Appendix S2: Simulation Study using MVGP Simulated data

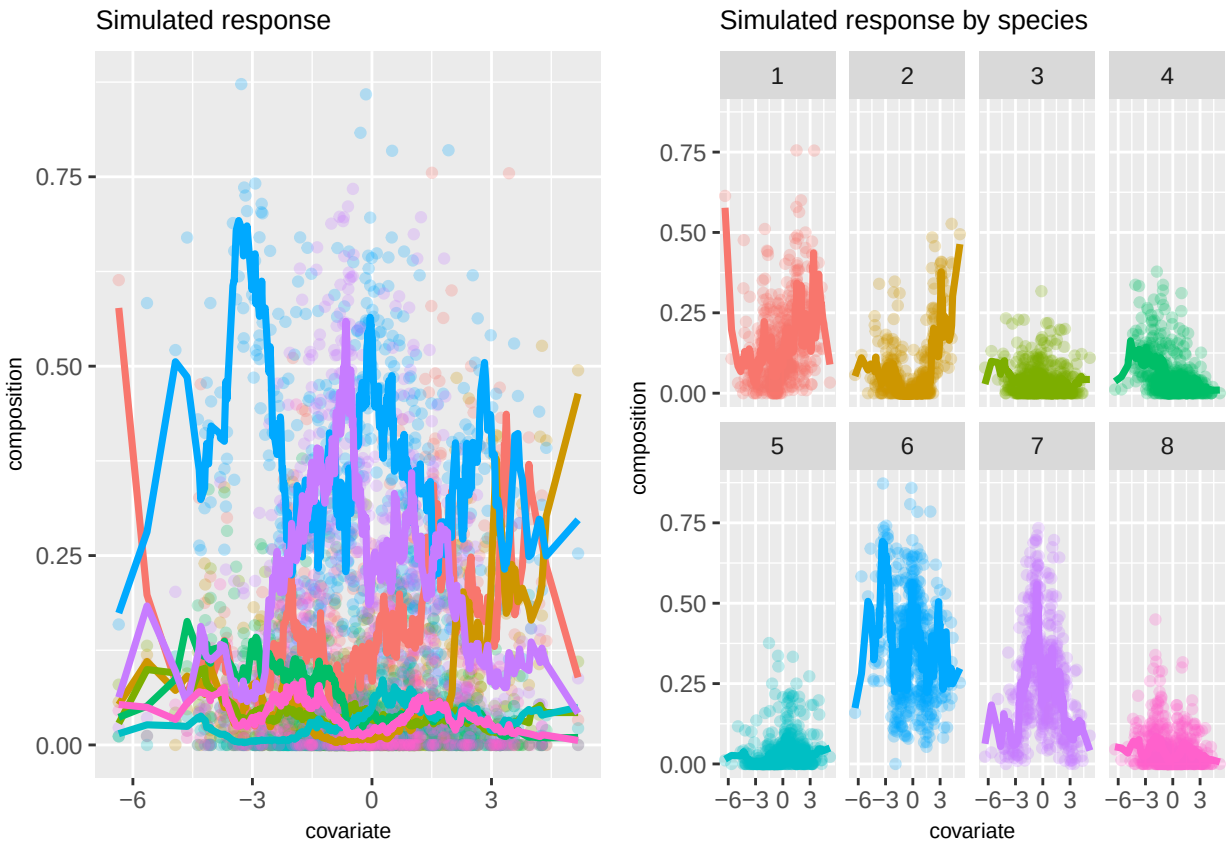
S2.1 Simulation Study

In this appendix, we simulated data using the multivariate Gaussian process model (MVGP) functional response model. We simulated data on the log-scale random effect $\boldsymbol{\alpha}_i$ (Equation (3) in the manuscript) setting $N = 500$ observations where the covariate is observed and $\tilde{N} = 200$ observations where the covariate is unobserved. We simulated the data with $d = 8$ species. The parameters used in simulation are generated according to the following: $\mu \sim \text{N}(0, 1)$, $\mathbf{R} \sim \text{LKJ}(1)$, $\tau_j \sim \text{gamma}(5, 2)$, $X \sim \text{N}(0, 16)$, $\sigma^2 = 1$, $\phi = 1/5$, and $\boldsymbol{\varepsilon}_i \equiv \mathbf{0}$. The simulation of the data using the `sim_compositional_data()` function in the `BayesComposition` package for the MVGP is shown below.

```
set.seed(101)
library(BayesComposition)
library(knitr)
library(here)
library(ggplot2)
library(GGally)
library(analogue)
library(rioja)
library(xtable)

## change these for your file structure
## output directory for MCMC output
save_directory <- "~/Google Drive/mvgp-test/"
## directory for MCMC monitoring output
progress_directory <- "./mvgp-test/"
```

```
## Function from BayesComposition to simulate data from MVGP model
N <- 500
N_pred <- 200
d <- 8

dat <- sim_compositional_data(
  N                          = N,
  N_pred                     = N_pred,
  d                          = d,
  likelihood                 = "dirichlet-multinomial",
  function_type              = "gaussian-process",
  predictive_process         = FALSE,
  correlation_function       = "exponential",
  phi                        = 1/5,
  multiplicative_correlation = TRUE,
  additive_correlation       = FALSE
)



p_alpha <- t(sapply(1:N, function(i) dat$alpha[i, ] / sum(dat$alpha[i, ])))
y_prop <- t(sapply(1:N, function(i) dat$y[i, ] / sum(dat$y[i, ])))
```

```r
simPlotData <- data.frame(
  species = as.factor(rep(1:d, each = N)),
  count   = c(y_prop),
  depth   = rep(dat$X, times = d),
  alpha   = c(p_alpha))

gsim1 <- ggplot(simPlotData, aes(x=depth, y=count, color=species,
                                 group=species)) +
  geom_point(alpha=0.25) +
  theme(legend.position="none",
        title = element_text(size=8)) +
  ggtitle("Simulated response") +
  labs(x = "covariate", y="composition") +
  geom_line(aes(x=depth, y=alpha, col = species), simPlotData, lwd=1.25)

gsim2 <- ggplot(simPlotData, aes(x=depth, y=count, color=species,
                                 group=species)) +
  geom_point(alpha=0.25) +
  theme(legend.position="none",
        title = element_text(size=8)) +
  ggtitle("Simulated response by species") +
  labs(x = "covariate", y="composition") +
  geom_line(aes(x=depth, y=alpha, col = species), simPlotData, lwd=1.25) +
  facet_wrap( ~ species, ncol = 4)

## generate the plot
multiplot(gsim1, gsim2, cols=2)
```



