Multinomial model with random effects

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Final Project

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The problem

Consider a random variable with multinomial distribution with three categories. In this case the probability function is given by

$$\mathbb{P}[X = x] = \frac{n!}{x_1!x_2!x_3!} p_1^{x_1} p_2^{x_2} p_3^{x_3}, \quad \text{with} \quad \sum_{i=1}^{3} p_i = 1.$$

Consider a situation with just one trial, made in n independent subjects.

On the Agenda

1. Find the MLEs. Provide some confidence intervals.
2. Consider two covariates for each subject and propose a regression model.
3. Do the maximum likelihood estimation for the proposed model.
4. Do a simulation study to evaluate the MLEs distribution.
5. Evaluate the coverage rate for the Wald and deviance intervals.
6. Propose a mixed model for multiple observations from the same subject.
7. Do the maximum likelihood estimation for the proposed model.

At first, getting some data

$n = 100$ independent subjects, one trial, $k = 3$ categories.

```r
probs <- c(.2, .6, .2) # probabilities for each category k
library(Matrix)
data_generator <- function(n, k = 3, p) {
    data <- t(rmultinom(n, 1, prob = p))
    colnames(data) <- paste0("p", seq(k))
    return(Matrix(data))
}
set.seed(1993)
data <- data_generator(n = 100, p = probs)
data[seq(5), ]
```

```
## 5 x 3 sparse Matrix of class "dgCMatrix"
##      p1 p2 p3
## [1,]  .  1  .
## [2,]  .  1  .
## [3,]  .  1  .
## [4,]  .  1  .
## [5,]  1  .  .
```

Maximum Likelihood Estimators

First, we write the log-likelihood function for a single subject j

$$L(\boldsymbol{p}) = f(x_j; \boldsymbol{p}) = \begin{cases} \frac{n!}{\prod_{i=1}^{k} x_i!} \prod_{i=1}^{k} p_i^{x_i}, & \text{when } \sum_{i=1}^{k} x_i = n \\ 0 & \text{otherwise,} \end{cases}, x_i \geq 0.$$

$$l(\boldsymbol{p}) = \log L(\boldsymbol{p}) = \log n! - \sum_{i=1}^{k} \log x_i! + \sum_{i=1}^{k} x_i \log p_i. \tag{1}$$

Second, we code it (next slide)

MLEs: mostrando o pau

```r
multinom_lkl <- function(par, xs) {
    N <- nrow(xs) ; k <- ncol(xs)
    ## k-1, since the last parameter is taken as the complementary
    for (i in 1:(k - 1)) assign(paste0("p", i), par[i])
    p <- unlist(mget(c(ls(pattern = glob2rx("^p\\d")))))
    ps <- c(p, 1 - sum(p))
    lkl_p <- rep(1, N) %*% xs %*% log(ps)
    ## normalizing constant
    lkl_c1 <- sum(lfactorial(rowSums(xs)))
    lkl_c2 <- sum(lfactorial(xs))
    lkl <- lkl_c1 - lkl_c2 + lkl_p
    ## returning the negative of it
    return(-as.numeric(lkl))
}
```

i.e., `lkl <-` $\sum_{j=1}^{N} \log n_j! - \sum_{j=1}^{N} \sum_{i=1}^{k} \log x_{ij}! + \sum_{j=1}^{N} \sum_{i=1}^{k} x_{ij} \log p_{ij}.$

MLEs: matando o gato

```r
initial_values <- c(1/3, 1/3)
library(bbmle)
names(initial_values) <- parnames(multinom_lkl) <- c("p1", "p2")
model_fit <- mle2(multinom_lkl,
                  start = initial_values, vecpar = TRUE,
                  data = list(xs = data))
## estimated probabilities
c(model_fit@coef, p3 = 1 - sum(model_fit@coef))
```

```
##        p1        p2        p3
## 0.2300425 0.5899757 0.1799818
```

Equal to the MLEs, x_i/n. Behold

```r
colSums(data)/nrow(data)
```

```
##   p1   p2   p3
## 0.23 0.59 0.18
```

