Fitting CoDa using the Logistic Gaussian distribution with Dirichlet covariance structure

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Joaquín Martínez-Minaya • jmarmin@eio.upv.es

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```r
  ### --- 0. Loading libraries --- ####
library(INLA)
library(dplyr)
library(ggplot2)
library(ggtern)
```

An introduction to the Logistic Normal Dirichlet Regression

As defined in Martínez-Minaya and Rue (2023), $\boldsymbol{y} \in \mathbb{S}^D$ follows a logistic-normal distribution with Dirichlet covariance $\mathcal{LND}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ if and only if $alr(\boldsymbol{y}) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, and:

$$
\begin{array}{rcl}
\Sigma_{dd} & = & \sigma_d^2 + \gamma\,,\ d = 1, \ldots, D-1 \\
\Sigma_{dk} & = & \gamma\,, d \neq k
\end{array}
$$

where $\sigma_d^2 + \gamma$ represents the variance of each log-ratio and γ is the covariance between log-ratios. From now on we will refer to $\mathcal{ND}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ as the multivariate normal with Dirichlet covariance structure.

Let $\boldsymbol{y}$ be a multivariate random variable such as $\boldsymbol{y} \sim \mathcal{LND}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, which by definition is equivalent to $alr(\boldsymbol{y}) \sim \mathcal{ND}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. Because of its easy interpretability in terms of log-ratios with the reference category, we focus on modelling $alr(\boldsymbol{y})$ as a $\mathcal{ND}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

Simulated example I (Type II)

The model with which we are going to operate in this example presents the following structure:

$$
\begin{array}{rcl}
alr(\boldsymbol{Y}) & \sim & \mathcal{ND}((\boldsymbol{\mu}^{(1)}, \ldots, \boldsymbol{\mu}^{(D)}), \boldsymbol{\Sigma}) \quad (1) \\
\boldsymbol{\mu}^{(d)} & = & \boldsymbol{X}\boldsymbol{\beta}^{(d)}\,, \quad (2)
\end{array}
$$

Note that this is the second structure presented in Martínez-Minaya and Rue (2023), where we are working under the assumption that covariates have different effect in each linear predictor. In particular, we consider $D = 3$, and the reference category is the third one. So, we are dealing with two alr-coordinates. Also, we just generate a covariate x scaled to have mean 0 and standard deviation 1.

$$
\begin{array}{rcl}
alr(\boldsymbol{Y}) & \sim & \mathcal{ND}((\boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}), \boldsymbol{\Sigma})\,, \quad (3) \\
\boldsymbol{\mu}^{(1)} & = & \beta_0^{(1)} + \beta_1^{(1)}\boldsymbol{x}\,, \\
\boldsymbol{\mu}^{(2)} & = & \beta_1^{(2)} + \beta_1^{(2)}\boldsymbol{x}\,. \quad (4)
\end{array}
$$

Data simulation

```
set.seed(201803)
inla.seed = sample.int(n=1E6, size=1)
options(width=70, digits=3)
```

Defining hyperparameters and dimensionality of the response

We start defining the hyperparameters of the likelihood: $\sigma_1^2 = 0.5$, $\sigma_2^2 = 0.4$ and $\gamma = 0.1$, and computing the correlation matrix of the *alr*-coordinates.

```
### --- 1. Simulation --- ####
# Parameters for the simulation
D <- 3
N <- 1000
sigma2 <- c(0.5, 0.4)
cov_param <- 0.1
sigma_diag <- sqrt(sigma2 + cov_param)
hypers_lik <- data.frame(hypers = c(sigma2, cov_param),
                         name1 = c("sigma2.1", "sigma2.2", "gamma"))
# We create the correlation parameters based on the previous idea
# We are going to have ((D-1)^2 - (D-1))/2 rhos
rho <- diag(1/sigma_diag) %*% matrix(cov_param, D-1, D-1) %*% diag(1/sigma_diag)
diag(rho) <- 1
rho
```

```
##       [,1]  [,2]
## [1,] 1.000 0.183
## [2,] 0.183 1.000
```

Simulating a covariate

We define the covariate $\boldsymbol{x}$ and also, the corresponding betas, constructing the corresponding linear predictor.

