Full Information Maximum Likelihood

Utrecht University Winter School: Missing Data in R

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Outline

FIML Intuition

FIML is an ML estimation method that is robust to ignorable nonresponse.

- FIML partitions the missing information out of the likelihood function so that the model is only estimated from the observed parts of the data.

After a minor alteration to the likelihood function, FIML reduces to simple ML estimation.

- So, let's review ML estimation before moving forward.

Maximum Likelihood Estimation

ML estimation simply finds the parameter values that are "most likely" to have given rise to the observed data.

- The *likelihood* function is just a probability density (or mass) function with the data treated as fixed and the parameters treated as random variables.
- Having such a framework allows us to ask: "Given that I've observed these data values, what parameter values most probably describe these data?"

Maximum Likelihood Estimation

ML estimation is usually employed when there is no closed form solution for the parameters we seek.

- This is why you don't usually see ML used to fit general linear models.

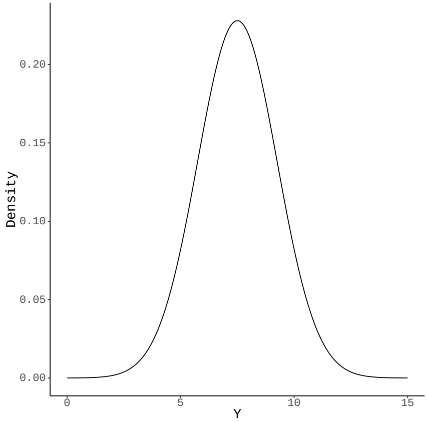
After choosing a likelihood function, we iteratively optimize the function to produce the ML estimated parameters.

- In practice, we nearly always work with the natural logarithm of the likelihood function (i.e., the *loglikelihood*).

Likelihoods

Suppose we have the following model:

$$Y \sim \mathrm{N}\left(\mu, \sigma^2\right).$$



Likelihoods

For a given Y_n, we have:

$$P\left(Y_n|\mu, \sigma^2\right) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(Y_n-\mu)^2}{2\sigma^2}}. \quad (1)$$

If we plug estimated parameters into Equation 1, we get the probability of observing Y_n given $\hat{\mu}$ and $\hat{\sigma}^2$:

$$P\left(Y_n|\hat{\mu}, \hat{\sigma}^2\right) = \frac{1}{\sqrt{2\pi\hat{\sigma}^2}} e^{-\frac{(Y_n-\hat{\mu})^2}{2\hat{\sigma}^2}}. \quad (2)$$

Applying Equation 2 to all N observations and multiplying the results produces a *likelihood*:

$$\hat{L}\left(\hat{\mu}, \hat{\sigma}^2\right) = \prod_{n=1}^{N} P\left(Y_n|\hat{\mu}, \hat{\sigma}^2\right).$$

Likelihoods

We generally want to work with the natural logarithm of Equation 2. Doing so gives the *loglikelihood*:

$$\begin{aligned}\hat{\mathcal{L}}\left(\hat{\mu}, \hat{\sigma}^2\right) &= \ln \prod_{n=1}^{N} P\left(Y_n | \hat{\mu}, \hat{\sigma}^2\right) \\ &= -\frac{N}{2} \ln 2\pi - N \ln \hat{\sigma} - \frac{1}{2\hat{\sigma}^2} \sum_{n=1}^{N} \left(Y_n - \hat{\mu}\right)^2\end{aligned}$$

ML tries to find the values of $\hat{\mu}$ and $\hat{\sigma}^2$ that maximize $\hat{\mathcal{L}}\left(\hat{\mu}, \hat{\sigma}^2\right)$.

- Find the values of $\hat{\mu}$ and $\hat{\sigma}^2$ that are *most likely*, given the observed values of Y.

Likelihoods

Suppose we have a linear regression model:

$$Y = \beta_0 + \beta_1 X + \varepsilon,$$

$$\varepsilon \sim \mathrm{N}\left(0, \sigma^2\right).$$

This model can be equivalently written as:

$$Y \sim \mathrm{N}\left(\beta_0 + \beta_1 X, \sigma^2\right)$$

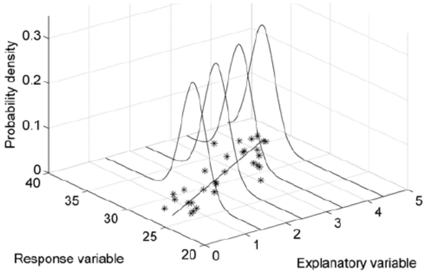


Image retrieved from:
`http://www.seaturtle.org/mtn/archives/mtn122/mtn122p1.shtml`

