FSAN/ELEG815: Statistical Learning

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6. Maximum Likelihood and Bayes Estimation

Maximum Likelihood and Bayes Estimation

Estimation

Estimation is the inference of unknown quantities. Two cases are considered:

1. Quantity is fixed, but unknown – parameter estimation
2. Quantity is random and unknown – random variable estimator

Parameter Estimation

Consider a set of observations forming a vector

$$\mathbf{x} = [x_1, x_2, \cdots, x_N]^T$$

Assumption: The x_i *RV*s come from a known density governed by unknown (but fixed) parameter θ

Objective: Estimate θ. What optimality criteria should be used?

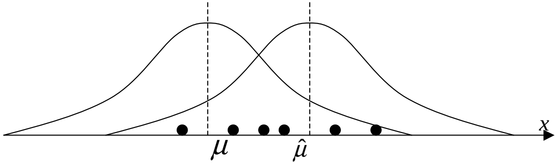
Definition (Maximum Likelihood Estimation)

The maximum likelihood estimate of θ is the value $\hat{\theta}_{\text{ML}}(\mathbf{x})$ which makes the $\mathbf{x}$ observations most likely

$$\hat{\theta}_{\text{ML}}(\mathbf{x}) = \underset{\theta}{\operatorname{argmax}} \, f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)$$

Example

Let $x_i \sim N(\mu, \sigma^2)$. Given N observations, find the ML estimate of μ.



For i.i.d. samples

$$\begin{aligned} f_{\mathbf{x}|\mu}(\mathbf{x}|\mu) &= \prod_{i=1}^{N} f_{x_i|\mu}(x_i|\mu) \\ &= \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}} \qquad \text{[Gaussian case]} \\ &\triangleq \text{likelihood function} \end{aligned}$$

Thus the estimate of the mean it is set as

$$\hat{\mu} = \underset{\mu}{\operatorname{argmax}} \, f_{\mathbf{x}|\mu}(\mathbf{x}|\mu)$$

Interpretation: Set the distribution mean to the value that makes obtaining the observed samples most likely.

Note: Maximizing $f_{\mathbf{x}|\mu}(\mathbf{x}|\mu)$ is equivalent to maximizing any monotonic function of $f_{\mathbf{x}|\mu}(\mathbf{x}|\mu)$. Choosing $\ln(\cdot)$

$$\begin{aligned}
\ln(f_{\mathbf{x}|\mu}(\mathbf{x}|\mu)) &= \ln\left(\prod_{i=1}^{N}\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}\right)\\
&= -N\ln(\sqrt{2\pi\sigma^2}) - \sum_{i=1}^{N}\frac{(x_i-\mu)^2}{2\sigma^2}\\
&= -N\ln(\sqrt{2\pi\sigma^2}) - \sum_{i=1}^{N}\frac{x_i^2}{2\sigma^2} + \mu\sum_{i=1}^{N}\frac{x_i}{\sigma^2} - \sum_{i=1}^{N}\frac{\mu^2}{2\sigma^2}
\end{aligned}$$

Taking the derivative and equating to 0,

$$\frac{\partial\ln(f_{\mathbf{x}|\mu}(\mathbf{x}|\mu))}{\partial\mu} = \sum_{i=1}^{N}\frac{x_i}{\sigma^2} - \frac{N\mu}{\sigma^2} = 0$$

$$\Rightarrow \hat{\mu} = \frac{1}{N}\sum_{i=1}^{N}x_i \triangleq \text{sample mean}$$

General Maximum Likelihood Result

General Statement: The ML estimate of θ is

$$\hat{\theta}_{\text{ML}}(\mathbf{x}) = \underset{\theta}{\operatorname{argmax}}\, f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)$$

Solution: The ML estimate of θ is obtained as the solution to

$$\left.\frac{\partial}{\partial\theta} f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)\right|_{\theta=\theta_{\text{ML}}} = 0$$

or

$$\left.\frac{\partial}{\partial\theta} \ln[f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)]\right|_{\theta=\theta_{\text{ML}}} = 0$$