S2.2 Fitting the MVGP model

To fit the model, we consider $n^\star = 30$ evenly spaced knots over a range larger than the observed data X to allow for potential predictions outside the range of the prediction. We have not found the inference to show much sensitivity in practical applications to the number of knots. The Gaussian process kernel uses an exponential covariance function; other covariance functions currently included in the software include a Gaussian covariance function. We fit the model for 150000 MCMC iterations, where the first 50000 iterations include adaptive tuning of the Metropolis-Hastings proposals and are used as a burn-in [Roberts and Rosenthal, 2009]. We fit 4 chains in parallel, keeping every 150th iteration to reduce memory and storage costs resulting in 4000 posterior samples.

```
## generate a sequence of knots that covers ranges outside
##    the observed values
n_knots <- 30
X_knots <- seq(
  min(dat$X, na.rm=TRUE) - 1.25 * sd(dat$X, na.rm=TRUE),
  max(dat$X, na.rm=TRUE) + 1.25 * sd(dat$X, na.rm=TRUE),
  length = n_knots)

## define the model parameters
params <- list(
  n_adapt                   = 50000,
  n_mcmc                    = 150000,
  n_thin                    = 150,
  correlation_function      = "exponential",
  likelihood                = "dirichlet-multinomial",
```

```
  function_type              = "gaussian-process",
  multiplicative_correlation = TRUE,
  additive_correlation       = FALSE,
  n_chains                   = 4,
  n_cores                    = 4,
  n_knots                    = n_knots,
  X_knots                    = X_knots)


if (file.exists(paste0(save_directory, "sim-mvgp-fit-mvgp.RData"))) {
  load(paste0(save_directory, "sim-mvgp-fit-mvgp.RData"))
} else {
  ## potentially long running MCMC code
  out <- fit_compositional_data(
    y                  = dat$y,
    X                  = dat$X,
    params             = params,
    progress_directory = progress_directory,
    progress_file      = "sim-mvgp-fit-mvgp.txt")
  ## save the output file
  save(out, file = paste0(save_directory, "sim-mvgp-fit-mvgp.RData"))

}
```

