Module 5: Statistical inference (II)

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Outline

This module we will review

- Basics of parametric inference
- Methods for generating parametric estimators
- Maximum likelihood estimators
- Delta method
- Optimization method for finding MLE in R (Newton-Raphson, EM algorithm)

Parametric inference

Definition (Parametric models)

$$\mathfrak{F} = \{f(x;\theta) : \theta \in \Theta\}$$

where the $\Theta \subset \mathbb{R}^k$ is the parameter space and $\theta = (\theta_1, \ldots, \theta_k)$ is the parameter.

Goal of parametric inference

- estimate the parametric θ (assume we known the form of the density).

Parameter of interest and nuisance parameter

Often, we are interested in estimating some function $T(\theta)$.

For example, if $X \sim N(\mu, \sigma^2)$, then

- Parameters: $\theta = (\mu, \sigma)$
- Parameter space: $\Theta = \{(\mu, \sigma) : \mu \in \mathbb{R}, \sigma > 0\}$

If the goal is to estimate the μ then

- Parameter of interest: $T(\theta) = \mu$
- Nuisance parameter: σ

Methods for generating parametric estimators

1. Method of moments
2. Maximum likelihood

Method of moments

Definitions

- $\mathbb{E}(X^k)$ is the k^{th} (theoretical) moment of the distribution, for $k = 1, 2, ...$
- $M_k = \frac{1}{n}\sum_{i=1}^{n} X_i^k$ is the k^{th} sample moment, for $k = 1, 2, ...$

Steps to find MoM

The basic idea behind this form of the method is to:

- Equate the first sample moment about the origin $M_1 = \frac{1}{n}\sum_{i=1}^{n} X_i = \bar{X}$ to the first theoretical moment $\mathbb{E}(X)$.
- Equate the second sample moment about the origin $M_2 = \frac{1}{n}\sum_{i=1}^{n} X_i^2$ to the second theoretical moment $\mathbb{E}(X^2)$.
- Continue equating sample moments about the origin until you have as many equations as you have parameters.
- Solve for the parameters

Example of MoM (Bernoulli)

Let $X_1, ..., X_n$ be Bernoulli random variables with parameter p. What is the method of moments estimator of p?

Example of MoM (Bernoulli)

Let $X_1, ..., X_n$ be Bernoulli random variables with parameter p. What is the method of moments estimator of p?

Only one parameter p, so we only need to equate the first moment.

$\mathbb{E}(X_i) = p = M_1 = \frac{1}{n}\sum_{i=1}^{n} X_i = \bar{X}$.

So,

$$\hat{p}_{MoM} = \bar{X}$$

Example of MoM (Normal)

Let $X_1, ..., X_n$ be normal random variables with mean μ and variance σ^2. What are the method of moments estimators of the mean μ and variance σ^2 ?

Example of MoM (Normal)

Let $X_1, ..., X_n$ be normal random variables with mean μ and variance σ^2. What are the method of moments estimators of the mean μ and variance σ^2 ?

Two parameters, so we need to equate the first and the second moment.

$E(X_i) = \mu = M_1, E(X_i^2) = \sigma^2 + \mu^2 = M_2.$

So,

$$\hat{\mu}_{MoM} = \bar{X}, \hat{\sigma}^2_{MoM} = \frac{1}{n}\sum_{i=1}^{n} X_i^2 - \bar{X}^2.$$

Asymptotic properties

Under mild regularity conditions, MoM estimators are

- *Consistent* $\rightarrow$ converge to the true value in probability as $n \rightarrow \infty$, i.e.

$$\lim_{n\rightarrow\infty} P(|\hat{\theta} - \theta| \leq \epsilon) = 1 \quad \forall \epsilon > 0$$

- *Asymptotically Normal* $\rightarrow \sqrt{n}(\hat{\theta} - \theta) \sim N\left(0, \sigma^2\right)$ for large n
- However, they are usually **NOT** *Asymptotically Efficient*