Likelihoods

For a given $\{Y_n, X_n\}$, we have:

$$P\left(Y_n|X_n, \beta_0, \beta_1, \sigma^2\right) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(Y_n - \beta_0 - \beta_1 X_n)^2}{2\sigma^2}}. \tag{3}$$

If we plug our estimated parameters into Equation 3, we get the probability of observing Y_n given $\hat{Y}_n = \hat{\beta}_0 + \hat{\beta}_1 X_n$ and $\hat{\sigma}^2$.

$$P\left(Y_n|X_n, \hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2\right) = \frac{1}{\sqrt{2\pi\hat{\sigma}^2}} e^{-\frac{\left(Y_n - \hat{\beta}_0 - \hat{\beta}_1 X_n\right)^2}{2\hat{\sigma}^2}} \tag{4}$$

Likelihoods

So, our final loglikelihood function would be the following:

$$\begin{aligned}\hat{\mathcal{L}}\left(\hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2\right) &= \ln \prod_{n=1}^{N} P\left(Y_n | X_n, \hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2\right) \\ &= -\frac{N}{2} \ln 2\pi - N \ln \hat{\sigma} - \frac{1}{2\hat{\sigma}^2} \sum_{n=1}^{N} \left(Y_n - \hat{\beta}_0 - \hat{\beta}_1 X_n\right)^2 .\end{aligned}$$

Example

```r
## Fit a model:
out1 <- lm(ldl ~ bp + glu + bmi, data = diabetes)

## Extract the predicted values and estimated residual
## standard error:
yHat <- predict(out1)
s    <- summary(out1)$sigma

## Compute the row-wise probabilities:
pY <- dnorm(diabetes$ldl, mean = yHat, sd = s)

## Compute the loglikelihood, and compare to R's version:
sum(log(pY)); logLik(out1)[1]

[1] -2109.939
[1] -2109.93
```

Multivariate Normal Distribution

The PDF for the multivariate normal distribution is:

$$P(\mathbf{Y}|\boldsymbol{\mu}, \Sigma) = \frac{1}{\sqrt{(2\pi)^P|\Sigma|}} e^{-\frac{1}{2}(\mathbf{Y}-\boldsymbol{\mu})^T\Sigma^{-1}(\mathbf{Y}-\boldsymbol{\mu})}.$$

So, the multivariate normal loglikelihood is:

$$\mathcal{L}\left(\boldsymbol{\mu}, \Sigma\right) = -\left[\frac{P}{2}\ln(2\pi) + \frac{1}{2}\ln|\Sigma| + \frac{1}{2}\right]\sum_{n=1}^{N}(\mathbf{Y}_n - \boldsymbol{\mu})^T\Sigma^{-1}(\mathbf{Y}_n - \boldsymbol{\mu}).$$

Which can be further simplified if we multiply through by -2:

$$-2\mathcal{L}\left(\boldsymbol{\mu}, \Sigma\right) = \left[P\ln(2\pi) + \ln|\Sigma|\right]\sum_{n=1}^{N}(\mathbf{Y}_n - \boldsymbol{\mu})^T\Sigma^{-1}(\mathbf{Y}_n - \boldsymbol{\mu}).$$

Steps of ML

1. Choose a probability distribution, $f(Y|\theta)$, to describe the distribution of the data, Y, given the parameters, θ.
2. Choose some estimate of θ, $\hat{\theta}^{(i)}$.
3. Compute each row's contribution to the loglikelihood function by evaluating: $\ln\left[f\left(Y_n|\hat{\theta}^{(i)}\right)\right]$.
4. Sum the individual loglikelihood contributions from Step 3 to find the loglikelihood value, $\hat{\mathcal{L}}$.
5. Choose a "better" estimate of the parameters, $\hat{\theta}^{(i+1)}$, and repeat Steps 3 and 4.
6. Repeat Steps 3 – 5 until the change between $LL^{(i-1)}$ and $LL^{(i)}$ falls below some trivially small threshold.
7. Take $\hat{\theta}^{(i)}$ as your estimated parameters.

