STA355
UTSG

Week 6 周课

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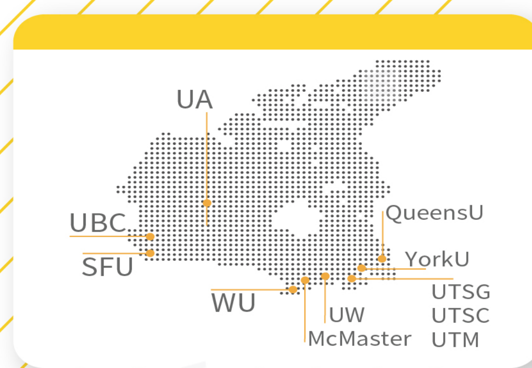

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今日内容:

1. Week 7 学校正课内容 (lectures 9-10)

From point estimation to interval estimation

- **Model:** We observe $X_1, \cdots, X_n$ assumed to have a distribution depending on some unknown parameter θ.
- **Point estimation:** Estimate the value of θ by a **point estimator** $\widehat{\theta} = \widehat{\theta}(X_1, \cdots, X_n)$.
- $\widehat{\theta}$ will have a **sampling distribution**, which will depend on θ as well as possibly other unknown parameters.
- The standard deviation of the sampling distribution is called the **standard error**.
    - We can often estimate the standard error using the Delta Method or jackknife method.
- **Interval estimation:** Define an interval

$$\mathcal{I} = [\ell(X_1, \cdots, X_n), u(X_1, \cdots, X_n)]$$

that we believe will contain θ with probability close to 1.

Interval estimation

- In this course, we'll talk about two approaches to interval estimation.
- **Confidence intervals:** These are typically defined in terms of the sampling distribution of a point estimator $\widehat{\theta}$ (or some related statistic).
  - We will often need to use approximations (e.g. normal approximations) to the sampling distributions.
  - The "confidence level" is defined in terms of repeated sampling.
- **Credible intervals:** These are based on the posterior distribution of θ given the observed data $x_1, \cdots, x_n$.
  - If $\pi(\theta | x_1, \cdots, x_n)$ is the posterior density of θ then $\mathcal{I}$ is a $100p\%$ credible interval if

$$\int_{\mathcal{I}} \pi(\theta | x_1, \cdots, x_n)\, d\theta = p.$$

  - Note that the "credible level" is defined in terms of the posterior distribution (which depends on the prior distribution and the data).

Confidence intervals

- **Definition:** An interval $\mathcal{I} = [\ell(X_1, \cdots, X_n), u(X_1, \cdots, X_n)]$ is a **confidence interval** (CI) with coverage $100p\%$ (or a $100p\%$ CI) if

$$\underbrace{P_\theta \left[\ell(X_1, \cdots, X_n) \le \theta \le u(X_1, \cdots, X_n)\right]}_{P_\theta(\theta \in \mathcal{I})} = p \ \text{ for all } \theta \in \Theta.$$

- If the probability statement above holds approximately (e.g. if n is large) then we often say that the interval is an approximate $100p\%$ CI for θ.
  - Typically, we have $\mathcal{I}_n = [\ell_n(X_1, \cdots, X_n), u_n(X_1, \cdots, X_n)]$ with

$$P_\theta(\theta \in \mathcal{I}_n) \to p \ \text{ as } n \to \infty$$

for all $\theta \in \Theta$.

Some comments on CIs

- In the definition of a CI, the interval $\mathcal{I}$ is actually a random interval (depending on the random variables $X_1, \cdots, X_n$) and a CI is defined in terms of the probability that the random interval contains θ.
- The data-based interval $[\ell(x_1, \cdots, x_n), u(x_1, \cdots, x_n)]$ **cannot** be interpreted in terms of the probability distribution of $(X_1, \cdots, X_n)$ – the interval either contains θ or it doesn't!
- However, the length of the CI gives us an idea about the uncertainty in the estimation of θ (much like an estimate of the standard error).
  - Many CIs are formed in terms of an estimator and its standard error.
  - For example, $\widehat{\theta} \pm z \times \widehat{\text{se}}(\widehat{\theta})$ for some z.

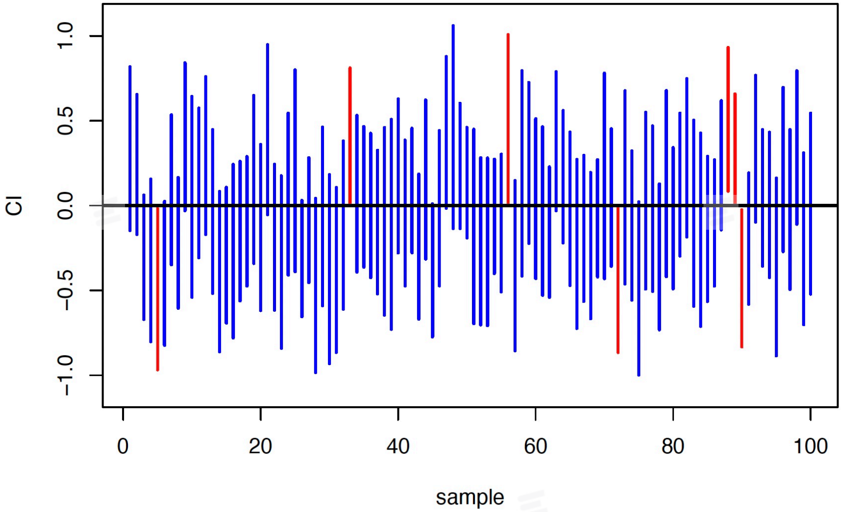
Example: CI demonstration

- **Model:** $X_1, \cdots, X_{20}$ independent $\mathcal{N}(\mu, \sigma^2)$ with both μ and σ^2 unknown.
- Classic 95% CI for μ:

$$\left[\bar{X} - 2.093\frac{S}{\sqrt{20}}, \bar{X} + 2.093\frac{S}{\sqrt{20}}\right]$$

  where $\bar{X}$ and S^2 are the sample mean and variance respectively.
  - 2.093 is the 0.975 quantile of Student's t distribution with 19 $(= 20 - 1)$ degrees of freedom.
  - Note that $\widehat{\text{se}}(\bar{X}) = S/\sqrt{n}$.
- **Simulation experiment:** Generate 100 samples of size 20 from a $\mathcal{N}(0, 1)$ distribution and compute 95% CIs for each sample.
  - Given the theory, we would expect that approximately 95 of the 100 constructed CIs will contain the true mean 0.

