Module 5: Statistical inference (II)

Jianhui Gao

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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 bout 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?

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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

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

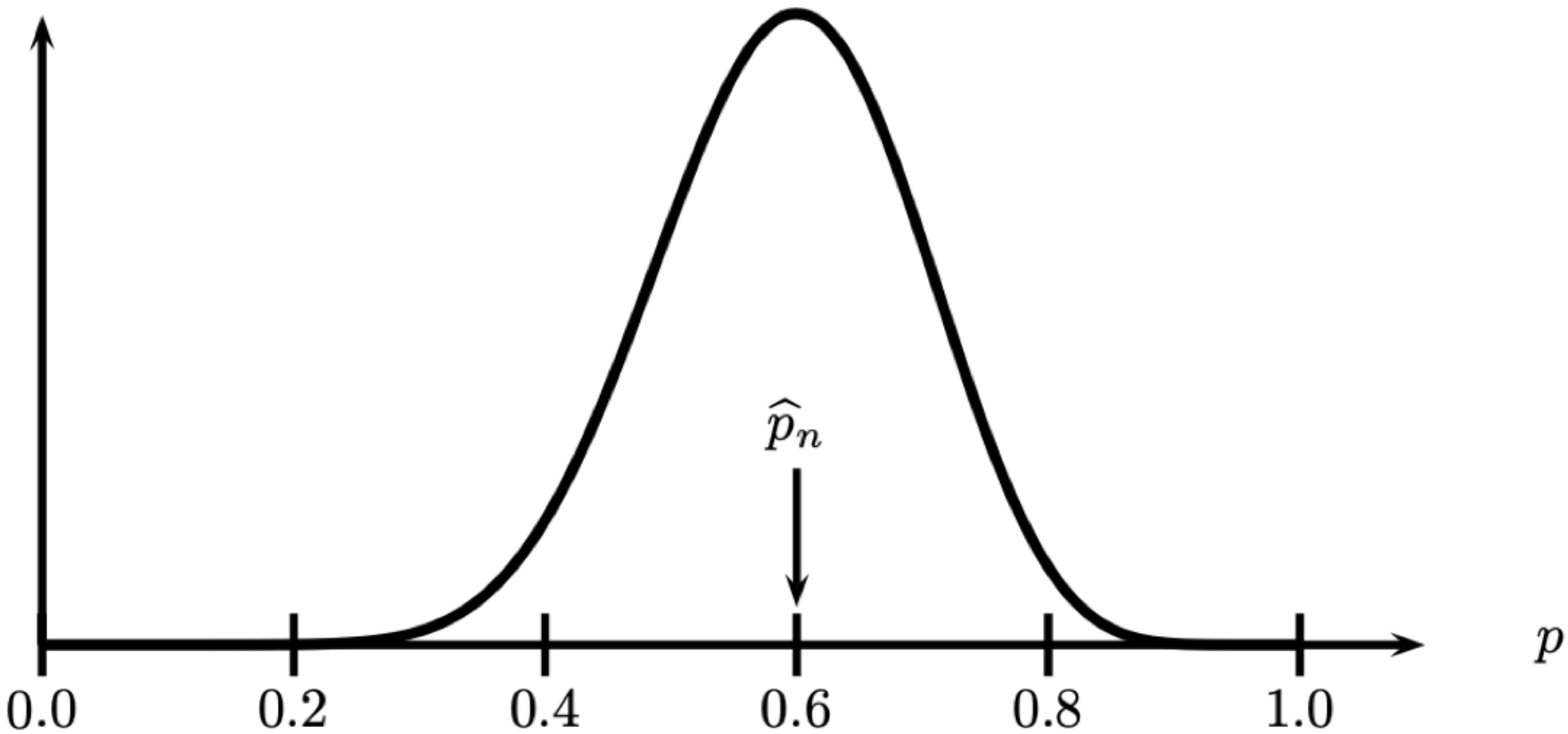
- The log-likelihood function

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

- 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

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

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

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

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

Exercise

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

1. The likelihood

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where $S = \sum_i X_i$

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 :