Some confidence intervals for the MLEs

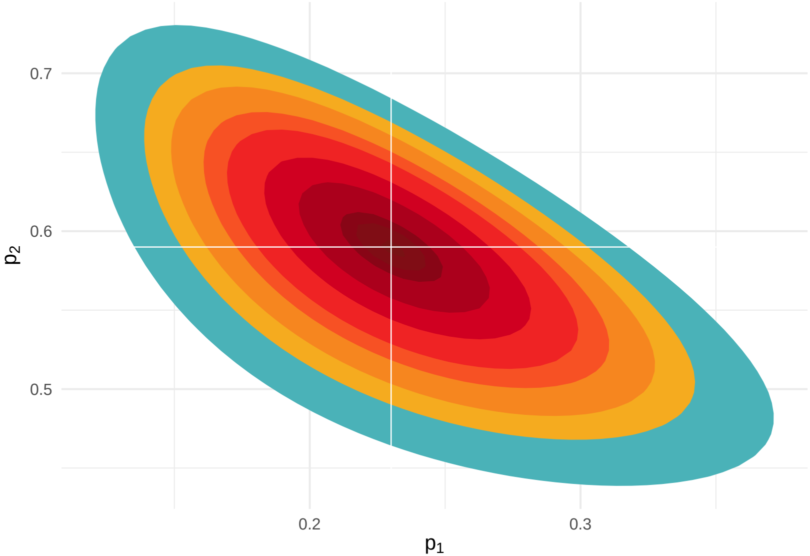
First, we write the deviance

$$\text{deviance} \equiv D(\boldsymbol{p}) = -2\left\{l(\boldsymbol{p}) - l(\hat{\boldsymbol{p}})\right\}.$$

It is much more simple and pretty if we work here with it, instead of the log-likelihood function itself.

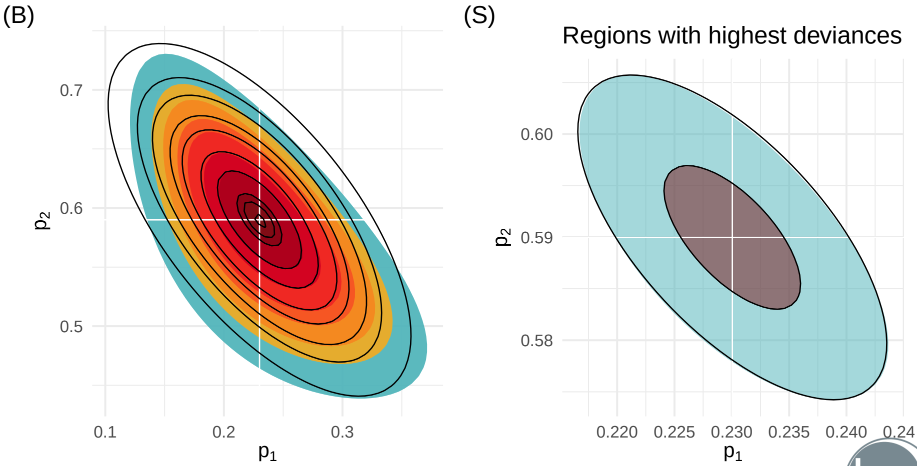
```
multinom_deviance <- function(p1, p2) {
    par <- c(p1, p2)
    log_ratio <- multinom_lkl(par, xs = data) - model_fit@min
    deviance <- 2 * (log_ratio)
    return(deviance)
}
multinom_deviance <- Vectorize(multinom_deviance, c("p1", "p2"))
```

Deviance contour



Deviance contour + quadratic approximation

Goal: confidence regions for the MLEs.



(B)ig picture and (S)mall picture.

Ok, but I also want some confidence intervals.

First, we need some stuff.

Key component: Fisher information matrix

$$I_{\text{Expected}}[\boldsymbol{p}] = \mathbb{E}\{I_{\text{Observed}}[\boldsymbol{p}]\} = \mathbb{E}\{-H_{\text{essian}}[\boldsymbol{p}]\} = \begin{bmatrix} \frac{n}{p_1} + \frac{n}{p_3} & \frac{n}{p_3} \\ \frac{n}{p_3} & \frac{n}{p_2} + \frac{n}{p_3} \end{bmatrix},$$

since $\mathbb{E}\{x_i\} = np_i$.