100 95% CIs for μ



CIs that do not include 0 are indicated by red bars.

Determining CIs: Heuristics

- **Model:** $X_1, \cdots, X_n$ independent with some (unknown) cdf F.
- Estimate $\theta = \theta(F)$ by $\widehat{\theta}$ where

$$\widehat{\theta} \approx \mathcal{N}(\theta, [\text{se}(\widehat{\theta})]^2).$$

- Thus if $\widehat{\text{se}}(\widehat{\theta})$ is a "good" estimator of $\text{se}(\widehat{\theta})$, we should have

$$\frac{\widehat{\theta} - \theta}{\widehat{\text{se}}(\widehat{\theta})} \approx \mathcal{N}(0, 1).$$

- Thus, for example,

$$P\left(-1.96 \leq \frac{\widehat{\theta} - \theta}{\widehat{\text{se}}(\widehat{\theta})} \leq 1.96\right) \approx 0.95$$

and so $\widehat{\theta} \pm 1.96\,\widehat{\text{se}}(\widehat{\theta})$ are the limits of an approximate 95% CI for θ.

The pivotal method

- It's not too difficult to formalize these heuristics.
- **Idea:** Find a random variable $g(X_1, \cdots, X_n, \theta)$ whose distribution is independent of θ and any other unknown parameters.
  - $P_\theta[g(X_1, \cdots, X_n, \theta) \leq x] = G(x)$ where $G(x)$ is completely known.
  - $g(X_1, \cdots, X_n, \theta)$ is called a **pivot**.
- Given the pivot, we choose a and b so that

$$p = P_\theta\left[a \leq g(X_1, \cdots, X_n, \theta) \leq b\right] = \underbrace{G(b) - G(a-)}_{independent\ \ of\ \ \theta}.$$

- From this, we get

$$\begin{aligned} p &= P_\theta\left[a \leq g(X_1, \cdots, X_n, \theta) \leq b\right] \\ &\quad \vdots \ (\textit{manipulation}!) \\ &= P_\theta\left[\ell(X_1, \cdots, X_n) \leq \theta \leq u(X_1, \cdots, X_n)\right]. \end{aligned}$$

Details of the pivotal method

- **Choice of pivot:**
  - If we have a point estimator $\widehat{\theta}$ then we can often define the pivot to be $g(\widehat{\theta}, \theta)$ where g is chosen to make its distribution independent of θ.
  - If we cannot find an exact pivot, we can sometimes find an approximate pivot $g(\widehat{\theta}, \theta)$ whose distribution is approximately independent of θ – for example,

$$\frac{\widehat{\theta} - \theta}{\widehat{\text{se}}(\widehat{\theta})} \approx \mathcal{N}(0, 1).$$

- **Choice of *a* and *b*:**
  - Ideally, we'd like to choose a and b to make the CI as short as possible.
  - However, if G is the cdf of the pivot then a good default is to define a so that $G(a) = (1 - p)/2$ and b so that $1 - G(b) = (1 - p)/2$.

Example: CIs for normal parameters

- **Model:** $X_1, \cdots, X_n$ independent $\mathcal{N}(\mu, \sigma^2)$.
- CI for μ: Pivot
$$\frac{\bar{X} - \mu}{S/\sqrt{n}} = \frac{\widehat{\mu} - \mu}{\widehat{\text{se}}(\widehat{\mu})} \sim \mathcal{T}(n-1)$$
where $\mathcal{T}(n-1)$ is a Student's t distribution with $n-1$ degrees of freedom.
- Define t_p so that
$$P\left(-t_p \leq \frac{\bar{X} - \mu}{S/\sqrt{n}} \leq t_p\right) = p.$$
- Then the $100p\%$ CI for μ is
$$\left[\bar{X} - t_p \frac{S}{\sqrt{n}}, \bar{X} + t_p \frac{S}{\sqrt{n}}\right].$$

Example: CIs for normal parameters (cont'd)

- For the variance, we have

$$\frac{(n-1)S^2}{\sigma^2} = \frac{1}{\sigma^2}\sum_{i=1}^{n}(X_i - \bar{X})^2 \sim \chi^2(n-1).$$

- Define a and b so that

$$P\left(a \le \frac{(n-1)S^2}{\sigma^2} \le b\right) = p$$

  from which a $100p\%$ CI for σ^2 is

$$\left[\frac{(n-1)S^2}{b}, \frac{(n-1)S^2}{a}\right].$$

- Choice of a and b:
  - Equal tail areas: $G(a) = 1 - G(b)$ with $G(b) - G(a) = p$.
  - Minimum length: minimize $a^{-1} - b^{-1}$ subject to $G(b) - G(a) = p$.