Maximum likelihood

- Parametric model: $f(x;\theta)$, $X_1,\ldots,X_n$ iid
- Likelihood function

$$\mathcal{L}_n(\theta)=\prod_{i=1}^{n} f\left(X_i;\theta\right)$$

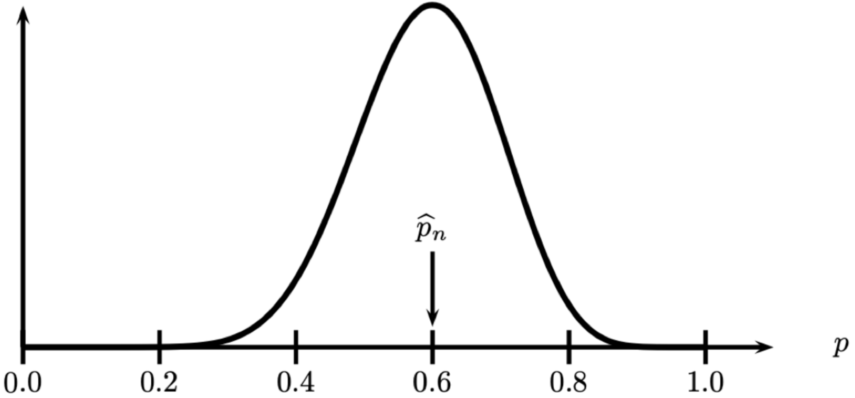
- The log-likelihood function

$$\ell_n(\theta)=\log \mathcal{L}_n(\theta)=\sum_{i=1}^{n} \log f\left(X_i;\theta\right)$$

- The maximum likelihood estimator (MLE)

$$\hat{\theta}_{MLE}=\arg\max_{\theta} \mathcal{L}(\theta)$$

An example of MLE



Likelihood function for Bernoulli with $n = 20$ and $\sum_{i=1}^{n} X_i = 12$. The MLE is $\widehat{p}_n = 12/20 = 0.6$.

Steps to find the MLE

1. Write out the likelihood

$$\mathcal{L}(\theta) = f(X_1, \ldots, X_n; \theta)$$

2. Simplify the log likelihood

$$\ell(\theta) = \log \mathcal{L}(\theta)$$

3. Take the derivative of $\ell(\theta)$ with respect to the parameter of interest, θ
   Set $= 0$
4. Solve for θ (get $\hat{\theta}_{MLE}$)
5. Check that $\hat{\theta}_{MLE}$ is a maximum $\left(\frac{\partial^2}{\partial\theta^2}\ell(\theta) < 0\right)$

Exercise

Suppose we have an iid sample $\{X_1, \ldots, X_n\}$ with $X_i \sim \text{Bernoulli}(p)$. Find the MLE for p.

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1. The likelihood

$$\mathcal{L}_n(p) = \prod_{i=1}^{n} f(X_i; p) = \prod_{i=1}^{n} p^{X_i}(1-p)^{1-X_i} = p^S(1-p)^{n-S}$$

where $S = \sum_i X_i$

Exercise

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2. Log-likelihood

$$\ell_n(p) = S \log p + (n - S) \log(1 - p)$$

Exercise

Suppose we have an iid sample $\{X_1, \ldots, X_n\}$ with $X_i \sim \text{Bernoulli}(p)$. Find the MLE for p.

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2. Log-likelihood

$$\ell_n(p) = S \log p + (n-S)\log(1-p)$$

3. MLE

$$\ell_n'(p) = 0$$

The MLE is $\widehat{p}_n = S/n$.

Asymptotics of MLE

Under mild regularity conditions, MLEs are

- *Consistent* $\rightarrow$ converge to the true value in probability as $n \rightarrow \infty$, i.e.

$$\lim_{n \rightarrow \infty} P(|\hat{\theta} - \theta| \leq \epsilon) = 1 \quad \forall \epsilon > 0$$

- *Asymptotically normal* $\rightarrow \sqrt{n}(\hat{\theta} - \theta) \sim N\left(0, \sigma^2\right)$ for large n
- *Asymptotically efficient*
- *equivariant* $\rightarrow$ if $\hat{\theta}$ is the MLE for θ then $g(\hat{\theta})$ is the MLE for $g(\theta)$

Asymptotic Efficiency

Cramér–Rao bound

The variance of any *unbiased* estimator $\hat{\theta}$ of θ is bounded by the reciprocal of the Fisher information $I(\theta)$:

$$\mathrm{Var}(\hat{\theta}) \geq \frac{1}{I(\theta)},$$

where $I(\theta) = n\mathbb{E}\left[\left(\frac{\partial \ell}{\partial \theta}\right)^2\right]$.