Thus, the asymptotic variance-covariance matrix is

$$I_{\text{Expected}}[\boldsymbol{p}]^{-1} = \begin{bmatrix} \frac{(p_2+p_3)(p_1p_2+p_1p_3+p_2p_3)}{np_2p_3} & -\frac{(p_1p_2+p_1p_3+p_2p_3)}{np_3} \\ -\frac{(p_1p_2+p_1p_3+p_2p_3)}{np_3} & \frac{(p_1+p_3)(p_1p_2+p_1p_3+p_2p_3)}{np_1p_3} \end{bmatrix}.$$

And the correlation between the estimates $\hat{p}_1$ and $\hat{p}_2$, $\hat{\rho}$, is given by

$$\hat{\rho}_{\hat{p}_1\hat{p}_2} = -\frac{\sqrt{\hat{p}_1\hat{p}_2}}{\sqrt{\hat{p}_1 + \hat{p}_3}\sqrt{\hat{p}_2 + \hat{p}_3}}.$$

The intervals,

A 95% Wald interval

$$\hat{p}_1 = 0.23: \quad \hat{p}_1 + \texttt{c(qnorm(0.025),qnorm(0.975))}\, I_{E\text{xpected}}[\hat{\boldsymbol{p}}]_{1,1}^{-1/2}$$

```
## [1] 0.1475502 0.3125348
```

$$\hat{p}_2 = 0.59: \quad \hat{p}_2 + \texttt{c(qnorm(0.025),qnorm(0.975))}\, I_{E\text{xpected}}[\hat{\boldsymbol{p}}]_{2,2}^{-1/2}$$

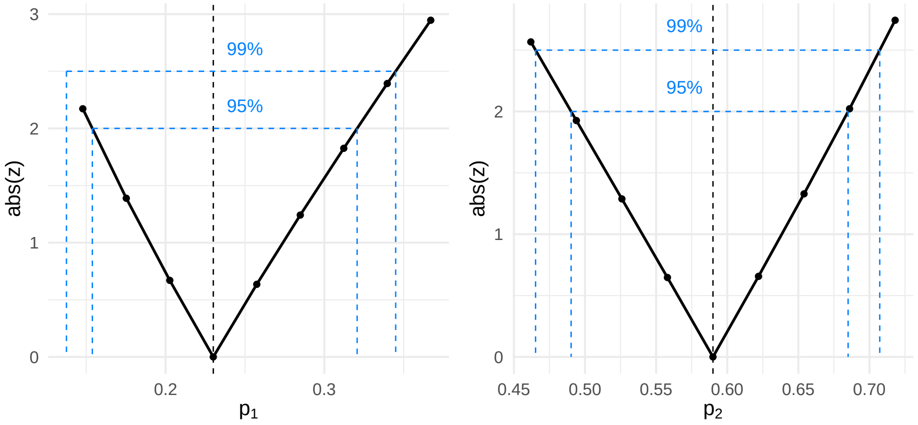
```
## [1] 0.4935764 0.6863750
```

And for $\hat{p}_3 = g(\hat{\boldsymbol{p}}) = 1 - \sum_{i=1}^{2} \hat{p}_i = 0.18$, we can get a 95% CI through the multiparameter Delta Method

$$g(\hat{\boldsymbol{p}}) \pm \texttt{qnorm(0.975)} \sqrt{(\nabla g(\hat{\boldsymbol{p}}))^\top I_{E\text{xpected}}[\hat{\boldsymbol{p}}]^{-1} \nabla g(\hat{\boldsymbol{p}})}$$

```
## [1] 0.1046884 0.2552752
```