Example: Exponential distribution

- **Model:** $X_1, \cdots, X_n$ independent Exponential random variables with pdf
$$f(x;\lambda) = \lambda \exp(-\lambda x) \text{ for } x \geq 0$$
where $\lambda > 0$ is unknown.
- We can estimate λ by $\widehat{\lambda} = 1/\bar{X}$.
- We can approximate the distribution of $\widehat{\lambda}$ as follows:
$$\begin{aligned} \sqrt{n}(\widehat{\lambda} - \lambda) &\approx \mathcal{N}(0, \lambda^2) \\ \text{or } \widehat{\lambda} &\approx \mathcal{N}(\lambda, \lambda^2/n). \end{aligned}$$
- From this, it follows that $\mathrm{se}(\widehat{\lambda})$ is approximately $\lambda/\sqrt{n}$ and this can be estimated by $\widehat{\mathrm{se}}(\widehat{\lambda}) = \widehat{\lambda}/\sqrt{n}$.

Example: Exponential distribution (cont'd)

- Look at 4 pivots for λ:
  1. $\lambda \sum_{i=1}^{n} X_i \sim \text{Gamma}(n, 1)$ (exact pivot).
  2. $\dfrac{\widehat{\lambda} - \lambda}{\lambda / \sqrt{n}} \approx \mathcal{N}(0, 1)$ (approximate pivot).
  3. $\dfrac{\widehat{\lambda} - \lambda}{\widehat{\lambda} / \sqrt{n}} \approx \mathcal{N}(0, 1)$ (approximate pivot).
  4. $\sqrt{n}\{\ln(\widehat{\lambda}) - \ln(\lambda)\} \approx \mathcal{N}(0, 1)$ (approximate pivot).

- Pivot 1 uses the fact that a sum of independent Exponential random variables has a Gamma distribution.

- Pivot 4 uses the variance stabilizing transformation discussed earlier.

Example: Exponential distribution (cont'd)

- The CIs resulting from the 4 pivots are:
  1. $\left[\frac{a}{\sum_{i=1}^n X_i}, \frac{b}{\sum_{i=1}^n X_i}\right]$ where a and b are such that
  $$P[a \leq \text{Gamma}(n,1) \leq b] = p;$$
  2. $\left[\frac{\widehat{\lambda}}{1 + z_p/\sqrt{n}}, \frac{\widehat{\lambda}}{1 - z_p/\sqrt{n}}\right]$ where z_p satisfies
  $$P[-z_p \leq \mathcal{N}(0,1) \leq z_p] = p;$$
  3. $\left[\widehat{\lambda}(1 - z_p/\sqrt{n}), \widehat{\lambda}(1 + z_p/\sqrt{n})\right]$;
  4. $\left[\widehat{\lambda}\exp(-z_p/\sqrt{n}), \widehat{\lambda}\exp(z_p/\sqrt{n})\right]$.

Simulation experiment: Coverage of the 4 CIs

- Generate $n = 20$ and $n = 100$ observations from an Exponential distribution and compute the four 95% CIs for 10000 samples.
  - We can estimate the coverage of each interval to within 0.005 with probability close to 1. ($\sqrt{0.05 \times 0.95/10000} \approx 0.002$).
  - Note that the true coverage for pivot 1 is exactly 0.95.

	Est'd coverage	
Pivot	$n = 20$	$n = 100$
1	0.949	0.949
2	0.922	0.945
3	0.954	0.950
4	0.946	0.947

- **Conclusions:**
  - Pivot 2 (i.e. $\sqrt{n}(\widehat{\lambda} - \lambda)/\lambda$) has the poorest coverage of the four CIs.
  - For $n = 100$, the coverage of all four is very close to the nominal 0.95.

Example: Unif$(0, \theta)$

- $X_1, \cdots, X_n$ independent Unif$(0, \theta)$ random variables with pdf

$$f(x; \theta) = \frac{1}{\theta} \quad \text{for } 0 \leq x \leq \theta.$$

- θ represents the maximum possible value of $X_1, \cdots, X_n$.
- **Pivot:** $X_{(n)}/\theta$. Why?
  - Since θ is the maximum possible value, $X_{(n)}$ should contain the most information about θ.
  - Distribution of $X_{(n)}/\theta$ is independent of θ:

$$P_\theta\left(\frac{X_{(n)}}{\theta} \leq x\right) = x^n \ \text{ for } 0 \leq x \leq 1.$$

Example: Unif$(0, \theta)$ (cont'd)

- How to construct a $100p\%$ CI for θ:
  - Take $0 \le a < b \le 1$ such that

$$P\left(a \le \frac{X_{(n)}}{\theta} \le b\right) = b^n - a^n = p.$$

  - Inverting this, we get

$$\left[\frac{X_{(n)}}{b}, \frac{X_{(n)}}{a}\right].$$

- "Optimal" choice of a, b:

$$b = 1 \quad a = (1-p)^{1/n}.$$

Example: CIs for quantiles $F^{-1}(\tau)$

- **Model:** $X_1, \cdots, X_n$ independent random variables with continuous cdf F and pdf f.
- **Goal:** Find a CI (e.g. 95% CI) for the quantile $\theta = F^{-1}(\tau)$.
- **Approach:** Use the pivot

$$g(X_1, \cdots, X_n, \theta) = \sum_{i=1}^{n} I(X_i \leq \theta) \sim \text{Binomial}(n, \tau).$$

- To use this pivot, note that if $a < b$ are integers between 1 and n then

$$\left\{\theta : a \leq \sum_{i=1}^{n} I(X_i \leq \theta) \leq b\right\} = \left\{\theta : X_{(a)} \leq \theta \leq X_{(b)}\right\}.$$

- Thus $[X_{(a)}, X_{(b)}]$ is a $100p\%$ CI for $\theta = F^{-1}(\tau)$ where

$$p = \sum_{k=a}^{b} \binom{n}{k} \tau^k (1-\tau)^{n-k}.$$

- This is a **distribution-free** CI for θ.