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

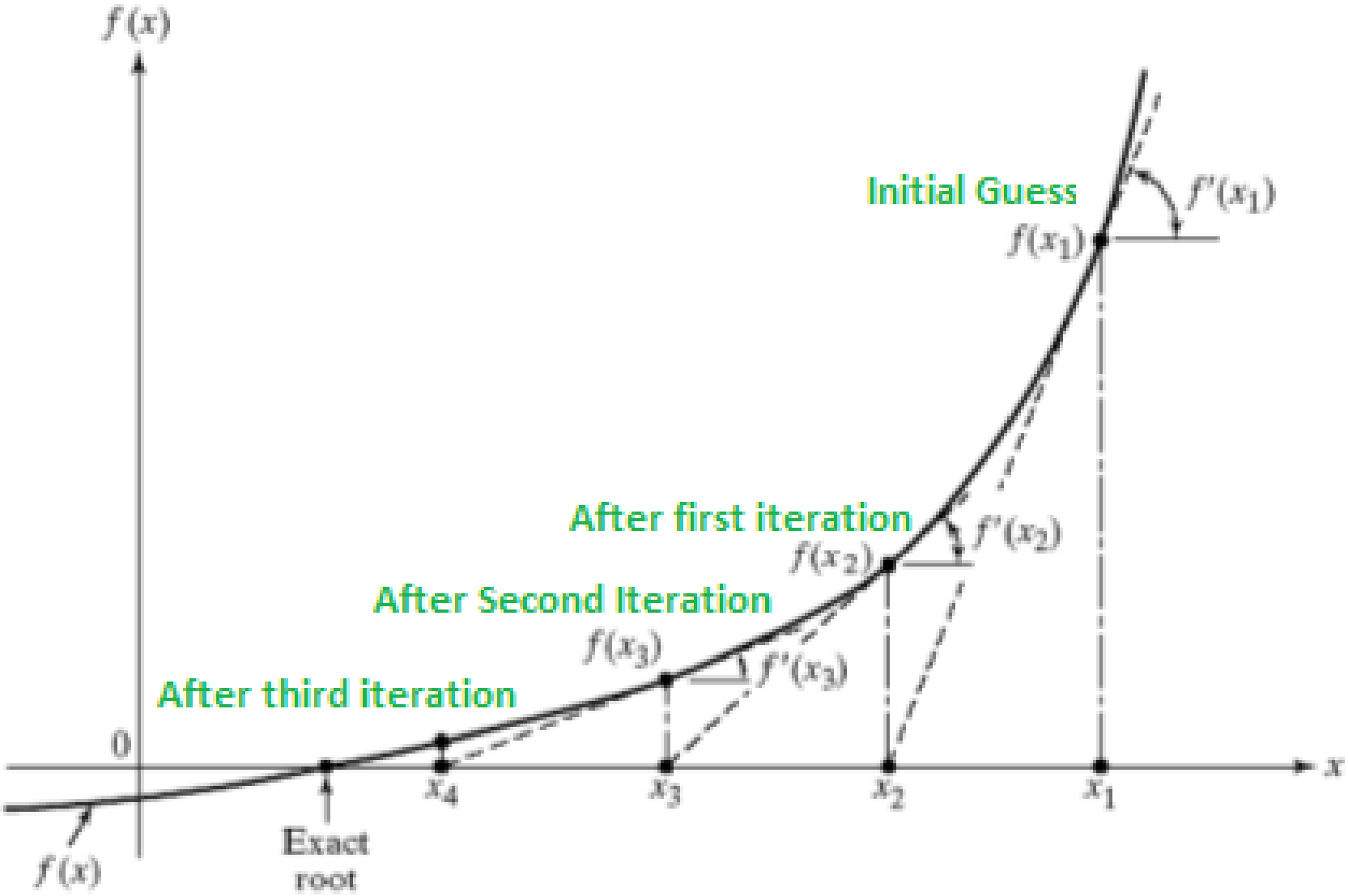
Solving for $\widehat{\theta}$ gives

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

This suggests the following iterative scheme:

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

Illustration

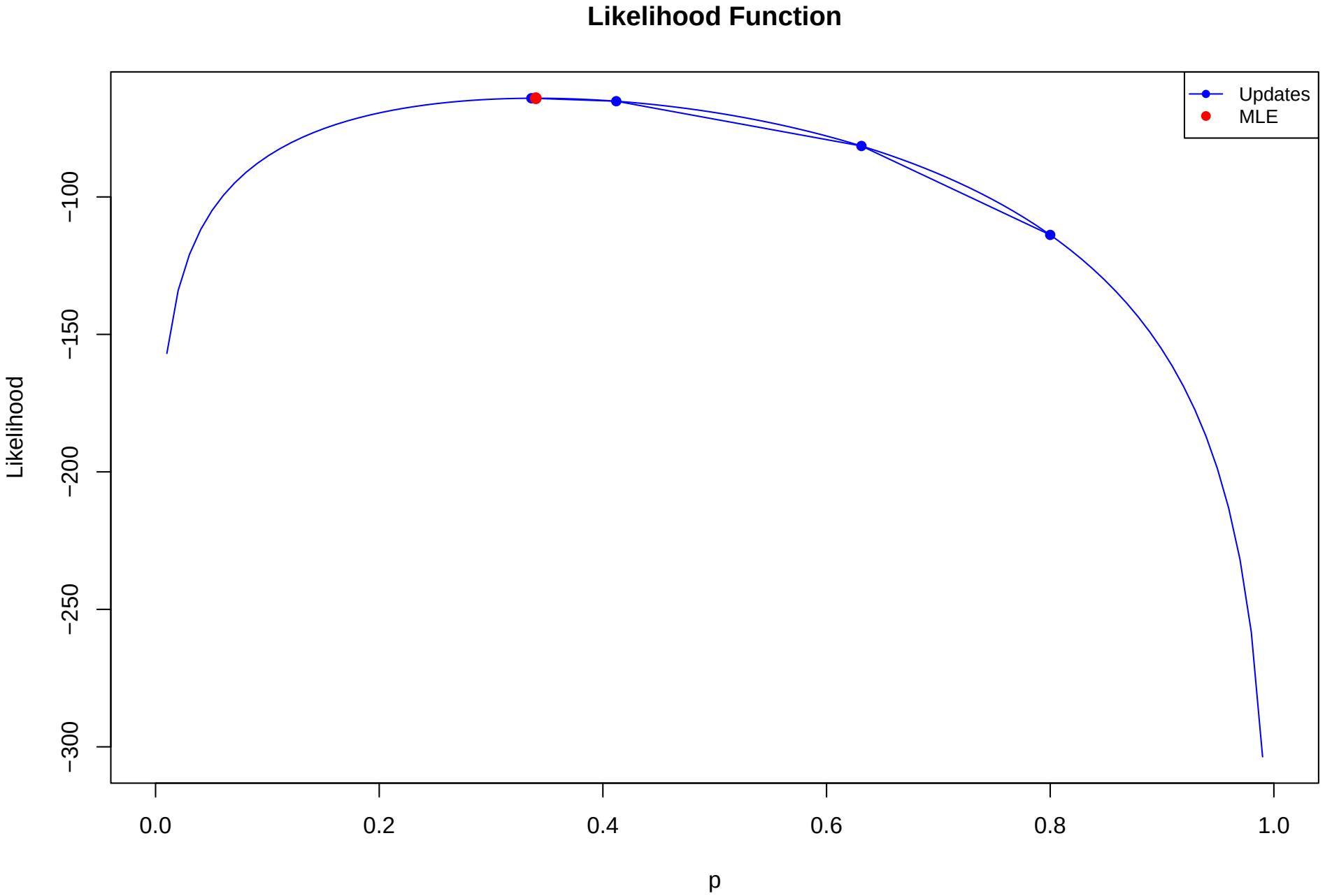


NR algorithm in R

```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

$$L(\theta|X_1, \ldots, X_n) = \prod *i = 1^n * \sum k = 1^K \pi_k N(x; \mu_k, \sigma_k^2)$$

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 $P(Z_i = k \mid X_i)$.
- Then with $P(Z_i = k \mid X_i)$ fixed, maximize the expected complete log-likelihood above with respect to μ_k, σ_k, π_k.