ML Example

Recall the *n*th observation's contribution to the multivariate normal loglikelihood function:

$$\mathcal{L}\left(\boldsymbol{\mu}, \Sigma\right)_n = -\frac{P}{2}\ln(2\pi) - \frac{1}{2}\ln|\Sigma| - \frac{1}{2}(\mathbf{Y}_n - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{Y}_n - \boldsymbol{\mu}).$$

It turns out that this function is readily available in R via the **mvtnorm** package:

```r
## Vector of row-wise contributions to the overall LL:
ll0 <- dmvnorm(y, mean = mu, sigma = sigma, log = TRUE)
```

ML Example

We can wrap the preceding code in a nice R function:

```r
## Complete data loglikelihood function:
ll <- function(par, data) {
    ## Extract the parameter matrices:
    p  <- ncol(data)
    mu <- par[1:p]

    ## Populate sigma from its Cholesky factor:
    sigma <- vecChol(tail(par, -p), p = p, revert = TRUE)

    ## Compute the row-wise contributions to the LL:
    ll0 <- dmvnorm(data, mean = mu, sigma = sigma, log = TRUE)

    sum(ll0)# return the overall LL value
}
```

ML Example

We'll also need the following helper function:

```r
## Convert from covariance matrix to vectorized Cholesky factor and back:
vecChol <- function(x, p, revert = FALSE) {
    if(revert) {
        tmp                    <- matrix(0, p, p)
        tmp[!lower.tri(tmp)] <- x
        crossprod(tmp)
    }
    else
        chol(x)[!lower.tri(x)]
}
```

ML Example

The **optimx** package can numerically optimize arbitrary functions.

- We can use it to (semi)manually implement ML.

```r
## Subset the 'diabetes' data:
dat1 <- diabetes[ , c("bmi", "ldl", "glu")] %>% as.matrix()

## Choose some starting values:
m0   <- rep(0, 3)
s0   <- diag(3) %>% vecChol()
par0 <- c(m0, s0)

## Use optimx() to numerically optimize the LL function:
mle <- optimx(par     = par0,
              fn      = ll,
              data    = dat1,
              method  = "BFGS",
              control = list(maximize = TRUE, maxit = 1000)
              )

Maximizing -- use negfn and neggr
```

ML Example

Finally, let's check convergence and extract the optimized parameters:

```
## Check convergence:
mle[c("convcode", "kkt1", "kkt2")]

     convcode kkt1 kkt2
BFGS        0 TRUE TRUE

## Get the optimize mean vector and covariance matrix:
muHat    <- mle[1:3]
sigmaHat <- mle[4:9] %>% as.numeric() %>% vecChol(p = 3, revert = TRUE)
```

ML Example

	bmi	ldl	glu
ML	26.376	115.437	91.260
Closed Form	26.376	115.439	91.260

Estimated Means

	bmi	ldl	glu
bmi	19.476	35.013	19.697
ldl	35.013	922.820	101.373
glu	19.697	101.373	131.864

ML Covariance Matrix

	bmi	ldl	glu
bmi	19.520	35.093	19.742
ldl	35.093	924.955	101.605
glu	19.742	101.605	132.166

Closed Form Covariance Matrix

Full Information Maximum Likelihood

From ML to FIML

The nth observation's contribution to the multivariate normal loglikelihood function would be the following:

$$\mathcal{L}\left(\boldsymbol{\mu}, \Sigma\right)_n = -\frac{P}{2}\ln(2\pi) - \frac{1}{2}\ln|\Sigma| - \frac{1}{2}(\mathbf{Y}_n - \boldsymbol{\mu})^T \Sigma^{-1}(\mathbf{Y}_n - \boldsymbol{\mu}). \tag{5}$$

From ML to FIML

The nth observation's contribution to the multivariate normal loglikelihood function would be the following:

$$\mathcal{L}\left(\boldsymbol{\mu}, \Sigma\right)_n = -\frac{P}{2}\ln(2\pi) - \frac{1}{2}\ln|\Sigma| - \frac{1}{2}(\mathbf{Y}_n - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{Y}_n - \boldsymbol{\mu}). \quad (5)$$

FIML just tweaks Equation 5 a tiny bit:

$$\mathcal{L}\left(\boldsymbol{\mu}, \Sigma\right)_{fiml,n} = -\frac{P}{2}\ln(2\pi) - \frac{1}{2}\ln|\Sigma_q| - \frac{1}{2}(\mathbf{Y}_n - \boldsymbol{\mu}_q)^T \Sigma_q^{-1} (\mathbf{Y}_n - \boldsymbol{\mu}_q).$$

Where $q = 1, 2, \ldots, Q$ indexes response patterns.

FIML Example

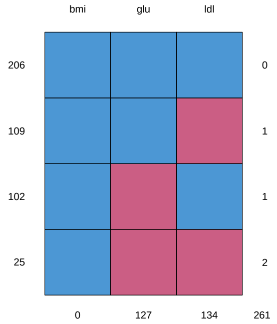
First things first, we need to punch some holes in our example data.

```r
## Impose MAR missing:
dat2 <- imposeMissData(data    = dat1,
                       targets = c("ldl", "glu"),
                       preds   = "bmi",
                       pm      = 0.3,
                       types   = c("low", "high"),
                       stdDat  = TRUE)
```

Visualize the Response Patterns

The data contain 4 unique response patterns.