And to finish this part, some likelihood profiles



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The model

$$
l(\beta) = \sum_{j=1}^{N} \log n_j! - \sum_{j=1}^{N} \sum_{i=1}^{k} \log y_{ij}! + \sum_{j=1}^{N} \sum_{i=1}^{k} y_{ij} \log p_{ij},
$$

$$
\text{with} \quad p_{ij} = \frac{\exp\{\boldsymbol{x}_j^\top \beta_i\}}{1 + \sum_{i=1}^{k-1} \exp\{\boldsymbol{x}_j^\top \beta_i\}}.
$$

- y represents the outcome for the subject j;
- i represents the multinomial category/level;
- p_{ij} is the probability of the subject j be classified in the category i, the so called inverse multinomial logit (logistic) function;
- β_i is the vector of coefficients for category i;
- and $\boldsymbol{x}_j$ is the row vector of covariates of the subject j.

Inverse multinomial logit function (the heart of everything)

```
inv_logit <- function(coefs, preds, data) {
    ## building objects
    ind_pred <- seq(preds) ; n_pred <- length(preds) ; k <- n_pred + 1
    betas <- split(coefs, substr(names(coefs), start = 3, stop = 3))
    list_X <- lapply(preds, model.matrix, data = data)
    ## computing the important stuff
    exp_xb <- sapply(seq(list_X),
                     function(i) exp(list_X[[i]] %*% betas[[i]]))
    link_denominator <- 1 + rowSums(exp_xb)
    ps <- sapply(ind_pred, function(i) exp_xb[ , i]/link_denominator)
    ps <- cbind(ps, 1 - rowSums(ps))
    colnames(ps) <- paste0("p", seq(k))
    return(list(y = data[ , seq(k)], ps = ps))
}
```

Now, simulating some probabilities

```r
n <- 100 ; k <- 3 # defining sample size and number of categories
naive_data <- function(n, k) {
    data <- as.data.frame(matrix(0, nrow = n, ncol = k))
    names(data) <- paste0("y", 1:k)
    return(data)
}
data <- naive_data(n, k)
set.seed(0080)
data$x1 <- rnorm(n, mean = 5, sd = 1) # covariates
data$x2 <- rnorm(n, mean = 1, sd = .5)
linear_pred <- list(y1 ~ x1 + x2, y2 ~ x1 + x2)
initial_values <- c("b01" = .4, "b11" = .1, "b21" = - .3,
                    "b02" = .2, "b12" = .5, "b22" = - .6)
probs <- inv_logit(initial_values, preds = linear_pred, data = data)$ps
```

After simulating the probabilities based in the covariates, we simulate the outcomes

```r
summary(probs)
```

```
##        p1                 p2               p3         
##  Min.   :0.05503   Min.   :0.4361   Min.   :0.01842  
##  1st Qu.:0.13533   1st Qu.:0.6810   1st Qu.:0.06418  
##  Median :0.16719   Median :0.7436   Median :0.09363  
##  Mean   :0.16954   Mean   :0.7323   Mean   :0.09813  
##  3rd Qu.:0.20092   3rd Qu.:0.8002   3rd Qu.:0.12448  
##  Max.   :0.32329   Max.   :0.9247   Max.   :0.24065  
```

```r
library(mc2d) # vectorized versions of {r, d}multinom
## finally, simulating the multinomial data
set.seed(1101)
data[ , seq(k)] <- rmultinomial(n, 1, prob = probs)
colSums(data[ , seq(k)]) # as expected, close to the ``probs`` means
```

```
## y1 y2 y3 
## 17 76  7 
```

