p} + z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}\right)$$

Cramer-Rao Lower Bound (CRLB)

There are many possible estimators for parameters (MME, MLE, etc). Is there a best one?

Theorem: Let $X_1, \ldots, X_n$ be i.i.d. with PDF/PMF $f(x \mid \theta)$. Let $T = t(X_1, \ldots, X_n)$ be an unbiased estimate for θ. Then, under smoothness assumptions on $f(x \mid \theta)$,

$$\text{Var}(T) \geq \frac{1}{n\mathcal{I}(\theta)}.$$

For the MLE $\widehat{\theta}$ of θ, recall $\widehat{\theta}$ is approx. $N\left(\theta,\ \frac{1}{n\mathcal{I}(\theta)}\right)$.

- The MLE is (asymptotically) unbiased
- The MLE's variance is (asymptotically) $\frac{1}{n\mathcal{I}(\theta)}$
- The MLE thus (asymptotically) achieves the CRLB

Is the MLE optimal?

- Not necessarily...
  there might be biased estimators with a smaller MSE

Lemma for the Proof of CRLB

If $\log f(X \mid \theta)$ is a smooth function of θ, it can be shown that

1. $\mathrm{E}\left(\frac{\partial}{\partial\theta}\log f(X \mid \theta)\right) = 0$
2. the Fisher information $\mathcal{I}(\theta)$ can also be calculated as

$$\mathcal{I}(\theta) = \mathrm{E}\left(\left(\frac{\partial}{\partial\theta}\log f(X \mid \theta)\right)^2\right)$$

The two points above combined also implies that

$$\mathrm{Var}\left(\frac{\partial}{\partial\theta}\log f(X \mid \theta)\right) = \mathrm{E}\left(\left(\frac{\partial}{\partial\theta}\log f(X \mid \theta)\right)^2\right) = \mathcal{I}(\theta).$$

since $\mathrm{E}\left(\frac{\partial}{\partial\theta}\log f(X \mid \theta)\right) = 0$

Proof of $\mathrm{E}\left(\frac{\partial}{\partial\theta}\log f(X \mid \theta)\right) = 0$

The proof will be done for case that X is continuous. The discrete case can be done similarly,

$$
\begin{aligned}
&\mathrm{E}\left(\frac{\partial}{\partial\theta}\log f(X \mid \theta)\right) \\
&= \int \frac{\partial}{\partial\theta}\log f(x \mid \theta) f(x \mid \theta)\mathrm{d}x \\
&= \int \frac{\frac{\partial}{\partial\theta} f(x \mid \theta)}{f(x \mid \theta)} f(x \mid \theta)\mathrm{d}x \\
&= \int \frac{\partial}{\partial\theta} f(x \mid \theta)\mathrm{d}x \\
&= \frac{\partial}{\partial\theta}\underbrace{\int f(x \mid \theta)\mathrm{d}x}_{=1} \quad \left(\begin{array}{c}\text{assume it's okay to swap the order} \\ \text{of integration \& differentiation}\end{array}\right) \\
&= \frac{\partial}{\partial\theta}1 = 0
\end{aligned}
$$

Proof that $\mathcal{I}(\theta) = \mathsf{E}\left(\left(\frac{\partial}{\partial\theta}\log f(X \mid \theta)\right)^2\right)$

From the proof in the previous page, we've obtained that

$$0 = \int \frac{\partial}{\partial\theta}\log f(x \mid \theta) f(x \mid \theta)\mathrm{d}x.$$

Taking another derivative of the preceding expressions, and swapping the order of differentiation and integration, we have

$$0 = \underbrace{\int \frac{\partial^2}{\partial\theta^2}\log f(x \mid \theta) f(x \mid \theta)\mathrm{d}x}_{=I} + \underbrace{\int \frac{\partial}{\partial\theta}\log f(x \mid \theta)\cdot\frac{\partial}{\partial\theta} f(x \mid \theta)\mathrm{d}x}_{=II}$$

where

$$I = \mathsf{E}\left[\frac{\partial^2}{\partial\theta^2}\log f(X_i \mid \theta)\right] = -\mathcal{I}(\theta).$$

$$
\begin{aligned}
II &= \int \frac{\partial}{\partial\theta} \log f(x \mid \theta) \cdot \frac{\partial}{\partial\theta} f(x \mid \theta) \mathrm{d}x \\
&= \int \frac{\partial}{\partial\theta} \log f(x \mid \theta) \cdot \underbrace{\frac{\frac{\partial}{\partial\theta} f(x \mid \theta)}{f(x \mid \theta)}}_{= \frac{\partial}{\partial\theta} \log f(x|\theta)} f(x \mid \theta) \mathrm{d}x \\
&= \int \left[\frac{\partial}{\partial\theta} \log f(x \mid \theta) \right]^2 f(x \mid \theta) \mathrm{d}x \\
&= \mathsf{E} \left(\left(\frac{\partial}{\partial\theta} \log f(X \mid \theta) \right)^2 \right)
\end{aligned}
$$

As $I + II = 0$, and $I = -\mathcal{I}(\theta)$, we have

$$
\mathcal{I}(\theta) = -I = II = \mathsf{E} \left(\left(\frac{\partial}{\partial\theta} \log f(X \mid \theta) \right)^2 \right).
$$

Proof of CRLB

Let

$$Z = \sum_{i=1}^{n} \frac{\partial}{\partial \theta} \log f(X_i \mid \theta) = \sum_{i=1}^{n} \frac{\frac{\partial}{\partial \theta} f(X_i \mid \theta)}{f(X_i \mid \theta)}.$$

As shown in the Lemma that $\text{Var}\left(\frac{\partial}{\partial\theta} \log f(X \mid \theta)\right) = \mathcal{I}(\theta)$, we have

$$\text{Var}(Z) = n\mathcal{I}(\theta).$$

The lemma also asserts $\text{E}(Z) = 0$ since $\text{E}\left(\frac{\partial}{\partial\theta} \log f(X \mid \theta)\right) = 0$

Recall that $T = t(X_1, \ldots, X_n)$ is an unbiased estimate for θ. We have

$$[\mathrm{Cov}(Z, T)]^2 \leq \mathrm{Var}(Z)\,\mathrm{Var}(T).$$

It remains to show that $\mathrm{Cov}(Z, T) = 1$, then CRLB would follows since

$$\mathrm{Var}(T) \geq \frac{[\mathrm{Cov}(Z, T)]^2}{\mathrm{Var}(Z)} = \frac{1}{n\mathcal{I}(\theta)}.$$

See p.301 of the textbook for the rest of the proof.