Example: CIs for $F^{-1}(\tau)$ (cont'd)

- For a given p (e.g. 0.95), we can find a and b using a normal approximation to the Binomial distribution so that

$$p \approx \sum_{k=a}^{b} \binom{n}{k} \tau^k (1-\tau)^{n-k}.$$

- If n is large enough then $\text{Binomial}(n,\tau) \approx \mathcal{N}(n\tau, n\tau(1-\tau))$.
- Using the normal approximation (with a continuity correction) we get

$$\begin{aligned} a &= \left\lfloor n\tau + \frac{1}{2} - z_p\sqrt{n\tau(1-\tau)} \right\rfloor \\ b &= \left\lceil n\tau - \frac{1}{2} + z_p\sqrt{n\tau(1-\tau)} \right\rceil \end{aligned}$$

where $\lfloor x \rfloor$ and $\lceil x \rceil$ round x, respectively, down and up to the nearest integer, for example:

$$\lfloor 3.5 \rfloor = 3 \quad \lceil 3.5 \rceil = 4.$$

补充笔记：

Consider the function:

$$g(X_1, X_2, \dots, X_n, \theta) = \sum_{i=1}^{n} I(X_i \leq \theta)$$

where $I(\cdot)$ is the indicator function, which equals 1 if the condition inside is true and 0 otherwise.
Given $\theta = F^{-1}(\tau)$, we have:

$$P(X_i \leq \theta) = P(X_i \leq F^{-1}(\tau)) = F(F^{-1}(\tau)) = \tau$$

Since the X_i are independent:

$$g(X_1, \dots, X_n, \theta) = \sum_{i=1}^{n} I(X_i \leq \theta) \sim \text{Binomial } (n, \tau)$$

This means g follows a Binomial distribution with parameters n (number of trials) and τ (probability of success).

The order statistics $X_{(1)} \leq X_{(2)} \leq \cdots \leq X_{(n)}$ are the sorted values of the sample.
If a and b are integers satisfying $1 \leq a < b \leq n$, consider the event:

$$a \leq g(X_1, \dots, X_n, \theta) \leq b$$

This event can be translated in terms of order statistics:

$$a \leq \sum_{i=1}^{n} I(X_i \leq \theta) \leq b \iff X_{(a)} \leq \theta \leq X_{(b)}$$

Explanation:

- $\sum_{i=1}^{n} I(X_i \leq \theta) \geq a$ implies that at least a observations are less than or equal to θ, meaning θ is at least as large as the a-th smallest observation $X_{(a)}$.
- Similarly, $\sum_{i=1}^{n} I(X_i \leq \theta) \leq b$ implies that at most b observations are less than or equal to θ, meaning θ is no larger than the b-th smallest observation $X_{(b)}$.

Thus, the interval $[X_{(a)}, X_{(b)}]$ serves as a confidence interval for θ.

We seek:

$$P(X_{(a)} \leq \theta \leq X_{(b)}) = P(a \leq g(X_1, \dots, X_n, \theta) \leq b) = p$$

where p is the desired confidence level (e.g., 95%).

Given that $g \sim \text{Binomial } (n, \tau)$, the probability p is:

$$p = \sum_{k=a}^{b} \binom{n}{k} \tau^k (1-\tau)^{n-k}$$

This sum represents the probability that the Binomial random variable falls between a and b, inclusive.

Thus, the interval $[X_{(a)}, X_{(b)}]$ is a $100p\%$ confidence interval for θ, independent of the underlying distribution F (hence, distribution-free).

When n is sufficiently large, the Binomial distribution $\text{Binomial}\ (n, \tau)$ can be approximated by a Normal distribution:

$$\text{Binomial}\ (n, \tau) \approx \mathcal{N}(\mu, \sigma^2)$$

where:

$$\mu = n\tau \ \text{ and } \ \sigma^2 = n\tau(1 - \tau)$$

The Binomial distribution is discrete, while the Normal distribution is continuous. To improve the approximation, especially for smaller n, we apply a continuity correction of ± 0.5.

$$p \approx P(a \leq \text{Binomial}\ (n, \tau) \leq b)$$

using the Normal approximation, solve for a and b such that:

$$P\left(\mu - z_p\sigma - \frac{1}{2} \leq \text{Binomial}\ (n, \tau) \leq \mu + z_p\sigma + \frac{1}{2}\right) \approx p$$

Rearranging, we obtain:

$$\begin{aligned} a &\approx \mu - z_p\sigma - \frac{1}{2} = n\tau - z_p\sqrt{n\tau(1 - \tau)} - \frac{1}{2} \\ b &\approx \mu + z_p\sigma + \frac{1}{2} = n\tau + z_p\sqrt{n\tau(1 - \tau)} + \frac{1}{2} \end{aligned}$$

Since a and b must be integers, we round them appropriately:

$$a = \left\lfloor n\tau + \frac{1}{2} - z_p\sqrt{n\tau(1 - \tau)} \right\rfloor$$
$$b = \left\lceil n\tau - \frac{1}{2} + z_p\sqrt{n\tau(1 - \tau)} \right\rceil$$

where:

- $\lfloor x \rfloor$ denotes the floor of x (rounding down to the nearest integer).
- $\lceil x \rceil$ denotes the ceiling of x (rounding up to the nearest integer).