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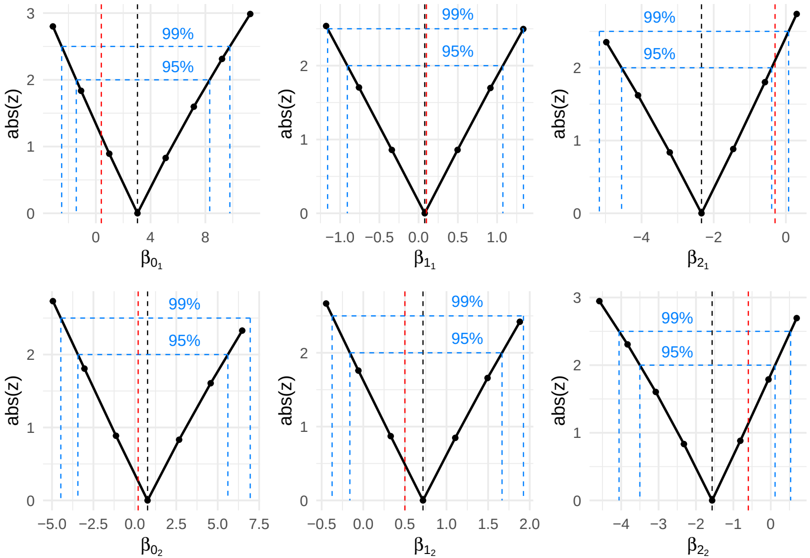
Maximum Likelihood Estimators

```
multi_lkl <- function(initial_values, linear_pred, data) {
    ilogit <- inv_logit(initial_values, preds = linear_pred, data = data)
    lkl_c1 <- with(ilogit, sum(lfactorial(rowSums(y))))
    lkl_c2 <- with(ilogit, sum(lfactorial(y)))
    lkl_p <- with(ilogit, sum(y * log(ps)))
    lkl <- lkl_c1 - lkl_c2 + lkl_p
    ## lkl <- sum(dmultinomial(as.matrix(ilogit$y), size = 1,
    ##                         prob = ilogit$ps, log = TRUE))
    return(-lkl)
}
parnames(multi_lkl) <- names(initial_values) # mle2 exigency
model_fit <- mle2(multi_lkl, start = initial_values,
                  data = list(linear_pred = linear_pred, data = data))
round(model_fit@coef, 6)
```

```
##       b01       b11       b21       b02       b12       b22
##  3.040304  0.078060 -2.338833  0.767001  0.717383 -1.568099
```

β's profile



Checking

```r
model_fit@coef
```

```
##         b01         b11         b21         b02         b12         b22
##  3.04030427  0.07805955 -2.33883295  0.76700112  0.71738285 -1.56809948
```

```r
fit_nnet <- nnet::multinom(y ~ x1 + x2, data_long)
```

```r
coef(fit_nnet)
```

```
##    (Intercept)         x1        x2
## y1   3.0412131 0.07785772 -2.338862
## y2   0.7677984 0.71720357 -1.568073
```

```r
fit_mlogit <- mlogit::mlogit(y ~ 0 | x1 + x2,
                             reflevel = 3, shape = "wide", data_long)
matrix(fit_mlogit$coef, nrow = 2, ncol = 3)
```

```
##           [,1]       [,2]      [,3]
## [1,] 3.0403108 0.07805888 -2.338837
## [2,] 0.7670852 0.71736537 -1.568101
```

Now, behold the estimated probabilities

```r
results <- lapply(
    seq(k),
    function(i) cbind(inv_logit(
                        model_fit@coef, linear_pred, data)$ps[ , i],
                        probs[ , i]))
results <- do.call(cbind, results)
colnames(results) <- c(sapply(seq(k),
                             function(i) c(paste0("p", i, "_est"),
                                            paste0("p", i, "_true"))))
head(round(results, 6), 8)
```

```
##        p1_est  p1_true   p2_est  p2_true   p3_est  p3_true
## [1,] 0.044708 0.214565 0.615056 0.607281 0.340236 0.178154
## [2,] 0.069857 0.142905 0.871300 0.774907 0.058844 0.082188
## [3,] 0.123282 0.155231 0.830405 0.760373 0.046313 0.084396
## [4,] 0.182925 0.125786 0.804101 0.819901 0.012974 0.054314
## [5,] 0.108773 0.162534 0.828098 0.743764 0.063129 0.093702
## [6,] 0.149994 0.190772 0.764336 0.693429 0.085670 0.115800
## [7,] 0.229920 0.144030 0.753823 0.791296 0.016257 0.064674
## [8,] 0.088643 0.200580 0.740493 0.658897 0.170864 0.140523
```

Hypothesis tests

Some β is significantly different from zero? Testing for $\beta_{1_1} = 0.078$.