Both MoM estimators are asymptotically unbiased, but MLE estimators achieves the CR lower bound.

MLE in R

Sometimes, there is no closed-form solution, so we need to use optimization methods to find the maximum of the log-likelihood.

- `optim()` find values of some parameters that **minimizes** some function.
- Newton-Raphson
- EM-algorithm

Example using optim()

```r
set.seed(42) # For reproducibility
sample_data <- rbinom(1000, size = 1, prob = 0.3) # Assuming success probability of 0.3

# Log-likelihood function for Bernoulli distribution
log_likelihood_bernoulli <- function(p, data) {
  n <- length(data)
  log_likelihood <- sum(data * log(p) + (1 - data) * log(1 - p))
  return(-log_likelihood) # Negative to be used with optimization functions (minimization)
}

# Initial parameter value for optimization (probability of success)
initial_param <- 0.8

# Find MLE using optim
result <- optim(
  par = initial_param, fn = log_likelihood_bernoulli,
  data = sample_data, method = "Brent", lower = 0, upper = 1
)

# MLE estimate of p
mle_p <- result$par

# Print the result
cat("MLE of p:", mle_p, "\n")
```

```
## MLE of p: 0.293
```

Newton-Raphson

Derivative of the log-likelihood around θ^j :

$$0 = \ell'(\widehat{\theta}) \approx \ell'\left(\theta^j\right) + \left(\widehat{\theta} - \theta^j\right) \ell''\left(\theta^j\right)$$

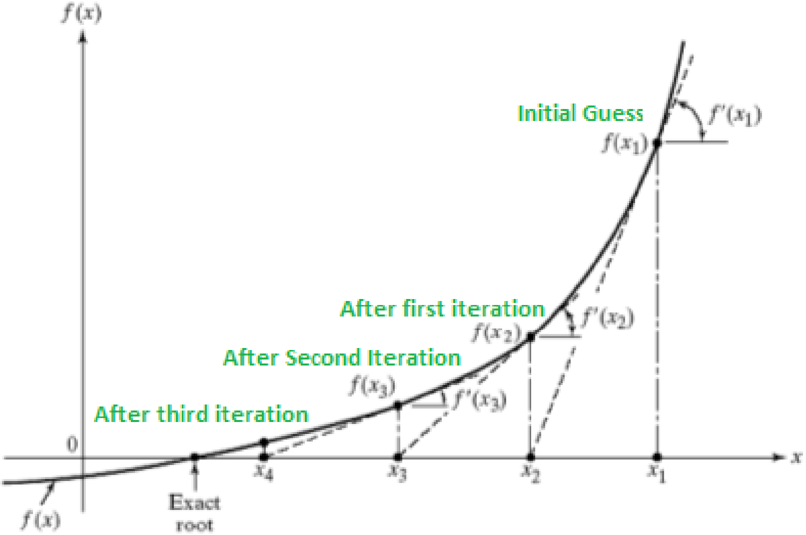
Solving for $\widehat{\theta}$ gives

$$\widehat{\theta} \approx \theta^j - \frac{\ell'\left(\theta^j\right)}{\ell''\left(\theta^j\right)}.$$

This suggests the following iterative scheme:

$$\widehat{\theta}^{j+1} = \theta^j - \frac{\ell'\left(\theta^j\right)}{\ell''\left(\theta^j\right)}$$