- $f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)$ is the likelihood function of θ.
- $\hat{\theta}_{\text{ML}}$ is a *RV* since it is a function of the *RVs* $x_1, x_2, \cdots, x_N$

Historical Note: ML estimation was pioneered by geneticist and statistician Sir R. A. Fisher between 1912 and 1922

Example

The time between customer arrivals at a bar is a *RV* with distribution

$$f_T(T) = \alpha e^{-\alpha T} U(T)$$

Objective: Estimate the arrival rate α based on N measured arrival intervals $T_1, T_2, \cdots, T_N$.

Assuming that the arrivals are independent,

$$\begin{aligned} f(T_1, T_2, \cdots, T_N) &= \prod_{i=1}^{N} f_T(T_i) \\ &= \prod_{i=1}^{N} \alpha e^{-\alpha T_i} = \alpha^N e^{-\alpha \sum_{i=1}^{N} T_i} \\ \Rightarrow \ln[f(T_1, T_2, \cdots, T_N)] &= [N \ln(\alpha) - \alpha \sum_{i=1}^{N} T_i] \end{aligned}$$

Taking the derivative and equating to 0,

$$\begin{aligned}\frac{\partial}{\partial\alpha}\ln[f(T_1,T_2,\cdots,T_N)] &= \frac{\partial}{\partial\alpha}[N\ln(\alpha)-\alpha\sum_{i=1}^{N}T_i] \\ &= \frac{N}{\alpha}-\sum_{i=1}^{N}T_i = 0\end{aligned}$$

Solving for α gives the ML estimate

$$\Rightarrow \hat{\alpha}_{\mathrm{ML}} = \frac{1}{\frac{1}{N}\sum_{i=1}^{N}T_i} = \frac{1}{\overline{\overline{T}}}$$

Result: The ML estimate of arival rate for exponentially distributed samples is the reciprocal of the sample mean arrival

Properties of Estimates

Since $\hat{\theta}_N$ is a function of *RVs* $x_1, x_2, \cdots, x_N$, estimates are*RVs* and we can state the following properties:

- An estimate $\hat{\theta}_N$ is unbiased if

$$E\{\hat{\theta}_N\} = \theta \qquad \text{bias} \triangleq E\{\hat{\theta}_N\} - \theta$$

- $\hat{\theta}_N$ is consistent (converges in probability) if

$$\lim_{N\to\infty} \Pr\{|\hat{\theta}_N - \theta| < \epsilon\} = 1 \quad \text{for arbitrary } \epsilon$$

- $\hat{\theta}_N$ is efficient in comparison to other estimators if

$$\text{var}(\hat{\theta}_N) < \text{var}(\hat{\theta}_{\text{other}})$$

Note: If $\hat{\theta}_N$ is unbiased and efficient with respect to $\hat{\theta}_{N-1}$ for all N (i.e., $\text{var}(\hat{\theta}_N)$ converges to 0), then $\hat{\theta}_N$ is a consistent estimate

To prove the consistent estimate result, note that by the Tchebycheff inequality

$$\Pr\{|\hat{\theta}_N - \theta| > \epsilon\} \leq \frac{\text{var}(\hat{\theta}_N)}{\epsilon^2}$$

If $\text{var}(\hat{\theta}_N) < \text{var}(\hat{\theta}_{N-1})$, the above gives

$$\lim_{N\to\infty} \Pr\{|\hat{\theta}_N - \theta| > \epsilon\} = 0$$

or

$$\lim_{N\to\infty} \Pr\{|\hat{\theta}_N - \theta| < \epsilon\} = 1$$

That is, it converges in probability, or is consistent

QED

Example

Let $\{x_i\}$ be WSS with uncorrelated samples. Is the sample mean a consistent estimator for this sequence?