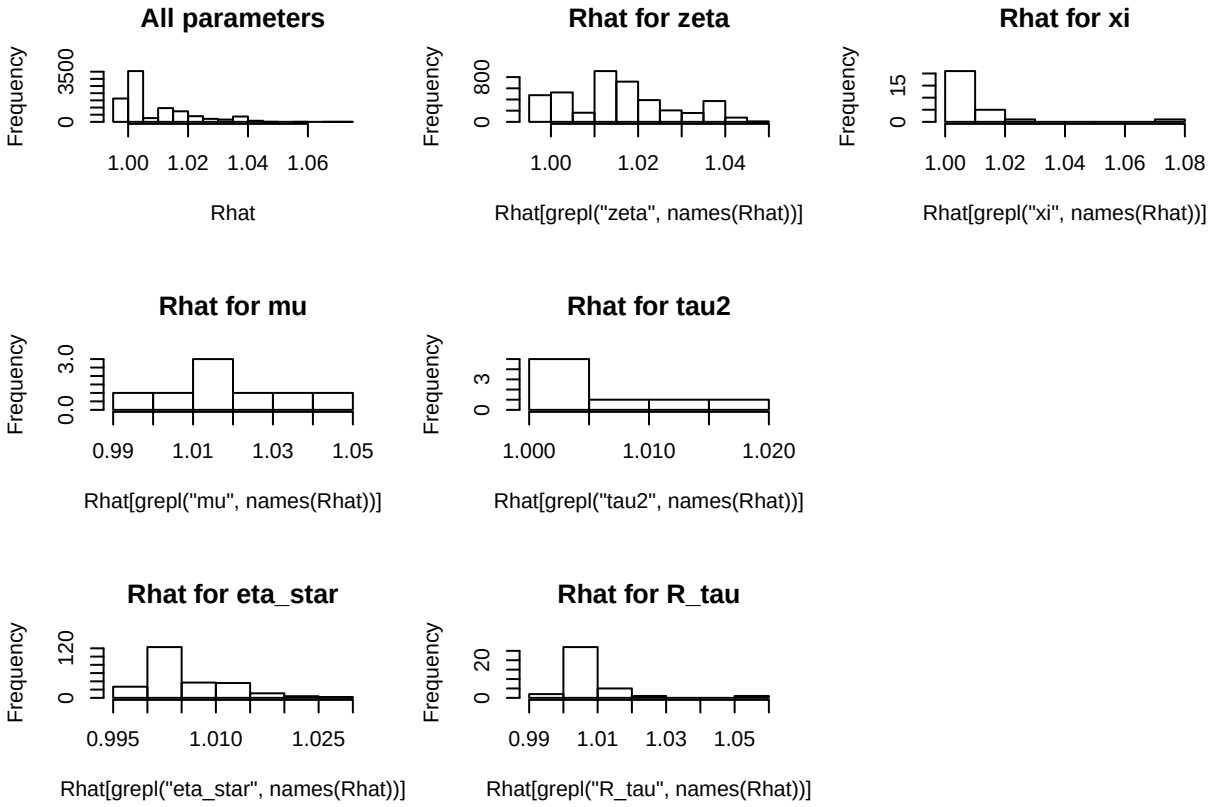
S2.2.1 MVGP convergence diagnostics

After fitting the model, the posterior samples are generated and MCMC convergence is assessed using the Gelman-Rubin $\hat{R}$ statistic. We see the distribution of $\hat{R}$ statistics is close to 1 with the largest $\hat{R} = 1.0706708 \leq 1.1$ at an acceptable value (Gelman et al. [2013], pp.287).

```
## extract posterior samples
samples <- extract_compositional_samples(out)
mu_post <- samples$mu
eta_star_post <- samples$eta_star
zeta_post <- samples$zeta
Omega_post <- samples$Omega
phi_post <- samples$phi
tau2_post <- samples$tau2
R_post <- samples$R
R_tau_post <- samples$R_tau
xi_post <- samples$xi
tau2_epsilon_post <- samples$tau2_epsilon
R_epsilon_post <- samples$R_epsilon
R_tau_epsilon_post <- samples$R_tau_epsilon
xi_epsilon_post <- samples$xi_epsilon

n_samples <- nrow(mu_post)

## Calculate Gelman-Rubin convergence statistic
Rhat <- make_gelman_rubin(out)
layout(matrix(1:9, 3, 3))
hist(Rhat, main="All parameters")
hist(Rhat[grepl("mu", names(Rhat))], main = "Rhat for mu")
```

```r
hist(Rhat[grepl("eta_star", names(Rhat))], main = "Rhat for eta_star")
hist(Rhat[grepl("zeta", names(Rhat))], main = "Rhat for zeta")
hist(Rhat[grepl("tau2", names(Rhat))], main = "Rhat for tau2")
hist(Rhat[grepl("R_tau", names(Rhat))], main = "Rhat for R_tau")
hist(Rhat[grepl("xi", names(Rhat))], main = "Rhat for xi")
Rhat[!is.finite(Rhat)] <- NA
max(unlist(na.omit(Rhat)))
```

```
## [1] 1.070671
```