Example of Rounding:

$$\lfloor 3.5 \rfloor = 3 \ \text{ and } \ \lceil 3.5 \rceil = 4$$

Example: Comparison of CIs for the normal mean

- **Model:** $X_1, \cdots, X_n$ independent $\mathcal{N}(\mu, \sigma^2)$ random variables.
  - Note that $\mu = E(X_i) = F^{-1}(1/2)$.
- Compare the two CIs:

$$\bar{X} \pm t_p \frac{S}{\sqrt{n}} \quad \text{versus} \quad [X_{(a)}, X_{(b)}].$$

- Compare the lengths of the two intervals when n is large:
  - $t_p \to z_p$ and $S \xrightarrow{p} \sigma$ so that length of parametric CI is approximately $2 z_p \sigma / \sqrt{n}$.
  - $X_{(b)} - X_{(a)} \approx z_p \sigma \sqrt{2\pi} / \sqrt{n}$.
- Thus

$$\frac{\text{length of dist. free CI}}{\text{length of parametric CI}} \approx \frac{\sqrt{2\pi}}{2} = 1.253$$

- **Tradeoff:** Distribution free CI is always valid but parametric CI will be shorter if that model is correct.

Example: CIs for the normal mean: $n = 20$

- Compare $\bar{X} \pm 2.093 \times S/\sqrt{n}$ to $[X_{(6)}, X_{(14)}]$.
  - Coverage for the latter CI is $\sum_{k=6}^{14} \binom{20}{k} \frac{1}{2^{20}} = 0.9586$.
- R code:

```
> len.t <- NULL
> len.df <- NULL
> for (i in 1:1000) {
+     x <- sort(rnorm(20))
+     len.t <- c(len.t, 2*qt(0.975,19)*sqrt(var(x)/20))
+     len.df <- c(len.df,x[14]-x[6])
+     }
> sum(len.t<len.df)/1000 # proportion of samples where len.t < len.df
[1] 0.664
> mean(len.t)
[1] 0.9239648
> mean(len.df)
[1] 1.029677
> mean(len.df/len.t)
[1] 1.114631
```

Example: Gamma pivot

- Sometimes, we may not be able to find pivotal quantities based on a point estimator $\hat{\theta}$.
- For samples from a continuous distribution with only **one unknown parameter**, we can always find at least one pivotal value.
- If X is continuous with CDF $F(x)$ and $U = F(X)$, then $U \sim \text{Unif}(0, 1)$.
- Suppose that $U \sim \text{Unif}(0, 1)$ and let $Y = -\ln U$. Therefore $y = g(u) = -\ln u$, $u = g^{-1}(y) = e^{-y}$. Note the range of Y here is $(0, \infty)$. The density of Y becomes

$$f_Y(y) = f_U(e^{-y})|-e^{-y}| = e^{-y} \quad \text{for } y \geq 0.$$

  That is $Y \sim \text{Exp}(1)$.
- For continuous X, we have $Y = -\ln F(X) \sim \text{Exp}(1)$.

Maximum likelihood estimation

- **Model:** $(X_1, \cdots, X_n)$ random variables with joint pdf or pmf $f(x_1, \cdots, x_n; \theta_1, \cdots, \theta_k)$ where $\theta_1, \cdots, \theta_k$ are unknown parameters.
- Given the data $x_1, \cdots, x_n$, we can define the **likelihood function**

$$\mathcal{L}(\theta_1, \cdots, \theta_k) = f(\underbrace{x_1, \cdots, x_n}_{data}; \theta_1, \cdots, \theta_k)$$

  which is a function over the parameter space (for fixed $x_1, \cdots, x_n$).
- **Definition:** Suppose that for each $\mathbf{x} = (x_1, \cdots, x_n)$, $(T_1(\mathbf{x}), \cdots, T_k(\mathbf{x}))$ maximize $\mathcal{L}(\theta_1, \cdots, \theta_k)$. Then **maximum likelihood estimators** (MLEs) of $\theta_1, \cdots, \theta_k$ are

$$\widehat{\theta}_j = T_j(X_1, \cdots, X_n) \text{ for } j = 1, \cdots, k.$$

Example: A non-regular model

- **Model:** $X_1, \cdots, X_n$ independent random variables with pdf

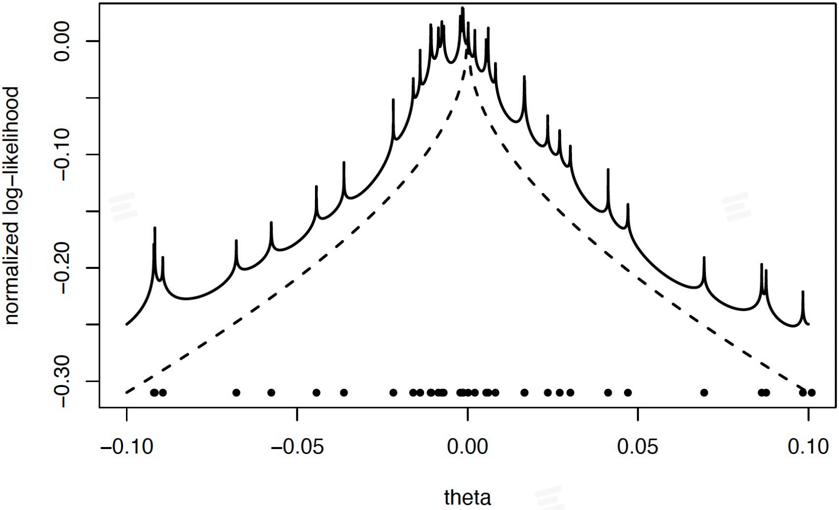
$$f(x;\theta) = \frac{|x-\theta|^{-1/2}}{2\sqrt{\pi}} \exp\left(-|x-\theta|\right).$$

- The likelihood function is

$$\mathcal{L}(\theta) = \prod_{i=1}^{n} \left\{ \frac{|x_i-\theta|^{-1/2}}{2\sqrt{\pi}} \exp\left(-|x_i-\theta|\right) \right\}.$$

- Note that as $\theta \to$ any x_i, $\mathcal{L}(\theta) \uparrow \infty$.
  - This suggests that either the MLE does not exist or that any X_i is an MLE of θ.
  - However, the likelihood function still provides a lot of information about θ.
- **Illustration:** Generate 100 observations from the model with $\theta = 0$ and plot $\ln \mathcal{L}(\theta)$.

