Maximum Likelihood Estimation

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1 Maximizing log-likelihood

In statistical inference, Maximum Likelihood Estimation (MLE) is a method of producing a model that best accounts for the observed data by maximizing the likelihood of the observed data; among all competing models, we should select the one that best predicts the observed data.

Optimizing the likelihood function becomes easier when we instead maximize the log-likelihood. We'll justify this alternative optimization in what follows.

Theorem 1 (Equivalence of Likelihood and Log-Likelihood Maximizers). Let $L(\theta \mid \mathbf{x})$ be the likelihood function for parameters θ given data \mathbf{x} , assumed to be positive. Let $\log L(\theta \mid \mathbf{x})$ be the corresponding log-likelihood function. A parameter value $\hat{\theta}$ maximizes the likelihood function if and only if it also maximizes the log-likelihood function. Formally:

$$\hat{\theta} = \argmax_{\theta} L(\theta \mid \mathbf{x}) \iff \hat{\theta} = \argmax_{\theta} \log L(\theta \mid \mathbf{x})$$

Proof. For the forward direction, assume that $\hat{\theta} = \underset{\theta}{\arg\max} L(\theta \mid \mathbf{x})$. By the definition of argument maximization, we have $L(\theta' \mid \mathbf{x}) \leq L(\hat{\theta} \mid \mathbf{x})$. Since $\log(x)$ is strictly increasing, $\log(L(\theta' \mid \mathbf{x})) \leq \log(L(\hat{\theta} \mid \mathbf{x}))$, so $\hat{\theta} = \arg\max\log L(\theta \mid \mathbf{x})$.

For the backward direction, assume that $\hat{\theta} = \underset{\theta}{\operatorname{arg\,max}} \log L(\theta \mid \mathbf{x})$. By the definition of argument maximization, we have $\log(L(\theta' \mid \mathbf{x})) \leq \log(L(\hat{\theta} \mid \mathbf{x}))$. Since e^x is strictly increasing, we have

$$e^{\log(L(\boldsymbol{\theta}'|\mathbf{x}))} < e^{\log(L(\hat{\boldsymbol{\theta}}|\mathbf{x}))}$$

, and by simplifying we get

$$L(\theta' \mid \mathbf{x}) < L(\hat{\theta} \mid \mathbf{x})$$

1.1 Example: MLE for a Normal Sample

Suppose $x_1, x_2, \dots x_n$ are iid with $x_i \sim \mathcal{N}(\mu, \sigma^2)$. First, we will derive the likelihood function:

$$L(\theta \mid x) = P(x_1, x_2, \dots, x_n \mid \mu, \sigma^2)$$

$$= \prod_{i=1}^n P(x_i \mid \mu, \sigma^2) \quad \text{(due to independence)}$$

$$= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i - \mu)^2}{2\sigma^2}}$$

$$= \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^n e^{-\sum_{i=1}^n \frac{(x_i - \mu)^2}{2\sigma^2}}$$

$$= \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^n e^{-\frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \mu)^2}$$

We can instead maximize the log-likelihood by theorem 1, so

$$\log(L(\theta \mid x)) = \log\left(\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^n e^{-\frac{1}{2\sigma^2}\sum_{i=1}^n(x_i-\mu)^2}\right)$$

$$= \log\left(\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^n\right) + \log\left(e^{-\frac{1}{2\sigma^2}\sum_{i=1}^n(x_i-\mu)^2}\right)$$

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

Maximizing the log-likelihood requires finding its partial derivatives:

$$\frac{\partial \log L}{\partial \mu} = \frac{\partial}{\partial \mu} \left[n \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} \right) - \frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \mu)^2 \right]$$

$$= \frac{\partial}{\partial \mu} \left[n \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} \right) \right] - \frac{\partial}{\partial \mu} \left[\frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \mu)^2 \right]$$

$$= \frac{1}{\sigma^2} \left(\left(\sum_{i=1}^n x_i \right) - n\mu \right)$$

Similarly,

$$\frac{\partial \log L}{\partial \sigma} = \frac{\partial}{\partial \sigma} \left[n \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} \right) - \frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \mu)^2 \right]$$

$$= \frac{\partial}{\partial \sigma} \left[n \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} \right) \right] - \frac{\partial}{\partial \sigma} \left[\frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \mu)^2 \right]$$

$$= -\frac{n}{\sigma} + \frac{\sum_{i=1}^n (x_i - \mu)^2}{\sigma^3}$$

We can set each partial derivative to 0 and solve, so with some algebra, the result is

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

$$\hat{\sigma} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (x_i - \mu)^2}$$

The critical points $(\hat{\mu}, \hat{\sigma})$ represent a global maximum due to the second derivative test.