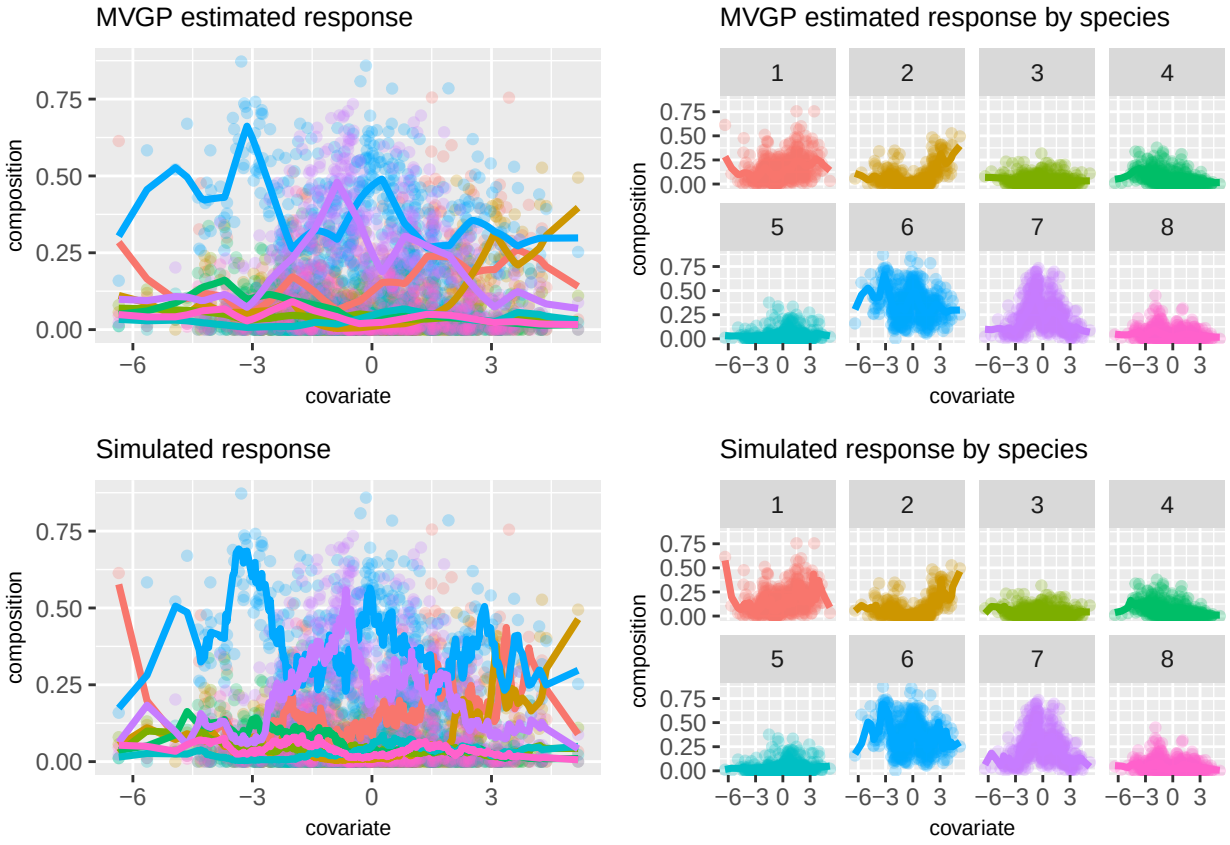


S2.2.2 MVGP functional response estimation

To compare how well the model reconstructs the unobserved latent functional relationships between the covariate and the observations, we plot both the simulated and fitted functional responses below. These show that the model is accurately estimating the latent functional responses, although the estimated functional responses are slightly smoother due to the predictive process approximation.

```r
alpha_post_mean <- exp(t(apply(mu_post, 2, mean) +
                         t(apply(zeta_post, c(2, 3), mean))))

p_alpha_post_mean <- t(sapply(1:N, function(i) {
  alpha_post_mean[i, ] / sum(alpha_post_mean[i, ])
}))

fitPlotData <- data.frame(species=as.factor(rep(1:d, each=N)),
                          count=c(y_prop),
                          depth=rep(dat$X, times=d),
                          alpha=c(p_alpha_post_mean))
```

```
g1_post <- ggplot(fitPlotData, aes(x=depth, y=count, color=species, group=species)) +
  geom_point(alpha=0.25) +
  theme(legend.position="none",
        title = element_text(size=8)) +
  ggtitle("MVGP estimated response") +
  labs(x = "covariate", y="composition") +
  geom_line(aes(x=depth, y=alpha, col = species), fitPlotData, lwd=1.25)

g2_post <- ggplot(fitPlotData, aes(x=depth, y=count, color=species, group=species)) +
  geom_point(alpha=0.25) +
  theme(legend.position="none",
        title = element_text(size=8)) +
  ggtitle("MVGP estimated response by species") +
  labs(x = "covariate", y="composition") +
  geom_line(aes(x=depth, y=alpha, col = species), fitPlotData, lwd=1.25) +
  facet_wrap( ~ species, ncol = 4)
multiplot(g1_post, g2_post, gsim1, gsim2, cols=2)
```



S2.2.3 Generate MVGP predictions

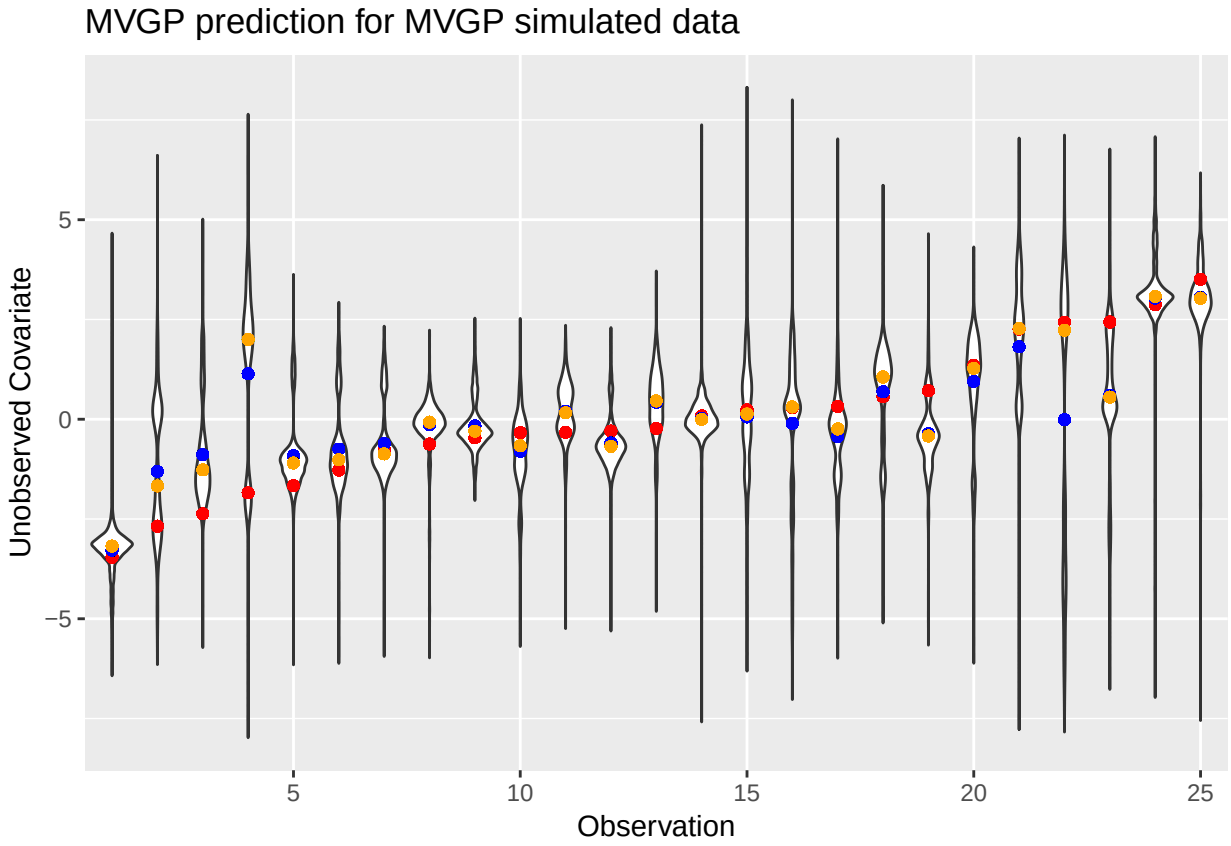
Using the elliptical slice sampler [Murray et al., 2010], we generate posterior predictions for the unobserved covariates using the posterior samples estimated from the MVGP calibration model. These estimates can be generated either jointly with the calibration model or estimated using a two-stage approach as presented here. We have found, there is little practical difference in model performance between joint and two-stage estimation and follow the convention in the transfer function literature of using two-stage estimation.

```
## Note, there might be some initial warnings about ESS shrunk to the
##    current position for the first few iterations. This is not a
##    major concern as long as the warnings don't continue.
if (file.exists(paste0(save_directory, "sim-mvgp-predict-mvgp.RData"))) {
  load(paste0(save_directory, "sim-mvgp-predict-mvgp.RData"))
} else {
  pred <- predict_compositional_data(
    dat$y_pred,
    dat$X,
    params,
    samples,
    progress_directory,
    "sim-mvgp-predict-mvgp.txt")
  save(pred, file = paste0(save_directory, "sim-mvgp-predict-mvgp.RData"))
}
```

