

# Fitting CoDa using the Logistic Gaussian distribution with Dirichlet covariance structure

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

## An introduction to the Logistic Normal Dirichlet Regression

As defined in @martinez-minaya2023,  $\mathbf{y} \in \mathbb{S}^D$  follows a logistic-normal distribution with Dirichlet covariance  $\mathcal{LND}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  if and only if  $alr(\mathbf{y}) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , and:

$$\begin{aligned}\Sigma_{dd} &= \sigma_d^2 + \gamma, \quad d = 1, \dots, D-1 \\ \Sigma_{dk} &= \gamma, \quad d \neq k\end{aligned}$$

where  $\sigma_d^2 + \gamma$  represents the variance of each log-ratio and  $\gamma$  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  $\mathbf{y}$  be a multivariate random variable such as  $\mathbf{y} \sim \mathcal{LND}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , which by definition is equivalent to  $alr(\mathbf{y}) \sim \mathcal{ND}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ . Because of its easy interpretability in terms of log-ratios with the reference category, we focus on modelling  $alr(\mathbf{y})$  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:

$$alr(\mathbf{Y}) \sim \mathcal{ND}((\boldsymbol{\mu}^{(1)}, \dots, \boldsymbol{\mu}^{(D)}), \boldsymbol{\Sigma}) \quad (1)$$

$$\boldsymbol{\mu}^{(d)} = \mathbf{X}\boldsymbol{\beta}^{(d)}, \quad (2)$$

Note that this is the second structure presented in @martinez-minaya2023, 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.

$$alr(\mathbf{Y}) \sim \mathcal{ND}((\boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}), \boldsymbol{\Sigma}), \quad (3)$$

$$\begin{aligned}\boldsymbol{\mu}^{(1)} &= \beta_0^{(1)} + \beta_1^{(1)} \mathbf{x}, \\ \boldsymbol{\mu}^{(2)} &= \beta_1^{(2)} + \beta_1^{(2)} \mathbf{x}.\end{aligned} \quad (4)$$

## 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  $\mathbf{x}$  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` from 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]
```

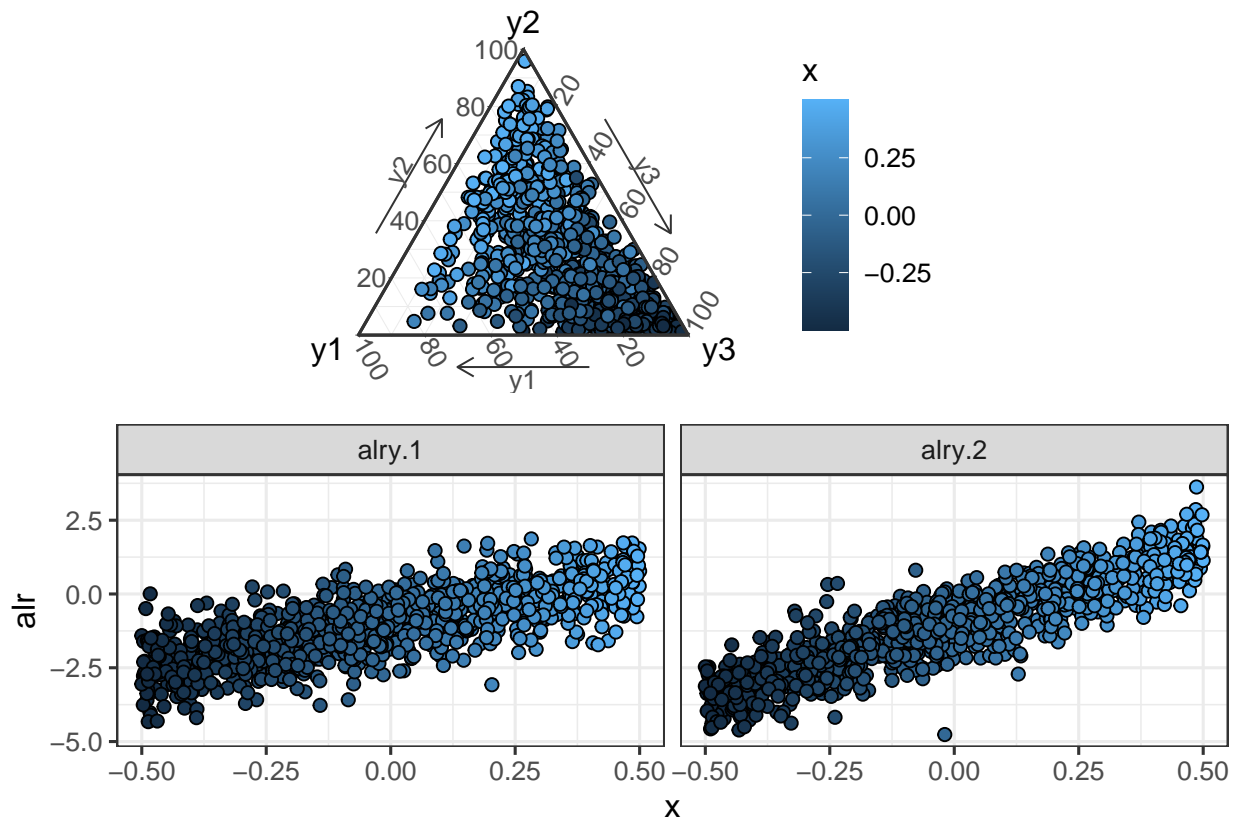


Figure 1: Simulated data in the Simplex and also using alr-coordinates in terms of  $x$

## Extending the dataset

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