Illustration

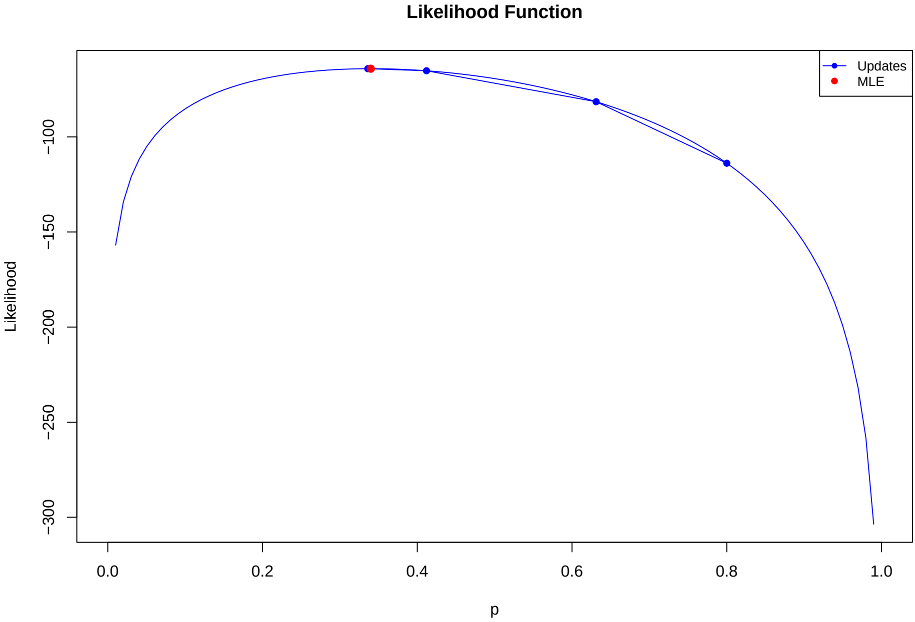


NR algorithm in R

```r
# First derivative of the log-likelihood function
log_likelihood_bernoulli_prime <- function(p, data) {
  n <- length(data)
  d_log_likelihood <- sum(data / p - (1 - data) / (1 - p))
  return(-d_log_likelihood) # Negative to be used with optimization functions (minimization)
}
# Second derivative of the log-likelihood function
log_likelihood_bernoulli_double_prime <- function(p, data) {
  n <- length(data)
  dd_log_likelihood <- sum(-data / p^2 - (1 - data) / (1 - p)^2)
  return(-dd_log_likelihood) # Negative to be used with optimization functions (minimization)
}
# Initial parameter value for optimization (probability of success)
initial_param <- 0.8
# Newton-Raphson algorithm for optimization
tolerance <- 1e-8
max_iterations <- 1000
p <- initial_param
for (i in 1:max_iterations) {
  p_new <- p - log_likelihood_bernoulli_prime(p, sample_data) /
    log_likelihood_bernoulli_double_prime(p, sample_data)
  if (abs(p_new - p) < tolerance) {
    break
  }
  p <- p_new
}
# Print the result
cat("MLE of p:", p, "\n")
```

```
## MLE of p: 0.293
```

Solution Trajectory



Expectation-Maximization (EM) algorithm

- We will introduce the expectation-maximization (EM) algorithm in the context of Gaussian mixture models.
- Let $N(\mu, \sigma^2)$ denote the probability distribution function for a normal random variable.
- In this scenario, we have that the conditional distribution $X_i | Z_i = k \sim N(\mu_k, \sigma_k^2)$

Likelihood Function

The marginal distribution of each X_i is

$$P(X_i = x) = \sum_{k=1}^{K} P(Z_i = k)P(X_i = x|Z_i = k) = \sum_{k=1}^{K} \pi_k N(x; \mu_k, \sigma_k^2)$$

Given the data is independent, the likelihood is

$$L(\theta|X_1, \ldots, X_n) = \prod_{i=1}^{n} \left[\sum_{k=1}^{K} \pi_k N(x_i; \mu_k, \sigma_k^2) \right]$$

and the log-likelihood is

$$\ell(\theta) = \sum_{i=1}^{n} \log \left[\sum_{k=1}^{K} \pi_k N(x; \mu_k, \sigma_k^2) \right]$$

where $\theta = \{\mu_1, ..., \mu_k, \sigma_1, ..., \sigma_k, \pi_1, ..., \pi_k\}$.

Complete Likelihood

The complete likelihood takes the form

$$P(X, Z \mid \mu, \sigma, \pi) = \prod_{i=1}^{n} \prod_{k=1}^{K} \pi_k^{I(Z_i=k)} N\left(x_i \mid \mu_k, \sigma_k\right)^{I(Z_i=k)}$$

so the complete log-likelihood takes the form:

$$\log(P(X, Z \mid \mu, \sigma, \pi)) = \sum_{i=1}^{n} \sum_{k=1}^{K} I\left(Z_i = k\right)\left(\log\left(\pi_k\right) + \log\left(N\left(x_i \mid \mu_k, \sigma_k\right)\right)\right)$$