```
x = runif(N)-0.5
# - mean 0 to not affect intercept
betas = matrix(c(-1, 3, -1, 5), nrow = D-1, byrow = TRUE)
X <- data.frame(1, x) %>% as.matrix(.)
lin.pred <- X %*% t(betas)
```

alr-coordinates

We construct the *alr*-coordinates

```
### ------- 1.2.3. Constructing the likelihood --- ####
Sigma <- matrix(sigma_diag, ncol = 1) %*% matrix(sigma_diag, nrow = 1)
Sigma <- Sigma*rho

lin.pred %>%
  apply(., 1, function(z)
    MASS::mvrnorm( n  = 1,
             mu = z,
             Sigma = Sigma)) %>%
  t(.)-> alry
```

Data in the simplex

We move back to the Simplex using the *alr*-inverse, in particular, we use the function `alrInv` form the R-package `compositions`.

```
  y.simplex <- compositions::alrInv(alry)
  y.simplex <- as.numeric(t(y.simplex)) %>% matrix(., ncol = D, byrow = TRUE)
  colnames(y.simplex) <- paste0("y", 1:D)
  data <- data.frame(alry, y.simplex, x)
colnames(data)[1:(D-1)] <- c(paste0("alry.", 1:(D-1)))
data %>% head(.)
```

```
##   alry.1 alry.2    y1     y2    y3       x
## 1 -1.580  -1.46 0.143 0.1620 0.695  0.0265
## 2 -1.345  -3.18 0.200 0.0318 0.768 -0.3708
## 3 -1.735  -1.52 0.126 0.1567 0.717  0.0819
## 4 -1.012  -2.01 0.243 0.0898 0.667 -0.0377
## 5 -0.584  -1.53 0.314 0.1224 0.563  0.0775
## 6 -0.041   2.10 0.095 0.8060 0.099  0.3962
```

Plotting the simulated data

```
### Ternary plot
ggtern::ggtern(data = data,
       aes(y1, y2, y3)) +
   #geom_mask() +
   geom_point(aes(fill = x), shape=21, size=2) +
   theme_bw() +
   theme_showarrows() +
   theme_clockwise() -> p_y

### Alr coordinates
data %>%
  tidyr::pivot_longer(., cols = ,starts_with("alr"),
                      names_to = "y.names", values_to = "y.resp") %>%
  ggplot(data = .) +
  geom_point(aes(x = x, y = y.resp, fill = x), shape = 21, size = 2) +
  ylab("alr") +
  facet_wrap(~y.names) +
  theme_bw() +
  theme(legend.position = "bottom") -> p_alr

#pdf("simulated_data.pdf", width = 8, height = 6)
grid.arrange(arrangeGrob(p_y,
                         p_alr + theme(legend.position = "none")))
```