```
data_ext <- data %>%
  tidyr::pivot_longer(., cols = all_of(paste0("alr.", 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 alr.y.1 -1.58
## 2 0.200  0.0318 0.768 -0.371     2 alr.y.1 -1.35
## 3 0.126  0.157  0.717  0.0819     3 alr.y.1 -1.74
## 4 0.243  0.0898 0.667 -0.0377     4 alr.y.1 -1.01
## 5 0.314  0.122  0.563  0.0775     5 alr.y.1 -0.584
## 6 0.0950 0.806  0.0990  0.396     6 alr.y.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("alr.", 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
```

```

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

```

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

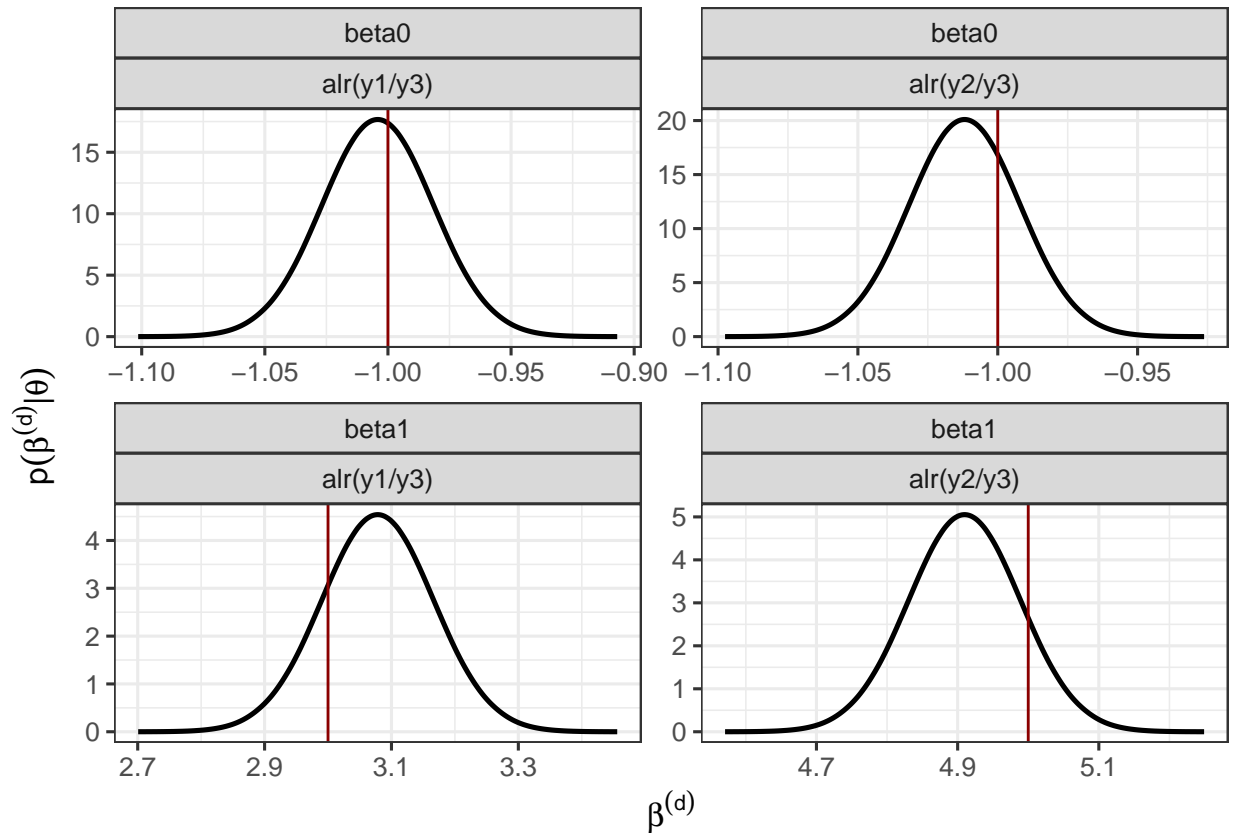
```

```

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