Step 1: Consider the bias

$$\begin{aligned} E\{\hat{\mu}_N\} &= E\left\{\frac{1}{N}\sum_{i=1}^{N} x_i\right\} \\ &= \frac{1}{N}(N\mu) = \mu \end{aligned}$$

Result: $\hat{\mu}_N$ is unbiased

Step 2: Consider the variance

$$\text{var}(\hat{\mu}_N) = E\left\{(\hat{\mu} - \mu)^2\right\}$$

$$
\begin{aligned}
\text{var}(\hat{\mu}_N) &= E\left\{(\hat{\mu}-\mu)^2\right\} \\
&= E\left\{\left(\left(\frac{1}{N}\sum_{i=1}^{N} x_i\right)-\mu\right)^2\right\} \\
&= \frac{1}{N^2}E\left\{\left(\sum_{i=1}^{N}(x_i-\mu)\right)^2\right\} \qquad \text{[assume uncorrelated]} \\
&= \frac{1}{N^2}\sum_{i=1}^{N}E\{(x_i-\mu)^2\} + \frac{1}{N^2}\underbrace{E(\text{cross terms})}_{=0} \\
&= \frac{1}{N^2}\sum_{i=1}^{N}E\{(x_i-\mu)^2\} = \frac{1}{N^2}(N\sigma^2) = \frac{\sigma^2}{N}
\end{aligned}
$$

Result: $\hat{\mu}_N$ is unbiased and $\text{var}(\hat{\mu}_N) < \text{var}(\hat{\theta}_{N-1}) \Rightarrow \hat{\mu}_N$ is consistent

Theorem (Cramer-Rao Bound (1945, 1946))

If $\hat{\theta}$ is an unbiased estimate of θ, then

$$var(\hat{\theta}) \geq \left(E\left\{ \left(\frac{\partial}{\partial \theta} \ln[f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)] \right)^2 \right\} \right)^{-1}$$

or equivalently

$$var(\hat{\theta}) \geq \left(-E\left\{ \frac{\partial^2}{\partial \theta^2} \ln[f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)] \right\} \right)^{-1}$$

where it is assumed

$$\frac{\partial}{\partial \theta} f_{\mathbf{x}|\theta}(\mathbf{x}|\theta) \quad \textit{and} \quad \frac{\partial^2}{\partial \theta^2} f_{\mathbf{x}|\theta}(\mathbf{x}|\theta) \quad \textit{exist}$$

Note: If any estimate satisfies the bound with equality, it is an efficient (minimum variance) estimate

Proof:

Since $\hat{\theta}$ is unbiased

$$E\{\hat{\theta}-\theta\} = \int_{-\infty}^{\infty} (\hat{\theta}-\theta) f_{\mathbf{x}|\theta}(\mathbf{x}|\theta) d\mathbf{x} = 0$$

Taking the derivative

$$\begin{aligned}
\frac{\partial}{\partial\theta}\int_{-\infty}^{\infty}(\hat{\theta}-\theta) f_{\mathbf{x}|\theta}(\mathbf{x}|\theta) d\mathbf{x} &= 0 \\
\Rightarrow \underbrace{-\int_{-\infty}^{\infty} f_{\mathbf{x}|\theta}(\mathbf{x}|\theta) d\mathbf{x}}_{-1} + \int_{-\infty}^{\infty} \frac{\partial f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)}{\partial\theta}(\hat{\theta}-\theta) d\mathbf{x} &= 0 \\
\Rightarrow \int_{-\infty}^{\infty} \frac{\partial f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)}{\partial\theta}(\hat{\theta}-\theta) d\mathbf{x} &= 1 \qquad (*)
\end{aligned}$$

Note the following equality

$$\frac{\partial \ln[f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)]}{\partial \theta} f_{\mathbf{x}|\theta}(\mathbf{x}|\theta) = \frac{\partial f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)}{\partial \theta}$$

Using this in $(*)$

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{\partial f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)}{\partial \theta}(\hat{\theta}-\theta) d\mathbf{x} &= 1 \\ \Rightarrow \int_{-\infty}^{\infty} \frac{\partial \ln[f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)]}{\partial \theta} f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)(\hat{\theta}-\theta) d\mathbf{x} &= 1 \end{aligned}$$

This can be equivalently expressed as

$$\left(\int_{-\infty}^{\infty} \left(\frac{\partial \ln[f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)]}{\partial \theta} \sqrt{f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)} \right) \left(\sqrt{f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)}(\hat{\theta}-\theta) \right) d\mathbf{x} \right)^2 = 1$$

Definition (Cauchy–Schwarz Inequality (1821 disc.; 1859 cont.))