```
#dev.off()
```

Data preparation for fitting

Index for individual

```
  data$id.z <- 1:dim(data)[1]
```

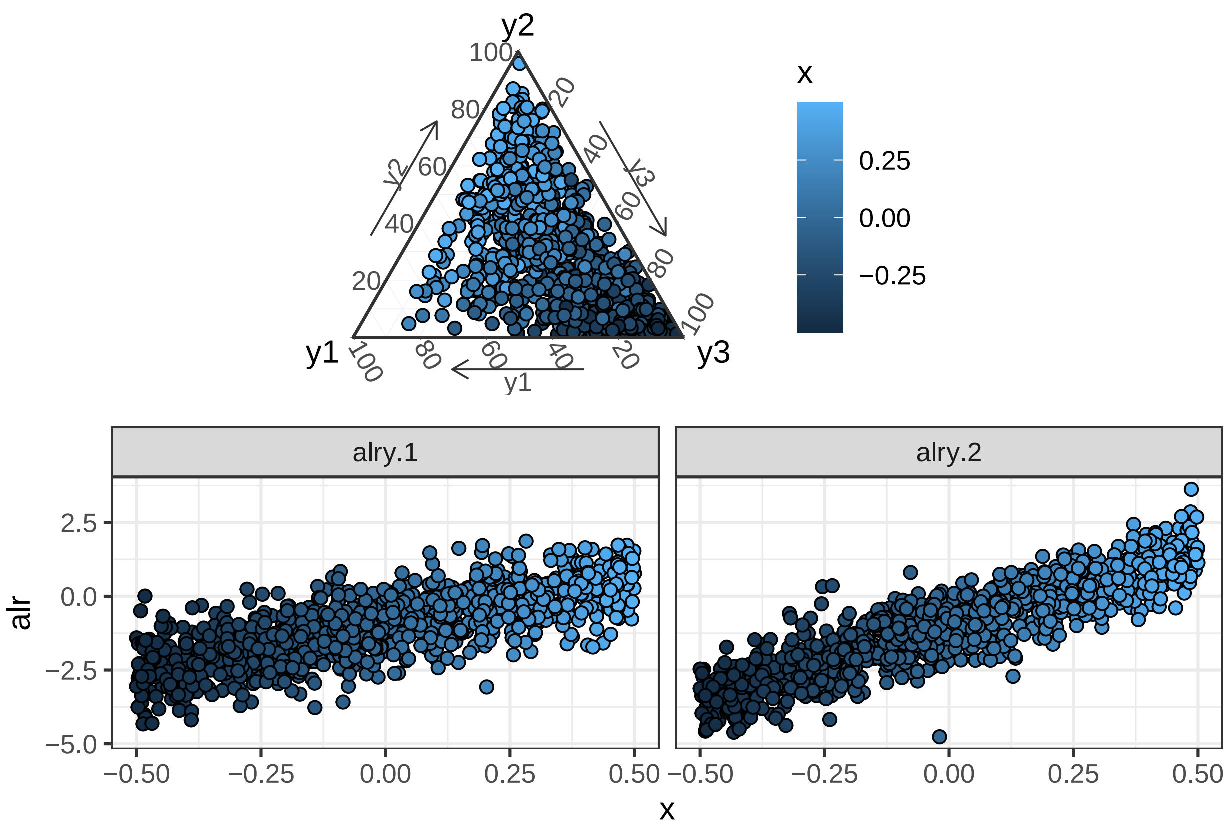


Figure 1: Simulated data in the Simplex and also using alr-coordinates in terms of x

Extending the dataset

We extent the data with *alr*-coordinates for introducing in `inla.stack`

```
data_ext <- data %>%
  tidyr::pivot_longer(., cols = all_of(paste0("alry.", 1:(D-1))),
                      names_to  = "y.names",
                      values_to = "y.resp") %>%
  .[order(ordered(.$y.names)),]
data_ext$y.names <- ordered(data_ext$y.names)
head(data_ext)
```

```
## # A tibble: 6 x 7
##       y1     y2     y3       x  id.z y.names  y.resp
##    <dbl>  <dbl>  <dbl>   <dbl> <int> <ord>     <dbl>
## 1 0.143  0.162  0.695   0.0265     1 alry.1  -1.58
## 2 0.200  0.0318 0.768  -0.371      2 alry.1  -1.35
## 3 0.126  0.157  0.717   0.0819     3 alry.1  -1.74
## 4 0.243  0.0898 0.667  -0.0377     4 alry.1  -1.01
## 5 0.314  0.122  0.563   0.0775     5 alry.1  -0.584
## 6 0.0950 0.806  0.0990  0.396      6 alry.1  -0.0410
```

Response in `R-INLA`

We create a matrix with dimension $(N \times (D-1)) \times (D-1)$ for including the multivariate response in `R-INLA`

```
names_y <- paste0("alry.", 1:(D-1))
1:length(names_y) %>%
  lapply(., function(i){
    data_ext %>%
      dplyr::filter(y.names == names_y[i]) -> data_comp_i
    #Response
    y_alr <- matrix(ncol = names_y %>% length(.), nrow = dim(data_comp_i)[1])
    y_alr[, i] <- data_comp_i$y.resp
  }) -> y.resp

1:length(names_y) %>%
  lapply(., function(i){
    y_aux <- data_ext %>%
      dplyr::select(y.resp, y.names) %>%
      dplyr::filter(y.names == names_y[i]) %>%
      dplyr::select(y.resp) %>%
      as.matrix(.)
    aux_vec <- rep(NA, (D-1))
    aux_vec[i] <- 1
    kronecker(aux_vec, y_aux)
  }) -> y_list

y_tot <- do.call(cbind, y_list)
y_tot %>% head(.)
```

```
##        [,1] [,2]
## [1,] -1.580   NA
## [2,] -1.345   NA
## [3,] -1.735   NA
## [4,] -1.012   NA
```

```
## [5,] -0.584   NA
## [6,] -0.041   NA
```

Covariates in R-INLA

Covariates are going to be included in the model as random effects with big variance. So, we need the values of the covariates, and also, an index indicating to which alr-coordinate it belongs.