E-step

In practice, we do not observe the latent variables, so we consider the expectation of the complete log-likelihood with respect to the posterior of the latent variables. The expected value of the complete log-likelihood is therefore:

$$
\begin{aligned}
& E_{Z|X}[\log(P(X, Z \mid \mu, \sigma, \pi))] \\
& = E_{Z|X}\left[\sum_{i=1}^{n} \sum_{k=1}^{K} I\left(Z_i = k\right)\left(\log\left(\pi_k\right) + \log\left(N\left(x_i \mid \mu_k, \sigma_k\right)\right)\right)\right] \\
& = \sum_{i=1}^{n} \sum_{k=1}^{K} P\left(Z_i = k \mid X\right)\left\{\log\left(\pi_k\right) + \log\left[N\left(x_i \mid \mu_k, \sigma_k\right)\right]\right\}
\end{aligned}
$$

Note that $P(Z_i = k|X)$ is the posterior distribution of Z_i given the observations:

$$
P\left(Z_i = k \mid X_i\right) = \frac{P\left(X_i \mid Z_i = k\right) P\left(Z_i = k\right)}{P\left(X_i\right)} = \frac{\pi_k N\left(\mu_k, \sigma_k^2\right)}{\sum_{k=1}^{K} \pi_k N\left(\mu_k, \sigma_k\right)}
$$

M-estp

- First choose initial values for μ, σ, π so you can compute $P\left(Z_i = k \mid X_i\right)$.
- Then with $P\left(Z_i = k \mid X_i\right)$ fixed, maximize the expected complete log-likelihood above with respect to μ_k, σ_k, π_k.

Example (Mixture of Two Normal)

Assume we have $K = 2$ components, so that:

$$X_i \mid Z_i = 0 \sim N(5, 1.5)$$
$$X_i \mid Z_i = 1 \sim N(10, 2)$$

The true mixture proportions will be $P(Z_i = 0) = 0.25$ and $P(Z_i = 1) = 0.75$. First we simulate data from this mixture model

EM in R

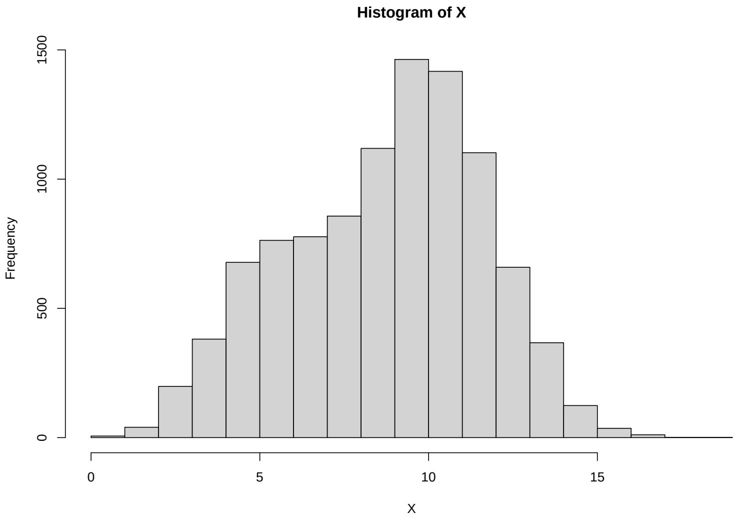
```r
# mixture components
mu.true <- c(5, 10)
sigma.true <- c(1.5, 2)

# determine Z_i
Z <- rbinom(10000, 1, 0.75)
# sample from mixture model

X <- rnorm(10000,
  mean = mu.true[Z + 1],
  sd = sigma.true[Z + 1]
)
```

EM in R

```
hist(X, breaks = 15)
```



EM in R

```r
log_likelihood_mixture <- function(theta, data) {
  mu1 <- theta[1]
  mu2 <- theta[2]
  sigma1 <- theta[3]
  sigma2 <- theta[4]
  pi <- theta[5]

  n <- length(data)
  log_likelihood <- sum(
    log(pi * dnorm(data, mean = mu1, sd = sigma1) +
      (1 - pi) * dnorm(data, mean = mu2, sd = sigma2))
  )

  return(log_likelihood)
}
```