- We'll define 4 different version of μ and Σ.
- We'll calculate each individual loglikelihood contributions using the appropriate flavor of μ and Σ.



FIML Example

```r
## Compute the within-pattern contributions to the LL:
ll0 <- function(i, mu, sigma, pats, ind, data) {
    ## Define the current response pattern:
    p1 <- pats[i, ]

    if(sum(p1) > 1) # More than one observed variable?
        dmvnorm(x     = data[ind == i, p1],
                mean  = mu[p1],
                sigma = sigma[p1, p1],
                log   = TRUE)
    else
        dnorm(x    = data[ind == i, p1],
              mean = mu[p1],
              sd   = sqrt(sigma[p1, p1]),
              log  = TRUE)
}
```

FIML Example

```r
## FIML loglikelihood function:
llm <- function(par, data, pats, ind) {
    ## Extract the parameter matrices:
    p  <- ncol(data)
    mu <- par[1:p]

    ## Populate sigma from its Cholesky factor:
    sigma <- vecChol(tail(par, -p), p = p, revert = TRUE)

    ## Compute the pattern-wise contributions to the LL:
    ll1 <- sapply(X     = 1:nrow(pats),
                  FUN   = ll0,
                  mu    = mu,
                  sigma = sigma,
                  pats  = pats,
                  ind   = ind,
                  data  = data)

    sum(unlist(ll1))
}
```

FIML Example

```r
## Summarize response patterns:
pats <- uniquecombs(!is.na(dat2))
ind  <- attr(pats, "index")

## Choose some starting values:
m0   <- colMeans(dat2, na.rm = TRUE)
s0   <- cov(dat2, use = "pairwise") %>% vecChol()
par0 <- c(m0, s0)

## Use optimx() to numerically optimize the LL function:
mle <- optimx(par     = par0,
              fn      = llm,
              data    = dat2,
              pats    = pats,
              ind     = ind,
              method  = "BFGS",
              control = list(maximize = TRUE, maxit = 1000)
              )

Maximizing -- use negfn and neggr
```

FIML Example

Check convergence and extract the optimized parameters:

```r
## Check convergence:
mle[c("convcode", "kkt1", "kkt2")]

     convcode kkt1 kkt2
BFGS        0 TRUE TRUE

## Get the optimize mean vector and covariance matrix:
muHat1    <- mle[1:3]
sigmaHat1 <- mle[4:9] %>% as.numeric() %>% vecChol(p = 3, revert = TRUE)
```

FIML Example

Just to make sure our results are plausible, we can do the same analysis using the `cfa()` function from the **lavaan** package:

```
## Define the model in lavaan syntax:
mod <- "
bmi ~~ ldl + glu
ldl ~~ glu
"

## Fit the model with lavaan::cfa():
fit <- cfa(mod, data = dat2, missing = "fiml")

## Extract the estimated parameters:
muHat2    <- inspect(fit, "est")$nu
sigmaHat2 <- inspect(fit, "theta")
```

FIML Example

	bmi	ldl	glu
Manual	26.376	116.634	91.686
Lavaan	26.376	116.636	91.686

Estimated Means

	bmi	ldl	glu
bmi	19.475	24.249	22.835
ldl	24.249	889.032	120.618
glu	22.835	120.618	140.543

Manual FIML Covariance Matrix

	bmi	ldl	glu
bmi	19.476	24.260	22.837
ldl	24.260	889.068	120.633
glu	22.837	120.633	140.544

Lavaan FIML Covariance Matrix

Auxiliary Variables

Satisfying the MAR Assumption

Like MI, FIML also requires MAR data.

- Parameters will be biased with MAR is violated.

Unlike MI, FIML directly treats the missing data while estimating the analysis model.

- The MAR predictors must be included in the analysis model.
- Otherwise, FIML reduces to pairwise deletion.

If the MAR predictors are not substantively interesting variables, naively included them in the analysis model can change the model's meaning.

Saturated Correlates Technique

Graham (2003) developed the *saturated correlates* approach to meet two desiderata:

1. Satisfy the MAR assumption by incorporating MAR predictors into the analysis model.
2. Do not affect the fit or substantive meaning of the analysis model.

The approach entails incorporating the MAR predictors via a fully-saturated covariance structure:

1. Allow all MAR predictors to co-vary with all other MAR predictors.
2. Allow all MAR predictors to co-vary with all observed variables in the analysis model (or their residuals).

References

Graham, J. W. (2003). Adding missing-data-relevant variables to FIML-based structural equation models. *Structural Equation Modeling: A Multidisciplinary Journal*, *10*(1), 80–100. doi: 10.1207/S15328007SEM1001_4