Cauchy-Schwarz's inequality states (for square–integrable complex–valued functions),

$$\left| \int f(x)g(x)\, dx \right|^2 \leq \int |f(x)|^2\, dx \cdot \int |g(x)|^2\, dx$$

with equality only if $f(x) = k \cdot g(x)$, where k is a constant

Thus

$$\left(\int_{-\infty}^{\infty} \left(\frac{\partial \ln[f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)]}{\partial \theta} \sqrt{f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)} \right) \left(\sqrt{f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)} (\hat{\theta} - \theta) \right) d\mathbf{x} \right)^2 = 1$$

$$\Rightarrow \left(\int_{-\infty}^{\infty} \left(\frac{\partial \ln[f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)]}{\partial \theta} \right)^2 f_{\mathbf{x}|\theta}(\mathbf{x}|\theta) d\mathbf{x} \right) \left(\int_{-\infty}^{\infty} (\hat{\theta} - \theta)^2 f_{\mathbf{x}|\theta}(\mathbf{x}|\theta) d\mathbf{x} \right) \geq 1$$

Note

$$\int_{-\infty}^{\infty}(\hat{\theta}-\theta)^2 f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)d\mathbf{x} = \text{var}(\hat{\theta}) \qquad (*)$$

and

$$\int_{-\infty}^{\infty}\left(\frac{\partial \ln[f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)]}{\partial\theta}\right)^2 f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)d\mathbf{x} = E\left\{\left(\frac{\partial \ln(f_{\mathbf{x}|\theta}(\mathbf{x}|\theta))}{\partial\theta}\right)^2\right\} \qquad (**)$$

Thus using $(*)$ and $(**)$ in

$$\left(\int_{-\infty}^{\infty}\left(\frac{\partial \ln[f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)]}{\partial\theta}\right)^2 f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)d\mathbf{x}\right)\left(\int_{-\infty}^{\infty}(\hat{\theta}-\theta)^2 f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)d\mathbf{x}\right) \geq 1$$

$$\Rightarrow \text{var}(\hat{\theta}) \geq \left[E\left\{\left(\frac{\partial \ln(f_{\mathbf{x}|\theta}(\mathbf{x}|\theta))}{\partial\theta}\right)^2\right\}\right]^{-1}$$

with equality iff

$$\frac{\partial}{\partial\theta}\ln(f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)) = k(\hat{\theta}-\theta)$$

QED

Thus the bound in met iff

$$\frac{\partial}{\partial\theta}\ln(f_{\mathbf{x}|\theta}(\mathbf{x}|\theta)) = k(\hat{\theta}-\theta)$$

Let $\theta = \hat{\theta}_{\text{ML}}$ in the above

$$\underbrace{\frac{\partial}{\partial\theta}\ln(f_{\mathbf{x}|\theta}(\mathbf{x}|\theta))\Big|_{\theta=\hat{\theta}_{\text{ML}}}}_{=0 \text{ by ML criteria}} = k(\hat{\theta}-\theta)\Big|_{\theta=\hat{\theta}_{\text{ML}}}$$

Therefore, the RHS must equal zero, or

$$\hat{\theta} = \hat{\theta}_{\text{ML}}$$

Result: If an efficient estimate (one that satisfies the bound with equality) exists, then it is the ML estimate

Note: If an efficient estimator doesn't exist, then we don't know how good $\hat{\theta}_{\text{ML}}$ is