EM in R

```r
# E-step: Compute the component proportions for each data point
e_step <- function(data, mu1, mu2, sigma1, sigma2, pi) {
  p1 <- pi * dnorm(data, mean = mu1, sd = sigma1)
  p2 <- (1 - pi) * dnorm(data, mean = mu2, sd = sigma2)

  # Compute the proportions for each data point
  proportions <- p1 / (p1 + p2)

  return(proportions)
}

# M-step: Update the parameters (means, variances, and mixture proportion)
m_step <- function(data, proportions) {
  pi <- mean(proportions)
  mu1 <- sum(proportions * data) / sum(proportions)
  mu2 <- sum((1 - proportions) * data) / sum(1 - proportions)
  sigma1 <- sqrt(sum(proportions * (data - mu1)^2) / sum(proportions))
  sigma2 <- sqrt(sum((1 - proportions) * (data - mu2)^2) / sum(1 - proportions))
  return(c(mu1, mu2, sigma1, sigma2, pi))
}
```

EM in R

```
# EM algorithm to estimate means and variances
em_algorithm <- function(data, max_iterations = 1000, tolerance = 1e-8, initial_params = NULL) {

  # Initial guesses for the parameters
  if (is.null(initial_params)) {
    initial_params <- c(mean(data), mean(data), sd(data), sd(data), 0.5)
  }

  params <- initial_params
  log_likelihood_prev <- -Inf

  for (i in 1:max_iterations) {
    # E-step: Compute the component proportions
    proportions <- e_step(data, params[1], params[2], params[3], params[4], params[5])

    # M-step: Update the parameters
    new_params <- m_step(data, proportions)

    # Compute the log-likelihood to check for convergence
    log_likelihood <- log_likelihood_mixture(new_params, data)

    # Check for convergence
    if (abs(log_likelihood - log_likelihood_prev) < tolerance) {
      cat("Total Number of Iterations:", i, "\n")
      break
    }

    # Update parameters and log-likelihood
    params <- new_params
    log_likelihood_prev <- log_likelihood
  }
  return(params)
}
```

EM in R

```r
# Run the EM algorithm on the generated data
estimated_params <- em_algorithm(X)
```

```
## Total Number of Iterations: 2
```

```r
# Print the estimated parameters
cat("Estimated mean 1:", estimated_params[1], "\n")
```

```
## Estimated mean 1: 8.730647
```

```r
cat("Estimated mean 2:", estimated_params[2], "\n")
```

```
## Estimated mean 2: 8.730647
```

```r
cat("Estimated variance 1:", estimated_params[3]^2, "\n")
```

```
## Estimated variance 1: 8.294363
```

```r
cat("Estimated variance 2:", estimated_params[4]^2, "\n")
```

```
## Estimated variance 2: 8.294363
```

```r
cat("Estimated mixture proportion:", estimated_params[5], "\n")
```

```
## Estimated mixture proportion: 0.5
```

What happened?

- There is no guarantee that the EM algorithm converges to a global maximum of the likelihood.
- To address this issue, one approach is to try different initial parameter values and run the EM algorithm multiple times.

EM in R

```r
# Run the EM algorithm with random initial parameter
estimated_params <- em_algorithm(X,
  initial_params = c(runif(2, min(X), max(X)),
                     runif(2, 0, max(X) - min(X)),
                     runif(1, 0, 1))
)
```

```
## Total Number of Iterations: 414
```

```r
# Print the estimated parameters
cat("Estimated mean 1:", estimated_params[1], "\n")
```

```
## Estimated mean 1: 5.012625
```

```r
cat("Estimated mean 2:", estimated_params[2], "\n")
```

```
## Estimated mean 2: 9.984025
```

```r
cat("Estimated variance 1:", estimated_params[3]^2, "\n")
```

```
## Estimated variance 1: 2.137282
```

```r
cat("Estimated variance 2:", estimated_params[4]^2, "\n")
```

```
## Estimated variance 2: 4.138926
```

```r
cat("Estimated mixture proportion:", estimated_params[5], "\n")
```

```
## Estimated mixture proportion: 0.2521176
```

EM in R

```r
# Run the EM algorithm with random initial parameter
estimated_params <- em_algorithm(X,
  initial_params = c(runif(2, min(X), max(X)),
                     runif(2, 0, max(X) - min(X)),
                     runif(1, 0, 1))
)
```

```
## Total Number of Iterations: 266
```

```r
# Print the estimated parameters
cat("Estimated mean 1:", estimated_params[1], "\n")
```

```
## Estimated mean 1: 9.984025
```

```r
cat("Estimated mean 2:", estimated_params[2], "\n")
```

```
## Estimated mean 2: 5.012624
```

```r
cat("Estimated variance 1:", estimated_params[3]^2, "\n")
```

```
## Estimated variance 1: 4.138927
```

```r
cat("Estimated variance 2:", estimated_params[4]^2, "\n")
```

```
## Estimated variance 2: 2.137281
```

```r
cat("Estimated mixture proportion:", estimated_params[5], "\n")
```

```
## Estimated mixture proportion: 0.7478825
```

