Statistical Methods for Data Science

Lesson 14 - Maximum likelihood estimation.

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Example: number of German tanks

- Tanks' ID drawn at random without replacement from $1, \dots, N$. Objective: estimate N.

Example: number of German tanks

- Let $x_1, \ldots, x_n$ be the observed ID's
- E.g., $61, 19, 56, 24, 16$ with $n = 5$
- They are realizations of $X_1, \ldots, X_n$ draws without replacement from $1, \ldots, N$
  - $X_1, \ldots, X_n$ is not a random sample, as they are not independent!
  - The marginal distribution is $X_i \sim U(1, N)$ **[prove it, or see Sect. 9.3]**

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- **Estimator based on the mean**
  - we have:

$$E[\bar{X}_n] = E[X_i] = \frac{N+1}{2}$$

  - We can define an estimator

$$T_1 = 2\bar{X}_n - 1$$

  - T_1 is unbiased: $E[T_1] = 2E[\bar{X}_n] - 1 = N$
  - E.g., $t_1 = 2(61 + 19 + 56 + 24 + 16)/5 - 1 = 69.4$

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- Let $x_1, \ldots, x_n$ be the observed ID's
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- **Estimator based on the maximum**
  - Let $M_n = \max\{X_1, \ldots, X_n\}$
  - We have: *[see Sect. 20.1]*

$$E[M_n] = n\frac{N+1}{n+1}$$

  - We can define an estimator

$$T_2 = \frac{n+1}{n}M_n - 1$$

  - T_2 is unbiased: $E[T_2] = \frac{n+1}{n}E[M_n] - 1 = N$
  - E.g., $t_2 = 6/5\max\{61, 19, 56, 24, 16\} - 1 = 72.2$

See R script

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- So far, estimators were naturally derived from parameter definition
- A general principle to derive estimators will be shown today

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Number of cycles	1	2	3	4	5	6	7	8	9	10	11	12	>12
Smokers	29	16	17	4	3	9	4	5	1	1	1	3	7
Nonsmokers	198	107	55	38	18	22	7	9	5	3	6	6	12

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$$P(X_i = k) = (1 - p)^{k-1} p$$

- What is an estimator for p? *[parametric inference]*
  - E.g., since $p = P(X_i = 1)$, we could use $S = \frac{|\{i \mid X_i = 1\}|}{n}$, and show $E[S] = p$
  - $p = 29/100$ for smokers, and $p = 198/486 = 0.41$ for non-smokers
  - But we did not use all of the available data!

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- For $k = 1, \ldots, 12$, $P(X_i = k) = (1-p)^{k-1}p$. Moreover, $P(X_i > 12) = (1-p)^{12}$

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- For $k = 1, \ldots, 12$, $P(X_i = k) = (1-p)^{k-1}p$. Moreover, $P(X_i > 12) = (1-p)^{12}$
- Since the X_i's are independent, we can write the probability of observing the dataset as:

$$L(p) = C \cdot P(X_i = 1)^{29} \cdot P(X_i = 2)^{16} \cdot \ldots \cdot P(X_i = 12)^3 \cdot P(X_i > 12)^7 = Cp^{93}(1-p)^{322}$$

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- $\log' L(p) = \frac{93}{p} - \frac{322}{1-p}$
- $\log' L(p) = 0$ for $322p = 93(1-p)$, i.e., $p = 93/(322+93) = 0.224$

See R script

Likelihood and log-likelihood

- Let $x_1, \ldots, x_n$ be realization of a random sample $X_1, \ldots, X_n$

Likelihood and log-likelihood functions

Let $f_\theta(x)$ be the density/p.m.f. of the distribution of $X_i's$, with parameter θ. The likelihood function is:

$$L(\theta) = P(X_1 = x_1, \ldots, X_n = x_n) = \prod_{i=1}^{n} f_\theta(x_i)$$

and the log-likelihood function is:

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MAXIMUM LIKELIHOOD ESTIMATES. The *maximum likelihood estimate of* θ is the value $t = h(x_1, x_2, \ldots, x_n)$ that maximizes the likelihood function $L(\theta)$. The corresponding random variable

$$T = h(X_1, X_2, \ldots, X_n)$$

is called the *maximum likelihood estimator* for θ.

Example: MLE of exponential distribution

- Random sample of $Exp(\lambda)$ $E[X] = {}^{1}/_{\lambda}$
- Since $f_\lambda(x) = \lambda e^{-\lambda x}$ for $x \geq 0$:

$$\ell(\lambda) = \sum_{i=1}^{n} (\log \lambda - \lambda x_i) = n \log \lambda - \lambda(x_1 + \ldots + x_n) = n(\log \lambda - \lambda \bar{x}_n)$$

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- It is biased!: $E[T] \geq 1/E[\bar{X}_n] = \lambda$ $\qquad$ *[Jensen's inequality]*

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- **Exercise at home**
  - show that $\bar{X}_n$ is an unbiased MLE of θ for a $Exp(1/\theta)$-distributed random sample

Example: upper point of a uniform distribution

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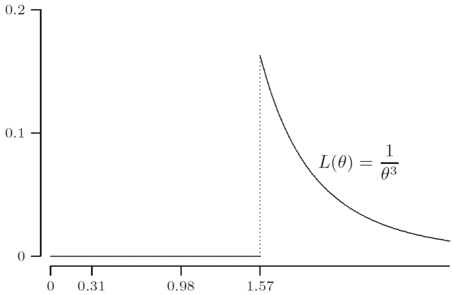