S2.2.4 Plot MVGP predictions

The predictions for 25 randomly chosen missing covariate observations are shown below. The simulated covariate values are shown as red dots and the posterior distribution shown as a violin plot where the width of the violin is proportional to the posterior density. The posterior mean is shown in blue and the posterior median is shown in orange. In general, the posterior distributions are doing a good job of estimating the unobserved covariate. For observations where the model is not performing as well (e.g. observations 2, 4, 22), there is still some of the multi-modal posterior mass covering the unobserved covariate value despite the posterior mean/median being far from the simulated value. Thus, the mean/median can be a poor summary of the posterior distribution leading to reduced performance on metrics like MSPE and MAE.

```
## sorted to increasing values for ease of display
idx <- order(dat$X_pred)
## randomly choose 25 observations to display
n_plot <- 25
plot_idx <- sort(sample(idx, n_plot))
n_samples <- length(pred$X[, 1])

sim_df <- data.frame(
  Covariate   = c(pred$X[, idx[plot_idx]]),
  Mean        = rep(apply(pred$X[, idx[plot_idx]], 2, mean), each = n_samples),
  Median      = rep(apply(pred$X[, idx[plot_idx]], 2, median), each = n_samples),
  Observation = factor(rep(1:n_plot, each = n_samples )),
  truth       = rep(dat$X_pred[idx[plot_idx]], each = n_samples))

ggplot(sim_df, aes(Observation, Covariate)) +
  geom_violin(position="identity") +
  geom_point(aes(Observation, truth), color="red") +
  geom_point(aes(Observation, Mean), color="blue") +
  geom_point(aes(Observation, Median), color="orange") +
  scale_x_discrete(breaks=seq(5, n_plot, 5)) +
  labs(x="Observation", y="Unobserved Covariate") +
    ggtitle("MVGP prediction for MVGP simulated data")
```

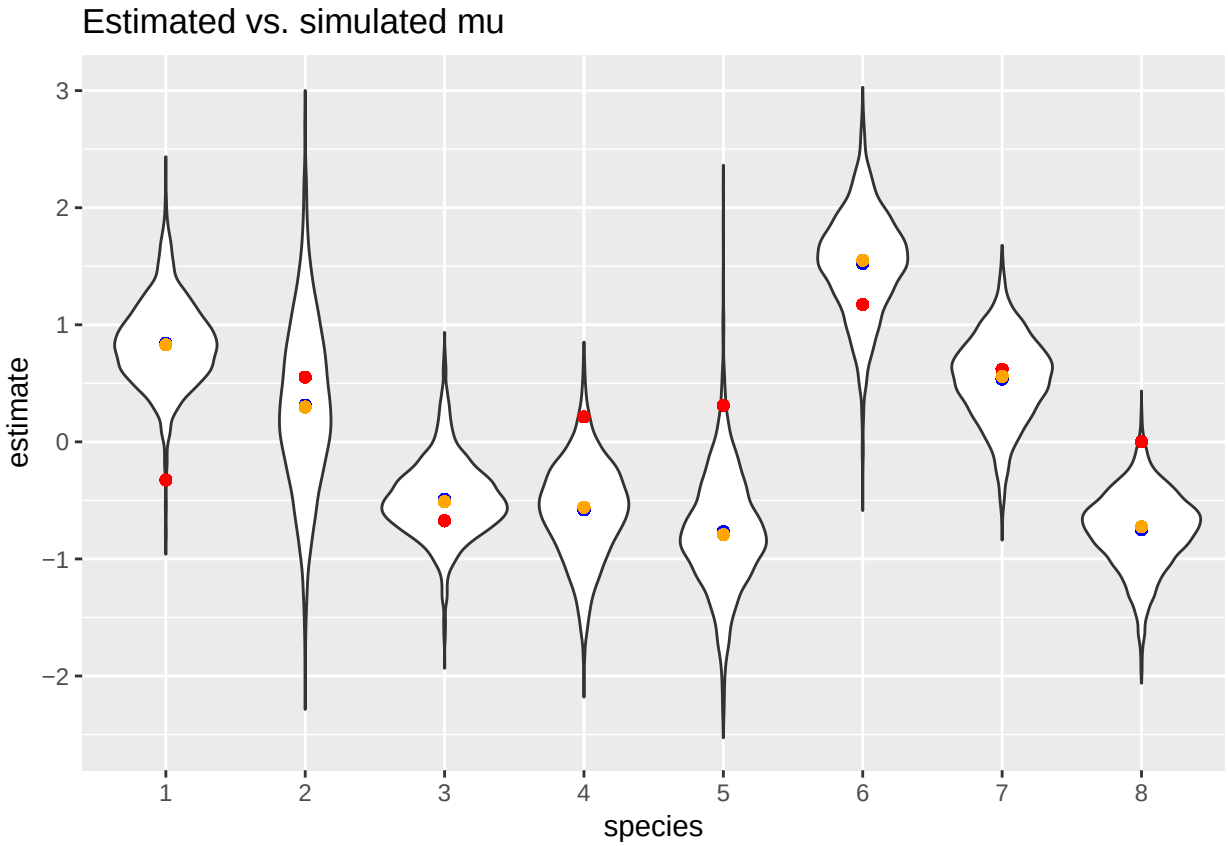


S2.2.5 Posterior estimates for simulated parameters

Finally, we compare the posterior estimates for the different families of parameters below. The simulated parameters fall within the posterior distribution estimates for almost every parameter indicating the model is accurately recovering the simulated parameters. The simulated values are shown in red dots and the posterior distribution shown as a violin plot where the width of the violin is proportional to the posterior density. The posterior mean is shown in blue and the posterior median is shown in orange.