```
variables <- c("intercept", data %>%
                 dplyr::select(starts_with("x")) %>%
                 colnames(.))
id.names <- paste0("id.", variables)
id.variables <- rep(data_ext$y.names %>% as.factor(.) %>% as.numeric(.),
                    length(variables)) %>%
  matrix(., ncol = length(variables), byrow = FALSE)
colnames(id.variables) <- id.names

variables
```

```
## [1] "intercept" "x"
```

```
id.variables %>% head(.)
```

```
##      id.intercept id.x
## [1,]            1    1
## [2,]            1    1
## [3,]            1    1
## [4,]            1    1
## [5,]            1    1
## [6,]            1    1
```

inla.stack

We create an `inla.stack` for estimation

```
stk.est <- inla.stack(data    = list(resp = y_tot),
                      A       = list(1),
                      effects = list(cbind(data_ext %>%
                                             dplyr::select(starts_with("x")),
                                           data_ext %>%
                                             dplyr::select(starts_with("id.z")),
                                           id.variables,
                                           intercept = 1)),
                      tag     = 'est')
```

Fitting the model

In this section, we fit a model (Type II in the manuscript), and we obtain the marginal posterior distribution of the parameters and hyperparameters

Fit in R-INLA

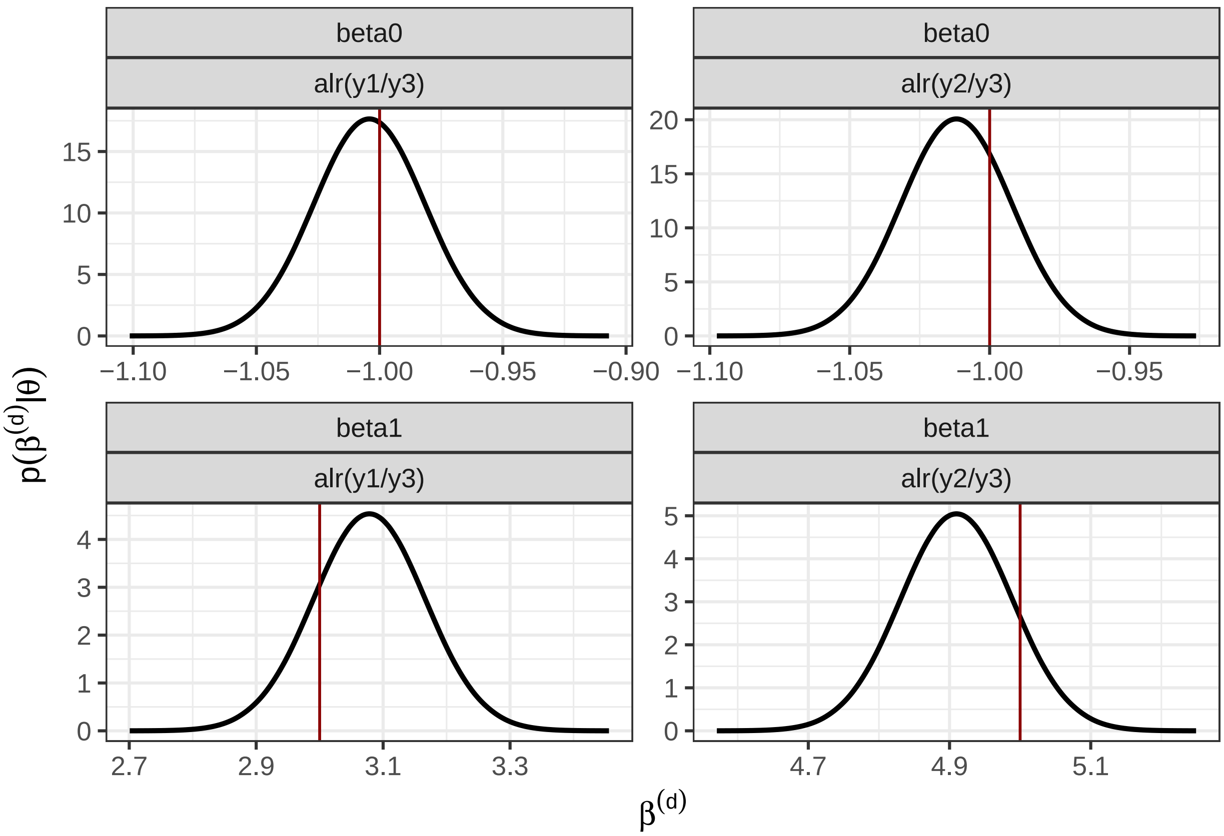
```
  # Have different parameters for fixed effects, and do not include spatial random effects.
list_prior <- rep(list(list(prior = "pc.prec", param = c(1, 0.01))), D-1)