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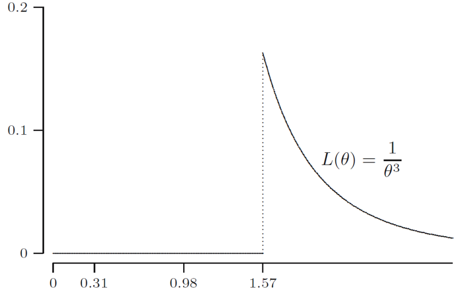

- In general, MLE estimator is $\max\{X_1, \ldots, X_n\}$

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- MLE of $\theta = (\mu, \sigma^2)$ where $f_{\mu,\sigma^2}(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$ *[we work on σ^2, not on σ]*

$$\ell(\mu, \sigma^2) = -n \log \sigma - n \log \sqrt{2\pi} - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (x_i - \mu)^2$$

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$$\frac{d}{d\mu} \ell(\mu, \sigma) = \frac{n}{\sigma^2} (\bar{x}_n - \mu) \qquad \frac{d}{d\sigma^2} \ell(\mu, \sigma) = \frac{1}{2\sigma^2} \left(\frac{1}{\sigma^2} \sum_{i=1}^{n} (x_i - \mu)^2 - n \right)$$

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- Partial derivatives at 0 for $\mu = \bar{x}_n$ and $\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2$ **[prove it is a maximum]**
- MLE estimators $\mu = \bar{X}_n$ (*unbiased*) and $\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(X_i - \mu)^2$ (*biased*)

See R script

Loss functions (to be minimized)

- Negative log-likelihood (nLL)

$$nLL(\theta) = -\ell(\theta)$$

- Akaike information criterion (AIC), balances model fit against model simplicity

$$AIC(\theta) = 2|\theta| - 2\ell(\theta)$$

- Bayesian information criterion (BIC), stronger balances over model simplicity

$$BIC(\theta) = |\theta| \log n - 2\ell(\theta)$$

Properties of MLE estimators

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- If T is the MLE estimator of θ and $g()$ is an invertible function, then $g(T)$ is the MLE estimator of $g(\theta)$ *[Invariance principle]*
  - E.g., MLE of σ for normal data is $\sqrt{\frac{1}{n} \sum_{i=1}^{n} (x_i - \mu)^2}$
  - but, $E[T] = \theta$ does **NOT** necessarily imply $E[g(T)] = g(\theta)$
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- Under mild assumptions, MLE estimators have asymptotically the smallest variance among unbiased estimators *[Asymptotic minimum variance]*

Minimum Variance Unbiased Estimators (MVUE)

- Consider a density function $f_\theta(x)$

Score function and Fisher information

The *score function* is the random variable:

$$S(\theta) = \frac{\partial}{\partial\theta}\ell(\theta) = \sum_{i=1}^{n} \frac{\partial}{\partial\theta} \log f_\theta(X_i)$$

The Fisher information is the variance of it:

$$I(\theta) = Var(S(\theta))$$

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- *Cramér-Rao's bound* for unbiased estimator T (under some assumptions):

$$Var(T) \geq \frac{1}{I(\theta)}$$

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- *Efficiency* of unbiased estimator is $e(T) = 1/(Var(T)I(\theta))$

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$$S(\theta) = \frac{\partial}{\partial\theta}\ell(\theta) = \sum_{i=1}^{n} \frac{\partial}{\partial\theta} \log f_\theta(X_i)$$

The Fisher information is the variance of it:

$$I(\theta) = Var(S(\theta))$$

- Since $E[S(\theta)] = 0$, we have $I(\theta) = E[S(\theta)^2]$
- *Cramér-Rao's bound* for unbiased estimator T (under some assumptions):

$$Var(T) \geq \frac{1}{I(\theta)}$$

- *Efficiency* of unbiased estimator is $e(T) = 1/(Var(T)I(\theta))$
- An unbiased estimator T such that $Var(T) = 1/I(\theta)$ (or $e(T) = 1$) is called a *MVUE*

Example

- Normal distribution and μ parameter: $f_{\mu}(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}$
- Unbiased MLE estimator of μ is $T = \bar{X}_n = (X_1 + \ldots + X_n)/n$.

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- Unbiased MLE estimator of μ is $T = \bar{X}_n = (X_1 + \ldots + X_n)/n$.
- The Fisher information is:

$$
\begin{aligned}
I(\theta) &= n\mathrm{E}\left[\left(\frac{\partial}{\partial\mu}\log f_\mu(X)\right)^2\right] \\
&= n\mathrm{E}\left[\left(\frac{X-\mu}{\sigma^2}\right)^2\right] \\
&= \frac{n}{\sigma^4}\mathrm{E}\left[(X-\mu)^2\right] \\
&= \frac{n}{\sigma^4}\mathrm{Var}(X) = \frac{n}{\sigma^4}\sigma^2 = \frac{n}{\sigma^2} = \frac{1}{\mathrm{Var}(\bar{X}_n)}
\end{aligned}
$$

where the last equality follows because for i.i.d. random variables $\mathrm{Var}(\bar{X}_n) = \sigma^2/n$.

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  where the last equality follows because for i.i.d. random variables $\mathrm{Var}(\bar{X}_n) = \sigma^2/n$.
- By taking the reciprocals: $Var(\bar{X}_n) = 1/I(\theta)$
- Hence $\bar{X}_n$ is a MVUE of μ