Plot of log-likelihood function



- $\mathcal{L}(x_i) = \infty$ for $i = 1, \cdots, 100$.
- Note that $\mathcal{L}(\theta)$ is generally largest for θ close to 0.

Example: The Neyman-Scott problem

- **Model:** $(X_1, Y_1), \cdots, (X_n, Y_n)$ independent pairs of independent Normal random variables.
  - Within each pair X_i and Y_i are independent $\mathcal{N}(\mu_i, \sigma^2)$ random variables.
- **Context:** X_i and Y_i are independent measurements of the same quantity.
  - σ represents the standard deviation of the measurement error.
- Unknown parameters: $\mu_1, \cdots, \mu_n$ and σ^2.
  - The number of unknown parameters $(n + 1)$ tends to infinity with n.
  - For each i, we have only two observations to estimate μ_i.
  - More information for estimating σ^2.

ML estimation of σ^2 and $\{\mu_i\}$

- Given data $(x_1, y_1), \cdots, (x_n, y_n)$, the likelihood function is

$$\mathcal{L}(\mu_1, \cdots, \mu_n, \sigma) = \prod_{i=1}^{n} \left\{ \frac{1}{2\pi\sigma^2} \exp\left[-\frac{(x_i - \mu_i)^2 + (y_i - \mu_i)^2}{2\sigma^2} \right] \right\}.$$

- $\widehat{\sigma}$ and $\{\widehat{\mu}_i\}$ are solutions to the following equations (**likelihood equations**):

$$\begin{aligned} \frac{1}{\widehat{\sigma}^2}(x_i + y_i - 2\widehat{\mu}_i) &= 0 \quad (i = 1, \cdots, n) \\ -\frac{2n}{\widehat{\sigma}} + \frac{1}{\widehat{\sigma}^3} \sum_{i=1}^{n} \left[(x_i - \widehat{\mu}_i)^2 + (y_i - \widehat{\mu}_i)^2 \right] &= 0. \end{aligned}$$

- MLEs:

$$\begin{aligned} \widehat{\mu}_i &= \frac{X_i + Y_i}{2} \quad (i = 1, \cdots, n) \\ \widehat{\sigma}^2 &= \frac{1}{4n} \sum_{i=1}^{n} (X_i - Y_i)^2. \end{aligned}$$

Inconsistency of $\widehat{\sigma}^2$

- Note that $X_i - Y_i \sim \mathcal{N}(0, 2\sigma^2)$ since X_i and Y_i are independent.
- Thus by the WLLN, we have

$$\frac{1}{n}\sum_{i=1}^{n}(X_i - Y_i) \xrightarrow{p} 2\sigma^2.$$

- Thus for the MLE of σ^2, we have

$$\widehat{\sigma}^2 = \frac{1}{4n}\sum_{i=1}^{n}(X_i - Y_i)^2 \xrightarrow{p} \frac{\sigma^2}{2}.$$

- Thus the MLE of σ^2 is not consistent.

Sufficiency

- Suppose we have $(X_1, \cdots, X_n)$ with joint pdf or pmf $f(x_1, \cdots, x_n; \theta)$.
  - θ may consist of k parameters so that $\theta = (\theta_1, \cdots, \theta_k)$.
- **Question:** Can we reduce $\mathbf{X} = (X_1, \cdots, X_n)$ to $\mathbf{T} = (T_1(\mathbf{X}), \cdots, T_m(\mathbf{X}))$ without losing any information about θ?
  - Ideally, we'd like m much smaller than n.
- For a given $\mathbf{T}$, look at the conditional distribution of $\mathbf{X}$ given $\mathbf{T} = \mathbf{t}$:
  - If this conditional distribution does not depend on θ then $\mathbf{T}$ contains the same information about θ as $\mathbf{X}$.
  - If $\mathbf{X}$ and $\mathbf{T}$ are both discrete, we can write

$$f(\mathbf{x}; \theta) = f_T(\mathbf{t}; \theta) f(\mathbf{x}|\mathbf{t}) \ \text{ where } \mathbf{t} = \mathbf{T}(\mathbf{x}).$$

- **Definition:** A statistic $\mathbf{T} = (T_1(\mathbf{X}), \cdots, T_m(\mathbf{X}))$ is a **sufficient statistic** for θ (or more generally a model) if the conditional distribution of $\mathbf{X}$ given $\mathbf{T} = \mathbf{t}$ depends only on $\mathbf{t}$ (and not θ).

Example: Order statistics

- $X_1, \cdots, X_n$ independent continuous random variables with unknown cdf F.
  - F is the parameter in this model.
- **Claim:** The order statistics $X_{(1)} \leq X_{(2)} \leq \cdots \leq X_{(n)}$ are a sufficient statistic for F.
- **Proof:** Look at the conditional distribution of $(X_1, \cdots, X_n)$ given $X_{(1)} = x_1, \cdots, X_{(n)} = x_n$ (where $x_1 \leq x_2 \leq \cdots \leq x_n$).
  - If $(y_1, \cdots, y_n)$ is a permutation of $(x_1, \cdots, x_n)$ then

$$P(X_1 = y_1, \cdots, X_n = y_n | X_{(1)} = x_1, \cdots, X_{(n)} = x_n) = \frac{1}{n!}$$

since all permutations of the ordered sample are equally likely given the order statistics.