### Fitting the model
```

```r
formula.typeII <- resp ~ -1 +
  f(id.intercept, intercept,
    model   = "iid",
    initial = log(1/1000),
    fixed   = TRUE) +
  f(id.x, x,
    model   = "iid",
    initial = log(1/1000),
    fixed   = TRUE) +
  f(id.z,
    model = "iid",
    hyper = list(prec = list(prior = "pc.prec",
                             param = c(1, 0.01))), constr = TRUE)
model.typeII <- inla(formula.typeII,
                     family         = rep("gaussian", D-1),
                     data           = inla.stack.data(stk.est),
                     control.compute = list(config = TRUE),
                     control.predictor = list(A = inla.stack.A(stk.est),
                                              compute = TRUE),
                     control.family = list_prior,
                     inla.mode = "experimental" ,
                     verbose = FALSE)
```

Marginal posterior distribution of the fixed effects

```r
### Posterior distribution of the fixed effects
data_fixed <- rbind(data.frame(inla.smarginal(model.typeII$marginals.random$id.x$index.1),
                               alr = "alr(y1/y3)",
                               var = "x",
                               param = "beta1",
                               real  = betas[1,2]),
                    data.frame(inla.smarginal(model.typeII$marginals.random$id.x$index.2),
                               alr = "alr(y2/y3)",
                               var = "x",
                               param = "beta1",
                               real  = betas[2,2]),
                    data.frame(inla.smarginal(model.typeII$marginals.random$id.intercept$index.1),
                               alr = "alr(y1/y3)",
                               var = "intercept",
                               param = "beta0",
                               real = betas[1,1]),
                    data.frame(inla.smarginal(model.typeII$marginals.random$id.intercept$index.2),
                               alr = "alr(y2/y3)",
                               var = "intercept",
                               param = "beta0",
                               real = betas[2,1]))

p_fixed <- ggplot() +
  geom_line(data = data_fixed, aes(x = x, y = y), size = 0.9) +
  #ggtitle("Effect of the covariate bio12") +
  theme_bw() +
  geom_vline(data = data_fixed, aes(xintercept = real), col = "red4") +
 # scale_color_manual(values=c("#E75F00", "#56B4E9"))+
```

```r
  theme(legend.position = "bottom") +
  facet_wrap(~param + alr, ncol = D-1, scales = "free") +
  xlab(expression(beta^(d))) +
  ylab(expression(p(beta^(d) *'|'* theta))) +
  theme(legend.title = element_blank())

#pdf("posterior_fixed.pdf", width = 6, height = 5)
p_fixed
```

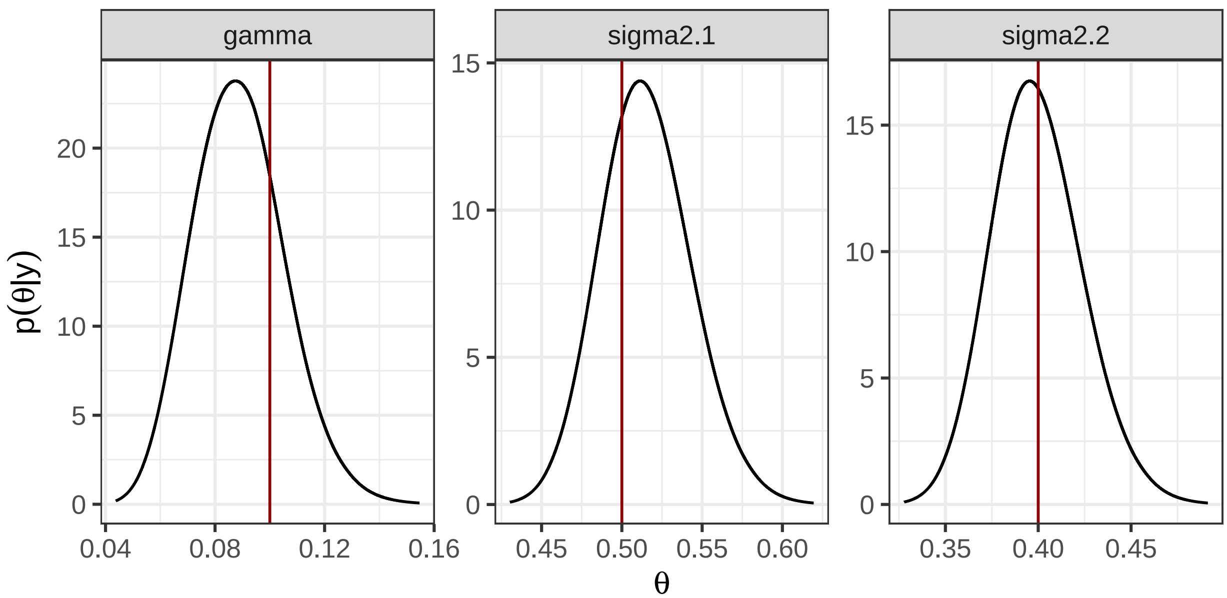