Example (Mixture of Two Normal)

In this example, we will assume our mixture components are fully specified Gaussian distributions (i.e the means and variances are known), and we are interested in finding the maximum likelihood estimates of the π_k 's. 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

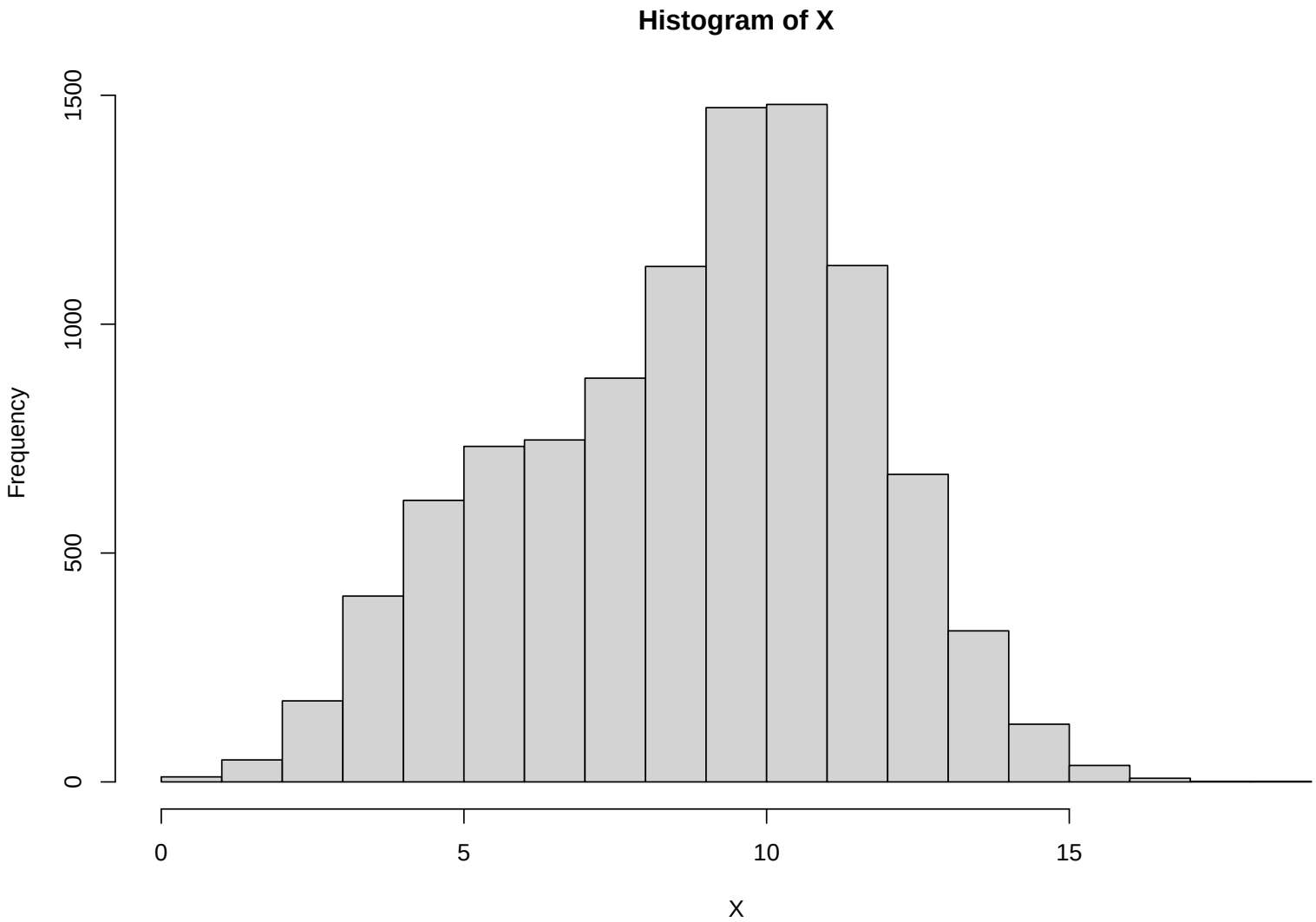
```r
# mixture components
mu.true <- c(5, 10)
sigma.true <- c(1.5, 2)