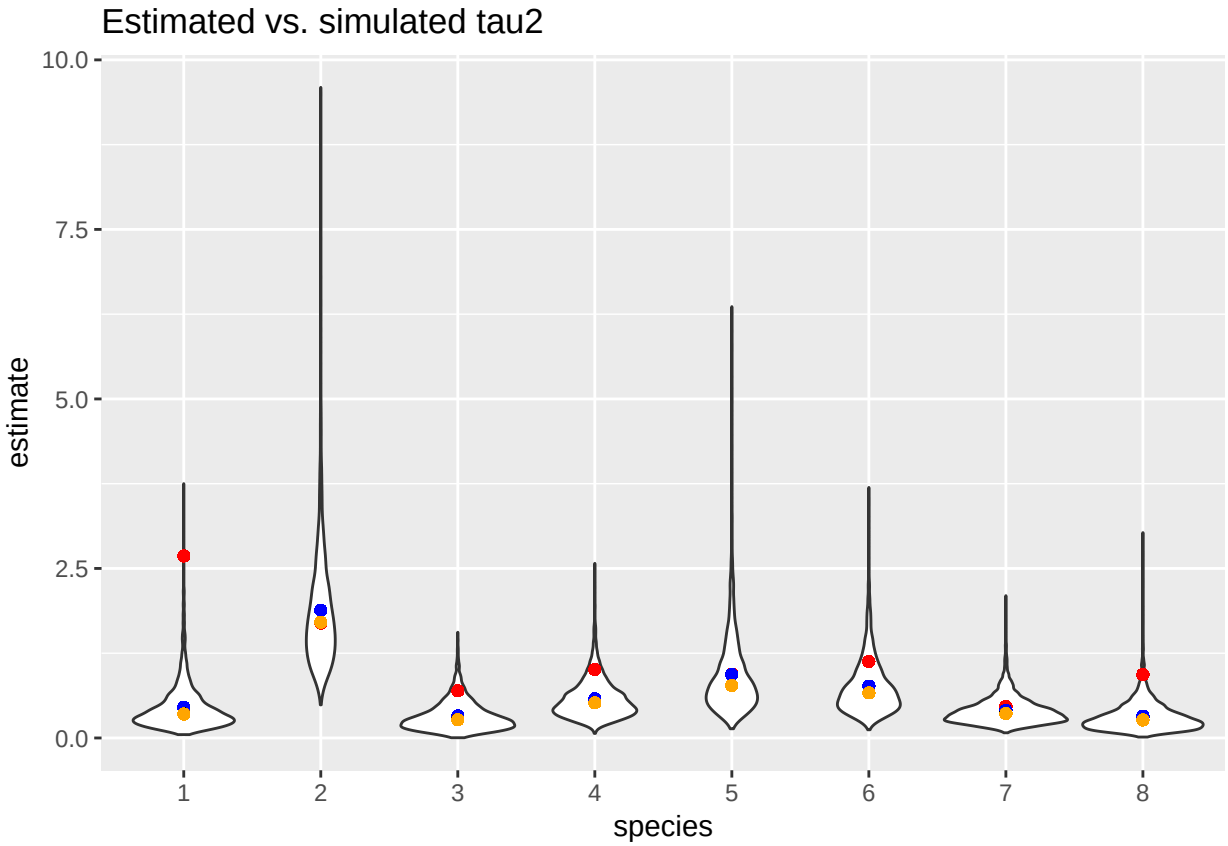
S2.2.5.1 Posterior estimates for the mean μ

```
mu_plot <- data.frame(
  species = as.factor(rep(1:d, each = n_samples)),
  estimate = c(mu_post),
  mean     = rep(apply(mu_post, 2, mean), each = n_samples),
  median   = rep(apply(mu_post, 2, median), each = n_samples),
  truth = rep(c(dat$mu), each = n_samples))

ggplot(mu_plot, aes(x = species, y = estimate)) +
  geom_violin() +
  geom_point(aes(x = species, y = truth), color = "red") +
  geom_point(aes(x = species, y = mean), color = "blue") +
  geom_point(aes(x = species, y = median), color = "orange") +
  ggtitle("Estimated vs. simulated mu")
```