EM in R

```
# Run the EM algorithm with random initial parameter
estimated_params <- em_algorithm(X,
  initial_params = c(runif(2, min(X), max(X)),
                     runif(2, 0, max(X) - min(X)),
                     runif(1, 0, 1))
)
```

```
## Total Number of Iterations: 367
```

```
# Print the estimated parameters
cat("Estimated mean 1:", estimated_params[1], "\n")
```

```
## Estimated mean 1: 5.012624
```

```
cat("Estimated mean 2:", estimated_params[2], "\n")
```

```
## Estimated mean 2: 9.984025
```

```
cat("Estimated variance 1:", estimated_params[3]^2, "\n")
```

```
## Estimated variance 1: 2.137281
```

```
cat("Estimated variance 2:", estimated_params[4]^2, "\n")
```

```
## Estimated variance 2: 4.138927
```

```
cat("Estimated mixture proportion:", estimated_params[5], "\n")
```

```
## Estimated mixture proportion: 0.2521175
```

Delta method

Theorem (The Delta Method).

Suppose that

$$\frac{\sqrt{n}\,(Y_n - \mu)}{\sigma} \rightsquigarrow N(0,1)$$

and that g is a differentiable function such that $g'(\mu) \neq 0$. Then

$$\frac{\sqrt{n}\,(g\,(Y_n) - g(\mu))}{|g'(\mu)|\,\sigma} \rightsquigarrow N(0,1).$$

In other words,

$$Y_n \approx N\left(\mu, \frac{\sigma^2}{n}\right) \quad \text{implies that} \quad g\,(Y_n) \approx N\left(g(\mu), (g'(\mu))^2\,\frac{\sigma^2}{n}\right).$$

Exercise

Let $X_1, \ldots, X_n \sim \text{Bernoulli}(p)$ and let $\psi = g(p) = \log(p/(1- p))$. Find the MLE of ψ and its asymptotic distribution.

Exercise

Let $X_1, \ldots, X_n \sim \text{Bernoulli}(p)$ and let $\psi = g(p) = \log(p/(1- \ p)\ )$. Find the MLE of ψ and its asymptotic distribution.

The MLE of p was derived previously as follows

$$\hat{p}_{\text{MLE}} = \frac{1}{n}\sum_{i=1}^{n} X_i = \bar{X}$$

Now, for $\psi = g(p) = \log\left(\frac{p}{1-p}\right)$, the MLE of ψ is obtained by plugging in the MLE of p:

$$\hat{\psi}_{\text{MLE}} = g(\hat{p}_{\text{MLE}}) = \log\left(\frac{\hat{p}_{\text{MLE}}}{1-\hat{p}_{\text{MLE}}}\right) = \log\left(\frac{\bar{X}}{1-\bar{X}}\right)$$

Exercise

By the Central Limit Theorem, as $n \to \infty$:

$$\sqrt{n}(\bar{X} - E[X_i]) \xrightarrow{D} N(0, \mathrm{Var}(X_i))$$

Therefore,

$$\sqrt{n}(\hat{p}_{\mathrm{MLE}} - p) \xrightarrow{D} N(0, p(1-p))$$

To apply delta method, we need to find the derivative of $g(p)$:

$$g'(p) = \frac{1}{p(1-p)}$$

and

$$[g'(p)]^2\sigma^2 = \left(\frac{1}{p(1-p)}\right)^2 \cdot p(1-p) = \frac{1}{p^2(1-p)^2} \cdot p(1-p) = \frac{1}{p(1-p)}$$

Therefore,

$$\sqrt{n}(\hat{\psi}_{\mathrm{MLE}} - \psi) \xrightarrow{D} N\left(0, \frac{1}{p(1-p)}\right)$$

Resources

This tutorial is based on

- Harvard Biostatistics Summer Pre Course [link]
- “All of Statistics” by Larry A. Wasserman [link]