```r
#dev.off()
```

Marginal Posterior distribution of the hyperparameters

```r
### Posterior distribution of the hyperparameters
prec <- list(sigma2.1 = model.typeII$marginals.hyperpar$`Precision for the Gaussian observations`,
             sigma2.2 = model.typeII$marginals.hyperpar$`Precision for the Gaussian observations[2]`,
             gamma = model.typeII$marginals.hyper$`Precision for id.z`)

hyper <- lapply(1:length(prec),
                function(x){
                  inla.smarginal(inla.tmarginal(prec[[x]], fun = function(y)(1/y))) %>%
                    data.frame(.)
                })
names(hyper) <- names(prec)

hyper.df <- lapply(1:length(hyper),
```

```
                    function(x){
                      cbind(data.frame(hyper[[x]]), name1 = names(hyper)[x])
                    })  %>%
  do.call(rbind.data.frame, .)

hyper.df$name1 <- ordered(hyper.df$name1,
                          levels = c("sigma2.1", "sigma2.2",
                                     "gamma"))
p.hyper <- ggplot(hyper.df) +
  geom_line(aes(x = x, y = y)) +
  geom_vline(data = hypers_lik, aes(xintercept = hypers), col = "red4") +
  facet_wrap(~ name1, scales = "free") +
  theme_bw() +
  xlab(expression(theta)) +
  ylab(expression(p(theta*'|'*y)))

#pdf("marginals_hyperpar.pdf", width = 6, height = 3)
print(p.hyper)
```




```
#dev.off()
```

Predicting for a new observation

This section, is devoted to explain how to make predictions. We want to predict, for the values of the covariate $x = -0.5, -0.2, 0.1, 0.4$. In particular, we show how to compute the posterior preditive distribution for the mean of the *alr*-coordinates. Posteriorly, we move back to the Simplex.

Preparing dataset for predictions

```
sim <- 1000
x.pred <- seq(-0.5, 0.5, 0.3)
n.pred <- length(x.pred)
cat("\n -------------------------------------------------- \n")
```

```
##
## ----------------------------------------------
```

```
cat("Creating the data.frame for predictions \n")
```

```
## Creating the data.frame for predictions
```

```
data_pred <- data.frame(intercept = 1,
                        x = rep(x.pred, D-1))
id.z.pred  <- rep((N + 1):(N + n.pred), D - 1) #random effect z to model the correlation

# Category
id.cat_pred <- rep(1:(D - 1), rep(n.pred, D - 1))
#Index for covariates
variables_pred <- c("intercept", data_pred %>%
                      dplyr::select(starts_with("x")) %>%
                      colnames(.))
id.names_pred <- paste0("id.", variables_pred)
id.variables_pred <- rep(id.cat_pred, length(variables_pred)) %>%
  matrix(., ncol = length(variables_pred), byrow = FALSE)
colnames(id.variables_pred) <- id.names_pred
```

Preparing inla.stack for predictions

```
stk.pred <- inla.stack(data    = list(resp = matrix(NA, ncol = D - 1,
                                                    nrow = n.pred*(D - 1))),
                       A       = list(1),
                       effects = list(cbind(data_pred,
                                            id.z = id.z.pred,
                                            id.variables_pred)),
                       tag     = 'pred')
### --- Total stack
stk <- inla.stack(stk.est, stk.pred)
```

Prediction