S2.2.5.2 Posterior estimates for the functional variances τ^2

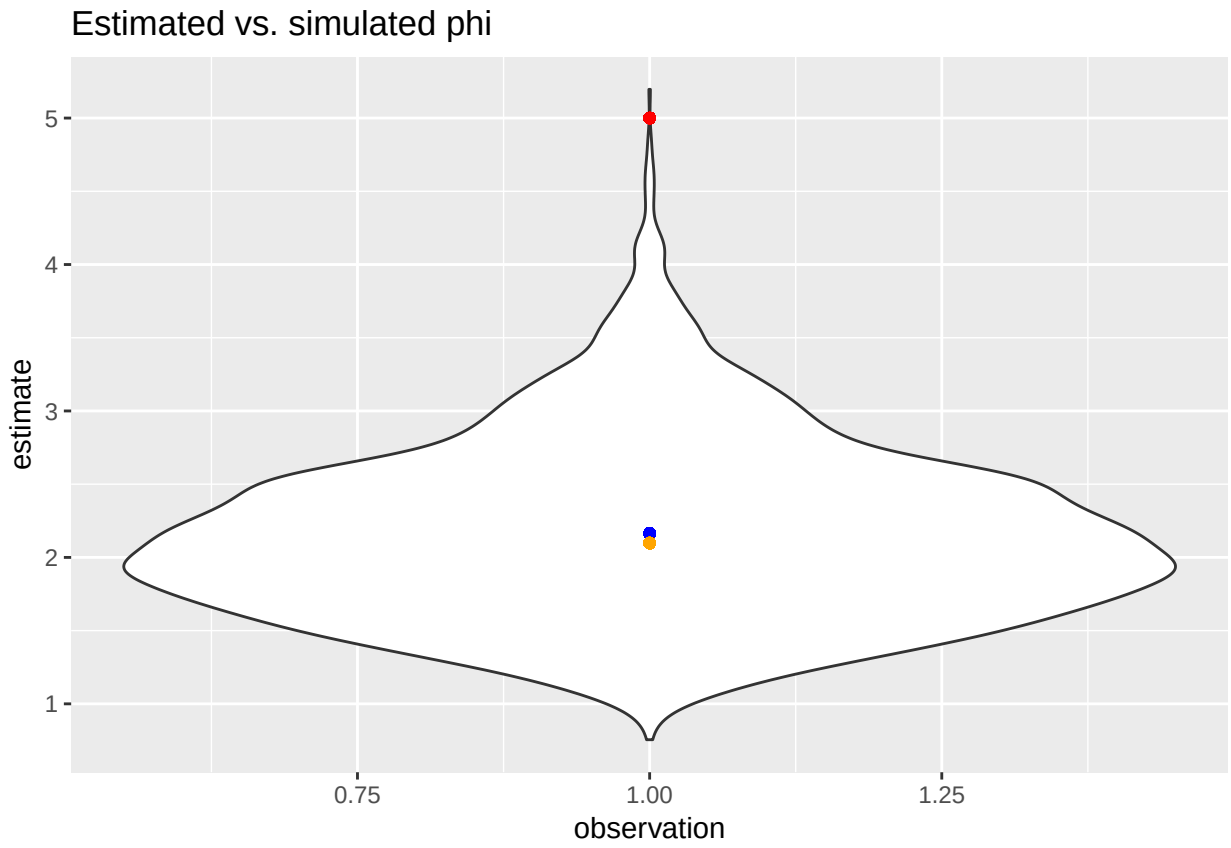
```
tau2_plot <- data.frame(
  species = as.factor(rep(1:d, each = n_samples)),
  estimate = c(tau2_post),
  mean     = rep(apply(tau2_post, 2, mean), each = n_samples),
  median   = rep(apply(tau2_post, 2, median), each = n_samples),
  truth = rep(c(dat$tau_multiplicative^2), each = n_samples))

ggplot(tau2_plot, aes(x = species, y = estimate)) +
  geom_violin() +
  geom_point(aes(x = species, y = truth), color = "red") +
  geom_point(aes(x = species, y = mean), color = "blue") +
  geom_point(aes(x = species, y = median), color = "orange") +
  ggtitle("Estimated vs. simulated tau2")
```



S2.2.5.3 Posterior estimate for the spatial range parameter ϕ

The estimate for the spatial range parameter ϕ is not being consistently estimated, but this is to expected [Zhang, 2004].

```
phi_plot <- data.frame(
  observation = rep(1, n_samples),
  estimate = c(phi_post),
  mean     = rep(mean(phi_post), each = n_samples),
  median   = rep(median(phi_post), each = n_samples),
  truth = rep(c(dat$phi), each = n_samples))

ggplot(phi_plot, aes(x = observation, y = estimate)) +
  geom_violin() +
  geom_point(aes(x = observation, y = truth), color = "red") +
  geom_point(aes(x = observation, y = mean), color = "blue") +
  geom_point(aes(x = observation, y = median), color = "orange") +
  ggtitle("Estimated vs. simulated phi")
```