```



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

## Marginal Posterior distribution of the hyperparameters

```

### 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.tsmarginal(prec[[x]], fun = function(y)(1/y))) %>%
                   data.frame(.)
               })
names(hyper) <- names(prec)

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

```



```

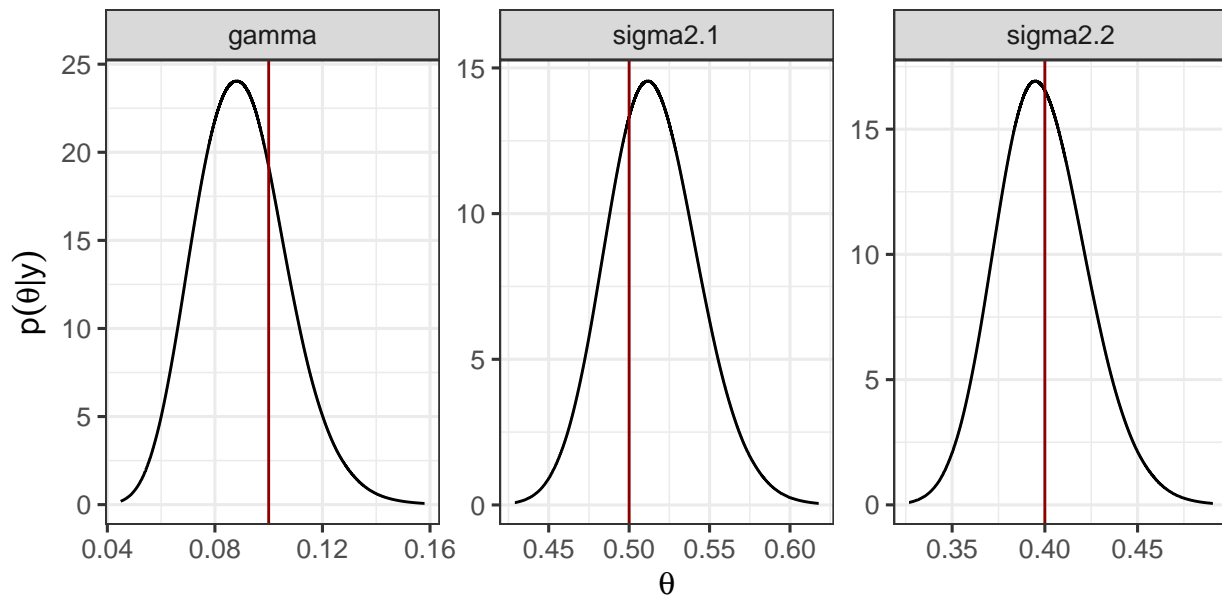
function(x){
  cbind(data.frame(hyper[[x]]), name1 = names(hyper)[x])
}) %>%
do.call(rbind.data.frame, .)

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 predictive 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(...){
```

```

  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 0.0488 alry.1  -0.5
## fun[2002] -1.620 0.0284 alry.1  -0.2
## fun[2003] -0.697 0.0246 alry.1   0.1
## fun[2004]  0.226 0.0421 alry.1   0.4
## fun[2005] -3.465 0.0435 alry.2  -0.5
## fun[2006] -1.993 0.0253 alry.2  -0.2
## fun[2007] -0.521 0.0218 alry.2   0.1
## fun[2008]  0.951 0.0374 alry.2   0.4

```

## Predictions in the simplex

```

#### 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 0.00320    y1  -0.5
## 2  0.0282 0.00118    y2  -0.5
## 3  0.9009 0.00347    y3  -0.5

```

## 4	0.1483	0.00356	y1	-0.2
## 5	0.1022	0.00231	y2	-0.2
## 6	0.7495	0.00390	y3	-0.2
## 7	0.2380	0.00462	y1	0.1
## 8	0.2839	0.00465	y2	0.1
## 9	0.4781	0.00418	y3	0.1
## 10	0.2589	0.00904	y1	0.4
## 11	0.5345	0.01036	y2	0.4
## 12	0.2066	0.00494	y3	0.4