$$\sum_{all\ \mathbf{y}} P(X_1 = y_1, \cdots, X_n = y_n | X_{(1)} = x_1, \cdots, X_{(n)} = x_n) = 1.$$

Sufficiency and the likelihood function

- **Neyman Factorization Theorem:** Suppose that the joint pdf or pmf of $\mathbf{X} = (X_1, \cdots, X_n)$ is $f(\mathbf{x}; \theta)$. Then the statistic $\mathbf{T} = (T_1(\mathbf{X}), \cdots, T_m(\mathbf{X}))$ is a sufficient statistic for θ if, and only if

$$f(\mathbf{x}; \theta) = g(\mathbf{T}(\mathbf{x}); \theta)h(\mathbf{x})$$

  where the function h does not depend on θ.
- Note that the likelihood function is

$$\begin{aligned} \mathcal{L}(\theta) &= f(\mathbf{x}; \theta) \\ &= g(\mathbf{T}(\mathbf{x}); \theta)h(\mathbf{x}). \end{aligned}$$

- Since $h(\mathbf{x})$ does not depend on θ, it is just a multiplicative constant in the likelihood function:
  - Maximizing $\mathcal{L}(\theta)$ is equivalent to maximizing $g(\mathbf{T}(\mathbf{x}); \theta)$.
  - Effectively, $\mathcal{L}(\theta)$ depends on the data $\mathbf{x}$ only through the value of $\mathbf{T}(\mathbf{x})$.
  - If the MLE is unique, it depends on $\mathbf{X}$ only through $\mathbf{T}(\mathbf{X})$.

Computing MLEs

- Likelihood function $\mathcal{L}(\theta)$.
  - Assume for simplicity that θ is real-valued.
- **Question:** How do we find $\widehat{\theta}$ maximizing $\mathcal{L}(\theta)$?
- Two general scenarios:
  1. $\mathcal{L}(\theta)$ is differentiable and the parameter space Θ is an open set (i.e. every point of Θ is an interior point). Then $\widehat{\theta}$ (if it exists) satisfies the **likelihood equation**
  $$\frac{d}{d\theta} \ln \mathcal{L}(\widehat{\theta}) = 0.$$
  In some cases, we can use the 2nd derivative to estimate the standard error.
  2. $\widehat{\theta}$ occurs at a “boundary”:
     - Boundary of Θ (if Θ is not an open set);
     - an extreme of the data (e.g. $\widehat{\theta} = X_{(n)}$).

  In these cases, we need to directly maximize $\mathcal{L}(\theta)$.

Example: Uniform distribution on $[0, \theta]$

- **Model:** $X_1, \cdots, X_n$ independent Unif$(0, \theta)$ random variables with $\theta > 0$ unknown:

$$
\begin{aligned}
f(x;\theta) &= \begin{cases} \theta^{-1} & \text{if } 0 \leq x \leq \theta \\ 0 & \text{otherwise} \end{cases} \\
&= \frac{1}{\theta} I(0 \leq x \leq \theta).
\end{aligned}
$$

- The likelihood function is

$$
\begin{aligned}
\mathcal{L}(\theta) &= \prod_{i=1}^{n} \left\{ \frac{1}{\theta} I(0 \leq x_i \leq \theta) \right\} \\
&= \frac{1}{\theta^n} \prod_{i=1}^{n} I(0 \leq x_i \leq \theta) \\
&= \frac{1}{\theta^n} I(\theta \geq \max\{x_1, \cdots, x_n\}).
\end{aligned}
$$

Example: Uniform distribution on $[0, \theta]$ (cont'd)

- Thus $\mathcal{L}(\theta) = 0$ for $\theta < \max\{x_1, \cdots, x_n\}$ while for $\theta \geq \max\{x_1, \cdots, x_n\}$, $\mathcal{L}(\theta) = \theta^{-n}$, which is decreasing as θ increases.
- Thus $\mathcal{L}(\theta)$ is maximized at $\max\{x_1, \cdots, x_n\}$ and so the MLE of θ is

$$\widehat{\theta} = \max\{X_1, \cdots, X_n\} = X_{(n)}.$$

- **Question:** What happens if we define $f(x; \theta) = \theta^{-1}$ for $0 < x < \theta$?
  - Then $\mathcal{L}(\theta) = 0$ for $\theta \leq \max\{x_1, \cdots, x_n\}$ and $\mathcal{L}(\theta) = \theta^{-n}$ for $\theta > \max\{x_1, \cdots, x_n\}$.
  - Technically, the MLE doesn't exist!
  - However, the likelihood function is largest for θ close to (and greater than) $\max\{x_1, \cdots, x_n\}$.

Example: Geometric distribution

- **Model:** $X_1, \cdots, X_n$ are independent Geometric(θ) random variables:
$$f(x;\theta) = \theta(1-\theta)^x \text{ for } x = 0, 1, 2, \cdots$$
where $0 < \theta < 1$.
- The likelihood and log-likelihood functions are
$$\begin{aligned} \mathcal{L}(\theta) &= \prod_{i=1}^{n} \{\theta(1-\theta)^{x_i}\} \\ \ln \mathcal{L}(\theta) &= n \ln(\theta) + \ln(1-\theta) \sum_{i=1}^{n} x_i. \end{aligned}$$
- Differentiating (with respect to θ), we get the likelihood equation
$$\frac{n}{\widehat{\theta}} - \frac{1}{1-\widehat{\theta}} \sum_{i=1}^{n} x_i = 0.$$

Example: Geometric distribution (cont'd)

- Provided that $\sum_{i=1}^{n} x_i > 0$, the likelihood equation has a unique solution

$$\widehat{\theta} = \frac{1}{1 + \bar{x}}.$$

- Does this maximize the log-likelihood function? Check second derivative:

$$\frac{d^2}{d\theta^2} \ln \mathcal{L}(\theta) = -\frac{n}{\theta^2} - \frac{1}{(1-\theta)^2} \sum_{i=1}^{n} x_i < 0.$$

- Therefore, the MLE is $\widehat{\theta} = (1 + \bar{X})^{-1}$ (provided $\bar{X} > 0$).