The simplest way is via the Wald test.

```
wald <- function(par, value, alpha) {
    mle <- as.numeric(model_fit@coef[par])
    test <- (mle - value)/sqrt(model_fit@vcov[par, par])
    critic <- qnorm(1 - alpha/2)
    print(ifelse(test <= critic, "Accept H0", "Reject H0"))
    return(c("Test" = test, "Critical_value" = critic))
}
wald(par = "b11", value = 0, alpha = .05)
```

```
## [1] "Accept H0"
```

```
##          Test Critical_value
##     0.1606135      1.9599640
```

Other options are the LRT and the Score test.

Likelihood Ratio Test (LRT)

```r
lrt <- function(model_h0, model_h1, alpha) {
    test <- 2 * (model_h0@min - model_h1@min)
    critic <- qchisq(1 - alpha, df = 1)
    print(ifelse(test <= critic, "Accept H0", "Reject H0"))
    return(c("Test" = test, "Critical_value" = critic))
}
```

```r
test_values <- c("b01" = .4,                "b21" = - .3,
                 "b02" = .2, "b12" = .5, "b22" = - .6)
```

```r
lrt(model_h0 = mle2(multi_lkl2, start = test_values,
                    data = list(
                        linear_pred = list(y1 ~ x2, y2 ~ x1 + x2),
                        data = data, "b11" = 0)),
    model_h1 = model_fit, alpha = .05)
```

```
## [1] "Accept H0"

##          Test Critical_value
##    0.02578236     3.84145882
```

Score test

```r
score <- function(par, ordered_Ie, alpha) {
    parpos <- which(colnames(ordered_Ie) == par)
    n <- ncol(ordered_Ie)
    I12 <- ordered_Ie[parpos, (parpos + 1):n]
    Vc <- ordered_Ie[parpos, parpos] -
        I12 %*% solve(ordered_Ie[-parpos, -parpos]) %*% I12
    test <- as.numeric(U[par] * 1/Vc * U[par])
    critic <- qchisq(1 - alpha, df = 1)
    print(ifelse(test <= critic, "Accept H0", "Reject H0"))
    return(c("Test" = test, "Critical_value" = critic))
}
score(par = "b11", ordered_Ie, alpha = .05)
```

```
## [1] "Accept H0"
```

```
##          Test Critical_value
##     0.02584964     3.84145882
```

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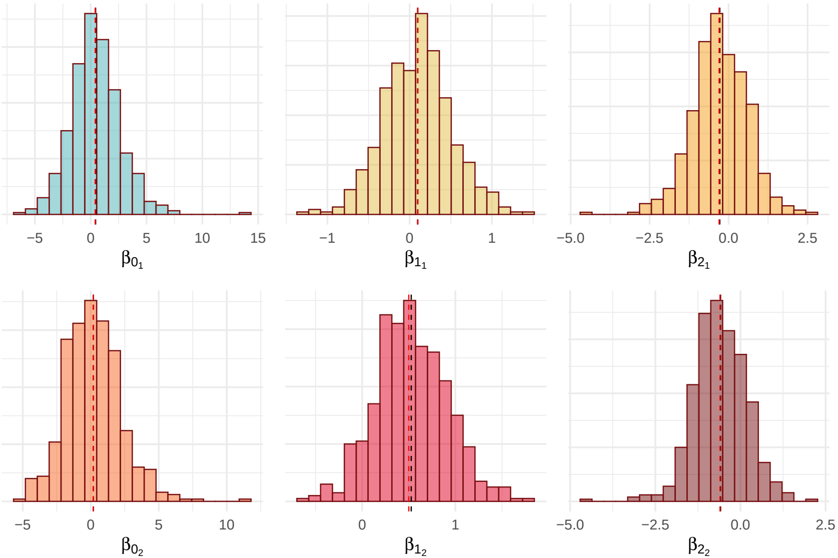
Running 500 simulations

```r
library(furrr)
plan(multiprocess)
parallel2run <- function(nsimu) {
    coefs <- Matrix(0, nrow = nsimu, ncol = 6)
    confint_profile <- confint_quad <- Matrix(0, nrow = nsimu, ncol = 12)
    data[ , seq(k)] <- rmultinomial(n, 1, prob = probs)
    fit <- try(mle2(multi_lkl, start = initial_values,
                    data = list(linear_pred = linear_pred, data = data)))
    if (class(fit) != "try-error") {
        coefs[nsimu, ] <- as.numeric(fit@coef)
        confint_profile[nsimu, ] <- c(confint(fit))
        confint_quad[nsimu, ] <- c(confint(fit, method = "quad"))
    }
    return(list(coefs = coefs, confint_profile = confint_profile,
                confint_quad = confint_quad))
}
nsimu <- 500 ; simu <- vector("list", nsimu)
simu <- future_map(rep(1, nsimu), parallel2run)
```