# determine Z_i
Z <- rbinom(500, 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

```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: 8.7721
```

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

```
## Estimated mean 2: 8.7721
```

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

```
## Estimated variance 1: 8.199793
```

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

```
## Estimated variance 2: 8.199793
```

```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: 383
```

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

```
## Estimated mean 1: 5.061732
```

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

```
## Estimated mean 2: 10.01453
```

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

```
## Estimated variance 1: 2.430693
```

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

```
## Estimated variance 2: 3.978077
```

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

```
## Estimated mixture proportion: 0.2508547
```

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: 407
```

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

```
## Estimated mean 1: 10.01453
```

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

```
## Estimated mean 2: 5.061732
```

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

```
## Estimated variance 1: 3.978077
```

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

```
## Estimated variance 2: 2.430693
```

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

```
## Estimated mixture proportion: 0.7491453
```

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: 304
```

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

```
## Estimated mean 1: 10.01453
```

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

```
## Estimated mean 2: 5.061733
```

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

```
## Estimated variance 1: 3.978076
```

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

```
## Estimated variance 2: 2.430694
```

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

```
## Estimated mixture proportion: 0.7491452
```

Delta method

Theorem (The Delta Method).

Suppose that

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

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

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

In other words,

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

Exercise

Let $X_1, \ldots, X_n \sim \text{Bernoulli}(p)$ and let $\psi = g(p) = \log(p/(1-p))$.

Exercise

Let $X_1, \ldots, X_n \sim \text{Bernoulli}(p)$ and let $\psi = g(p) = \log(p/(1- p)\ )$.

The Fisher information function is $I(p) = 1/(p(1-p))$

Exercise

Let $X_1, \ldots, X_n \sim \text{Bernoulli}(p)$ and let $\psi = g(p) = \log(p/(1- p))$.

The Fisher information function is $I(p) = 1/(p(1-p))$

The estimated standard error of the MLE $\widehat{p}_n$ is

$$\widehat{\text{se}} = \sqrt{\frac{\widehat{p}_n\,(1-\widehat{p}_n)}{n}}$$

Exercise

Let $X_1, \ldots, X_n \sim \text{Bernoulli}(p)$ and let $\psi = g(p) = \log(p/(1- p))$.

The Fisher information function is $I(p) = 1/(p(1-p))$

The estimated standard error of the MLE $\widehat{p}_n$ is

$$\widehat{\text{se}} = \sqrt{\frac{\widehat{p}_n (1-\widehat{p}_n)}{n}}$$

The MLE of ψ is $\widehat{\psi} = \log \widehat{p}/(1-\widehat{p})$. Since, $g'(p) = 1/(p(1-p))$, according to the delta method

$$\widehat{\text{se}}\left(\widehat{\psi}_n\right) = \left|g'\left(\widehat{p}_n\right)\right| \widehat{\text{se}}\left(\widehat{p}_n\right) = \frac{1}{\sqrt{n\widehat{p}_n\left(1-\widehat{p}_n\right)}}$$

Exercise

Let $X_1, \ldots, X_n \sim \text{Bernoulli}(p)$ and let $\psi = g(p) = \log(p/(1- p))$.

The Fisher information function is $I(p) = 1/(p(1-p))$

The estimated standard error of the MLE $\widehat{p}_n$ is

$$\widehat{\text{se}} = \sqrt{\frac{\widehat{p}_n (1-\widehat{p}_n)}{n}}$$

The MLE of ψ is $\widehat{\psi} = \log \widehat{p}/(1-\widehat{p})$. Since, $g'(p) = 1/(p(1-p))$, according to the delta method

$$\widehat{\text{se}}\left(\widehat{\psi}_n\right) = \left|g'\left(\widehat{p}_n\right)\right| \widehat{\text{se}}\left(\widehat{p}_n\right) = \frac{1}{\sqrt{n\widehat{p}_n\left(1-\widehat{p}_n\right)}}$$

An approximate 95 percent confidence interval is

$$\widehat{\psi}_n \pm \frac{2}{\sqrt{n\widehat{p}_n\left(1-\widehat{p}_n\right)}}$$

Resources

This tutorial is based on

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