Example: Geometric distribution (cont'd)

- **Question:** How can we estimate the standard error of $\widehat{\theta} = (1 + \bar{X})^{-1}$?
  - We could use the Delta Method – we need to find $\mathrm{Var}_\theta(X_i)$.
  - We can also base an estimate on the second derivative of the log-likelihood.
- Given the MLE $\widehat{\theta}$, we define the **observed Fisher information** as

$$-\frac{d^2}{d\theta^2} \ln \mathcal{L}(\widehat{\theta}).$$

- We can then estimate the standard error of $\widehat{\theta}$ by

$$\widehat{\mathrm{se}}(\widehat{\theta}) = \left\{-\frac{d^2}{d\theta^2} \ln \mathcal{L}(\widehat{\theta})\right\}^{-1/2} = \left(\frac{\bar{X}}{n(1 + \bar{X})^3}\right)^{1/2}.$$

- **Question:** Why does this work?

Example: Exponential distribution

- **Model:** $X_1, \cdots, X_n$ are independent Exponential random variables with pdf
$$f(x; \lambda) = \lambda \exp(-\lambda x) \text{ for } x \geq 0$$
where $\lambda > 0$ is unknown.
- The log-likelihood function is
$$\ln \mathcal{L}(\lambda) = n \ln(\lambda) - \lambda \sum_{i=1}^{n} x_i.$$
- Differentiating we get the likelihood equation
$$\frac{n}{\widehat{\lambda}} - \sum_{i=1}^{n} x_i = 0$$
and note that the 2nd derivative is $-n/\lambda^2 < 0$.
- Thus the MLE is $\widehat{\lambda} = 1/\bar{X}$.

Example: Exponential distribution (cont'd)

- We noted in the Geometric example that we could estimate the standard error of the MLE using the observed Fisher information obtained from the 2nd derivative of the log-likelihood function.
- In this case, the observed Fisher information is

$$-\frac{d^2}{d\lambda^2} \ln \mathcal{L}(\widehat{\lambda}) = \frac{n}{\widehat{\lambda}^2}.$$

- Therefore, we obtain the standard error estimator

$$\widehat{\text{se}}(\widehat{\lambda}) = \left(\frac{n}{\widehat{\lambda}^2}\right)^{-1/2} = \frac{\widehat{\lambda}}{\sqrt{n}}.$$

- Note that this is the same as the estimator obtained via the Delta Method.

Example: Gamma distribution

- **Model:** $X_1, \cdots, X_n$ are independent Gamma random variables with pdf
$$f(x;\alpha,\beta) = \frac{x^{\alpha-1}\exp(-x/\beta)}{\beta^\alpha \Gamma(\alpha)} \quad \text{for } x \geq 0$$
where $\alpha, \beta > 0$ are unknown.
- The log-likelihood function is
$$\ln \mathcal{L}(\alpha,\beta) = -n\alpha \ln(\beta) - n \ln \Gamma(\alpha) + (\alpha - 1) \ln \left(\prod_{i=1}^{n} x_i \right) - \frac{1}{\beta} \sum_{i=1}^{n} x_i.$$
- The partial derivatives are
$$\frac{d}{d\alpha} \ln L(\alpha,\beta) = -n \ln(\beta) - n\frac{\Gamma'(\alpha)}{\Gamma(\alpha)} + \ln \left(\prod_{i=1}^{n} x_i \right);$$
$$\frac{d}{d\beta} \ln L(\alpha,\beta) = -\frac{n\alpha}{\beta} + \frac{1}{\beta^2} \sum_{i=1}^{n} x_i.$$

Example: Gamma distribution (cont'd)

- Now, define

$$\psi(\alpha) := \frac{d}{d\alpha} \ln \Gamma(\alpha) = \frac{\Gamma'(\alpha)}{\Gamma(\alpha)} \quad \text{and } \tilde{x}_n = \left(\prod_{i=1}^{n} x_i \right)^{1/n}$$

  where $\psi(\cdot)$ is called the **digamma function** and $\tilde{x}_n$ is the **geometric mean** of $x_1, \ldots, x_n$.

- Setting the partial derivatives to 0, we obtain the maximum likelihood equations

$$\beta = \frac{\overline{x}_n}{\alpha}$$

$$\ln(\alpha) - \psi(\alpha) - \ln(\overline{x}_n / \tilde{x}_n) = 0.$$

- There is no closed form solution for these equations, but they can be solved numerically.

MLE: Invariance property

Invariance property of MLEs

If $\hat{\theta}$ is the MLE of θ and if $u(\theta)$ is a function of θ, then $u(\hat{\theta})$ is an MLE for $u(\theta)$.

- **Examples:**
  1. Let $X_1, \ldots, X_n$ be a random sample from an Exponential distribution with scale parameter β. What is the MLE for estimating $p(\beta) = P(X \geq 1) = e^{-1/\beta}$? Since $\overline{X}_n$ is the MLE for β, we have $\widehat{p(\beta)} = p(\hat{\beta}) = e^{-1/\overline{X}_n}$.
  2. Let $X_1, \ldots, X_n$ be a random sample from a Poisson distribution with parameter $\lambda > 0$. What is the MLE for estimating $p(\lambda) = P(X = 0) = e^{-\lambda}$? Since $\overline{X}_n$ is the MLE for λ, we have $\widehat{p(\lambda)} = p(\hat{\lambda}) = e^{-\overline{X}_n}$.