MLEs distribution



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Coverage rate: Deviance and Wald intervals

```
coverage <- function(method) {
    coverage <- Matrix(0, nrow = 6, ncol = nsimu)
    for (i in seq(6))
        for (j in seq(nsimu))
            coverage[i, j] <-
                initial_values[i] >= simu[[j]][[method]][i] &
                initial_values[i] <= simu[[j]][[method]][i + 6]
    means <- rowMeans(coverage, na.rm = TRUE)
    names(means) <- names(initial_values)
    return(round(means, 3))}
coverage(method = 2) # deviance interval
```

```
##   b01   b11   b21   b02   b12   b22
## 0.950 0.956 0.950 0.934 0.948 0.952
```

```
coverage(method = 3) # wald interval
```

```
##   b01   b11   b21   b02   b12   b22
## 0.962 0.970 0.960 0.950 0.954 0.966
```

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For a subject i, with measurements j, we have

$$y_{ij} \mid \alpha_{1i}, \alpha_{2i} \sim \text{Multinomial}(p_{1ij}, p_{2ij}, p_{3ij}),$$

$$\text{with} \quad \begin{bmatrix} \alpha_{1i} \\ \alpha_{2i} \end{bmatrix} \sim \mathcal{N}\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma_{\alpha_1}^2 & \sigma_{\alpha_1}\sigma_{\alpha_2}\rho \\ \sigma_{\alpha_1}\sigma_{\alpha_2}\rho & \sigma_{\alpha_2}^2 \end{bmatrix} \right],$$

$$\text{and} \quad p_{kij} = \frac{\exp\{\boldsymbol{x}_{kij}\boldsymbol{\beta}_{kj} + \alpha_{ki}\}}{1 + \sum_{k=1}^{K-1} \exp\{\boldsymbol{x}_{kij}\boldsymbol{\beta}_{kj} + \alpha_{ki}\}}.$$

The likelihood for a random sample, and $\boldsymbol{\theta} = [\boldsymbol{\beta}, \rho, \sigma_{\alpha_1}^2, \sigma_{\alpha_1}^2]^\top$, is given by

$$L(\boldsymbol{\theta}; y) = \prod_{i=1}^{N} \int_{\Re} \int_{\Re} \prod_{j=1}^{n_i} \left[\binom{n_{ij}}{y_{1ij}, y_{2ij}, y_{3ij}} \prod_{k=1}^{K} p_{kij}^{y_{kij}} \right] \times$$

$$\frac{\exp\left\{ -\frac{1}{2(1-\rho^2)} \left(\frac{\alpha_{1i}^2}{\sigma_{\alpha_1}^2} + \frac{\alpha_{2i}^2}{\sigma_{\alpha_2}^2} - \frac{2\alpha_{1i}\alpha_{2i}\rho}{\sigma_{\alpha_1}\sigma_{\alpha_2}} \right) \right\}}{2\pi\sigma_{\alpha_1}\sigma_{\alpha_2}\sqrt{1-\rho^2}} \, d\alpha_{1i} \, d\alpha_{2i}.$$

$$\text{i.e.,} \quad L(\boldsymbol{\theta}; y_i) = \int_{\Re} \int_{\Re} f(y_i \mid \alpha_{1i}, \alpha_{2i}) \, f(\alpha_{1i}, \alpha_{2i}) \, d\alpha_{1i} \, d\alpha_{2i}.$$

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and. . .