```
mod.pred <- inla(formula.typeII,
                 family         = rep("gaussian", D - 1),
                 data              = inla.stack.data(stk),
                 control.compute   = list(config = TRUE),
                 control.predictor = list(A = inla.stack.A(stk), compute = TRUE, link = 1),
                 control.mode      = list(theta = model.typeII$mode$theta, restart = TRUE),
                 control.family = list_prior,
                 num.threads       = 2,
                 inla.mode = "experimental" ,
                 verbose           = FALSE)
```

Extracting predictions using inla.posterior.sample

```
pred.values.mean <- mod.pred$summary.fitted.values$mean[inla.stack.index(stk, 'pred')$data] %>%
  matrix(., ncol = D - 1, byrow = FALSE)

post_sim_pred <- inla.posterior.sample(n = sim, result = mod.pred)
post_sim_predictor <- inla.posterior.sample.eval(fun = function(...){
```

```r
  APredictor}, post_sim_pred, return.matrix = TRUE)
post_sim_idz <- inla.posterior.sample.eval(fun = function(...){
  id.z}, post_sim_pred, return.matrix = TRUE)

ind.pred <- inla.stack.index(stk, 'pred')$data
ind.idz <- inla.stack.index(stk, 'est')$data #This is the shared random effect
ind.idz <- ind.idz[1:(length(ind.idz)/(D - 1))]

post_sim_predictor[ind.pred, ] <- post_sim_predictor[ind.pred, ]-
  kronecker(rep(1, D-1), post_sim_idz[-ind.idz,])

post_sim_pred_alr <- post_sim_predictor[ind.pred,]

#Computing mean and sd
pred_alr_summary <- t(apply(post_sim_pred_alr, 1, function(x){c(mean(x), sd(x))}))
pred_alr_summary <- data.frame(pred_alr_summary,
                               y.names = rep(names_y, rep(n.pred, D-1)),
                               x.pred = rep(x.pred, D-1))
colnames(pred_alr_summary)[1:2] <- c("mean", "sd")

pred_alr_summary
```

```
##             mean     sd y.names x.pred
## fun[2001] -2.543 0.0494  alry.1   -0.5
## fun[2002] -1.619 0.0279  alry.1   -0.2
## fun[2003] -0.696 0.0244  alry.1    0.1
## fun[2004]  0.227 0.0434  alry.1    0.4
## fun[2005] -3.466 0.0445  alry.2   -0.5
## fun[2006] -1.994 0.0255  alry.2   -0.2
## fun[2007] -0.522 0.0213  alry.2    0.1
## fun[2008]  0.950 0.0373  alry.2    0.4
```

Predictions in the simplex

```r
###  Prediction in the simplex --- #####
apply(post_sim_predictor[ind.pred,], 2, function(x){
  alr_pred <- matrix(x, ncol = D - 1)
  pred_simplex <- compositions::alrInv(alr_pred)
  as.numeric(t(pred_simplex)) #Byrows
}) -> post_sim_pred_simplex

#Computing credible intervals
pred_simplex_summary <- t(apply(post_sim_pred_simplex, 1, function(x){c(mean(x), sd(x))}))
pred_simplex_summary <- data.frame(pred_simplex_summary,
                                   y.names = rep(c("y1", "y2", "y3"), n.pred),
                                   x.pred  = rep(x.pred, rep(D, n.pred)))
colnames(pred_simplex_summary)[1:2] <- c("mean", "sd")

pred_simplex_summary
```

```
##      mean      sd y.names x.pred
## 1  0.0709 0.00324      y1   -0.5
## 2  0.0282 0.00121      y2   -0.5
## 3  0.9009 0.00347      y3   -0.5
```

```
## 4  0.1485 0.00352      y1   -0.2
## 5  0.1021 0.00234      y2   -0.2
## 6  0.7495 0.00379      y3   -0.2
## 7  0.2384 0.00463      y1    0.1
## 8  0.2837 0.00461      y2    0.1
## 9  0.4780 0.00404      y3    0.1
## 10 0.2594 0.00949      y1    0.4
## 11 0.5341 0.01070      y2    0.4
## 12 0.2065 0.00486      y3    0.4
```

References

Martínez-Minaya, Joaquín, and Haavard Rue. 2023. "A Flexible Bayesian Tool for CoDa Mixed Models: Logistic-Normal Distribution with Dirichlet Covariance." https://arxiv.org/abs/2308.13928.