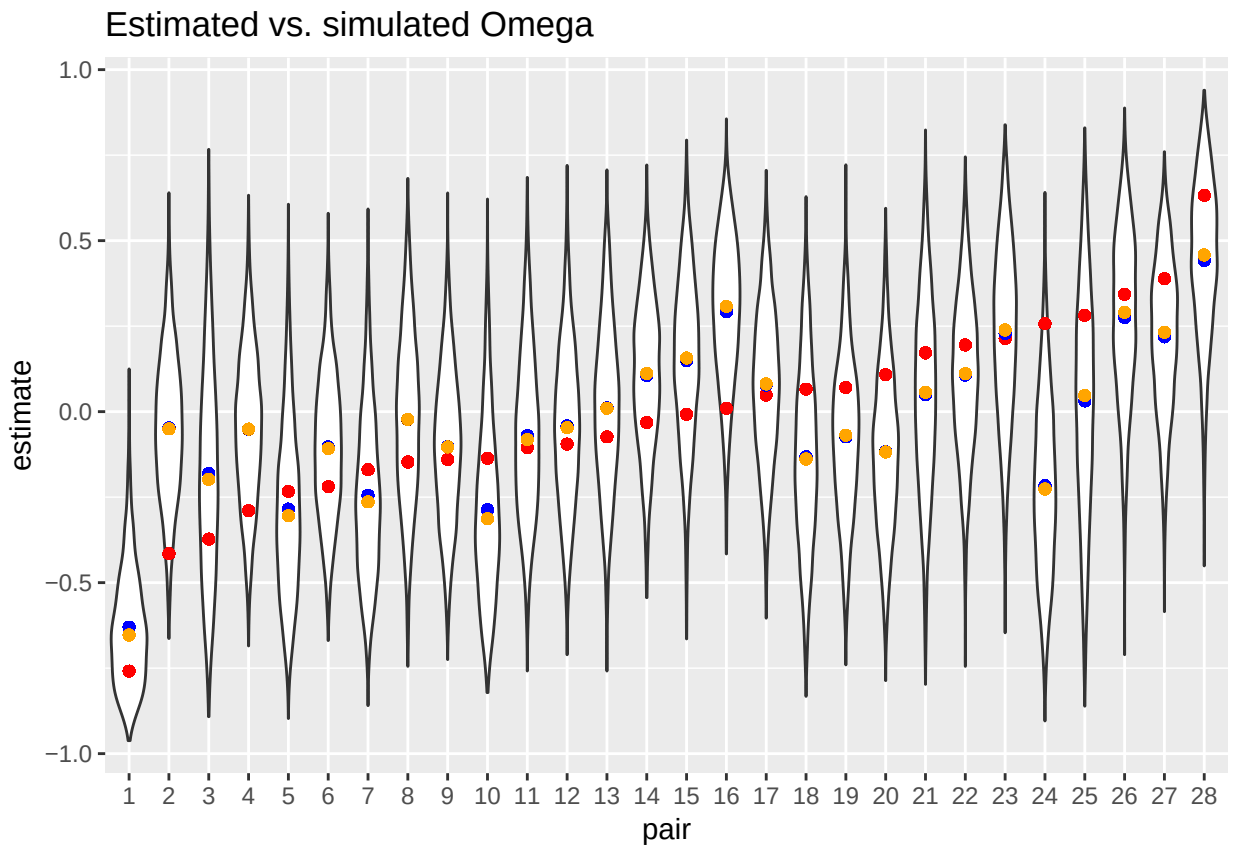


S2.2.5.4 Posterior estimates of the simulated functional correlations Ω

Here we show the posterior distribution for each of the estimated functional correlations.

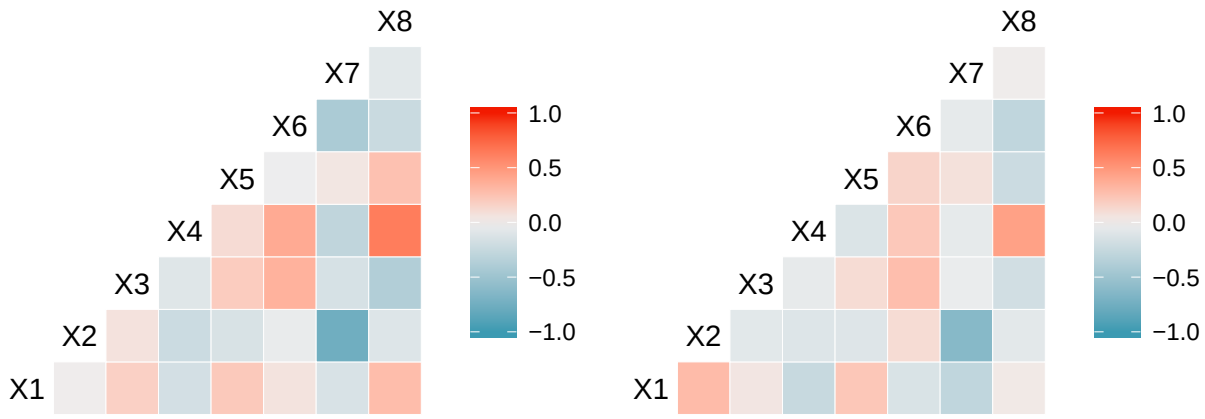
```
Omega_idx <- lower.tri(diag(d))

Omega_post <- array(0, dim = c(n_samples, d, d))
Omega_post_estimates <- matrix(0, n_samples, sum(Omega_idx))
for (i in 1:n_samples) {
  Omega_post[i, , ] <- t(R_post[i, , ]) %*% R_post[i, , ]
  Omega_post_estimates[i, ] <- Omega_post[i, , ][Omega_idx]
}

Omega <- t(dat$R_multiplicative) %*% dat$R_multiplicative
Omega_estimates <- (Omega)[Omega_idx]
Omega_order <- order(Omega_estimates)

Omega_plot <- data.frame(
  pair = as.factor(rep(1:(d * (d - 1) / 2), each = n_samples)),
  estimate = c(Omega_post_estimates[, Omega_order]),
  mean     = rep(apply(Omega_post_estimates, 2, mean)[Omega_order],
                 each = n_samples),
  median   = rep(apply(Omega_post_estimates, 2, median)[Omega_order],
                 each = n_samples),
  truth = rep(c(Omega_estimates[Omega_order]), each = n_samples))
```

```
ggplot(Omega_plot, aes(x = pair, y = estimate)) +
  geom_violin() +
  geom_point(aes(x = pair, y = truth), color = "red") +
  geom_point(aes(x = pair, y = mean), color = "blue") +
  geom_point(aes(x = pair, y = median), color = "orange") +
  ggtitle("Estimated vs. simulated Omega")
```



Below we show the simulated functional correlations along with the posterior mean estimates of the functional correlations. Below, we see that the MVGP model is capable of reconstructing the general structure of the functional covariance matrix.

```
Omega_post_mean <- apply(Omega_post, c(2, 3), mean)

multiplot(ggcorr(data=NULL, cor_matrix=cov2cor(Omega)) +
            ggtitle("Simulated Correlation"),
          ggcorr(data=NULL, cor_matrix=Omega_post_mean) +
            ggtitle("Estimated Posterior Mean Correlation"),
          cols=2)
```



S2.2.6 Fitting the GAM model

The GAM model is a simplification to the full MVGP model. The `BayesComposition` package has an option for fitting the GAM model. We fit the model for 200,000 MCMC iterations, discarding the first 50,000 iterations with adaptive Metropolis-Hastings proposals as burn in and thinning every 150 iterations. The model is run for 4 chains resulting in 4,000 posterior samples. The GAM model was fit using a cubic B-spline basis with 10 degrees of freedom and hierarchical pooling priors on the B-spline coefficients β using a log-link function.

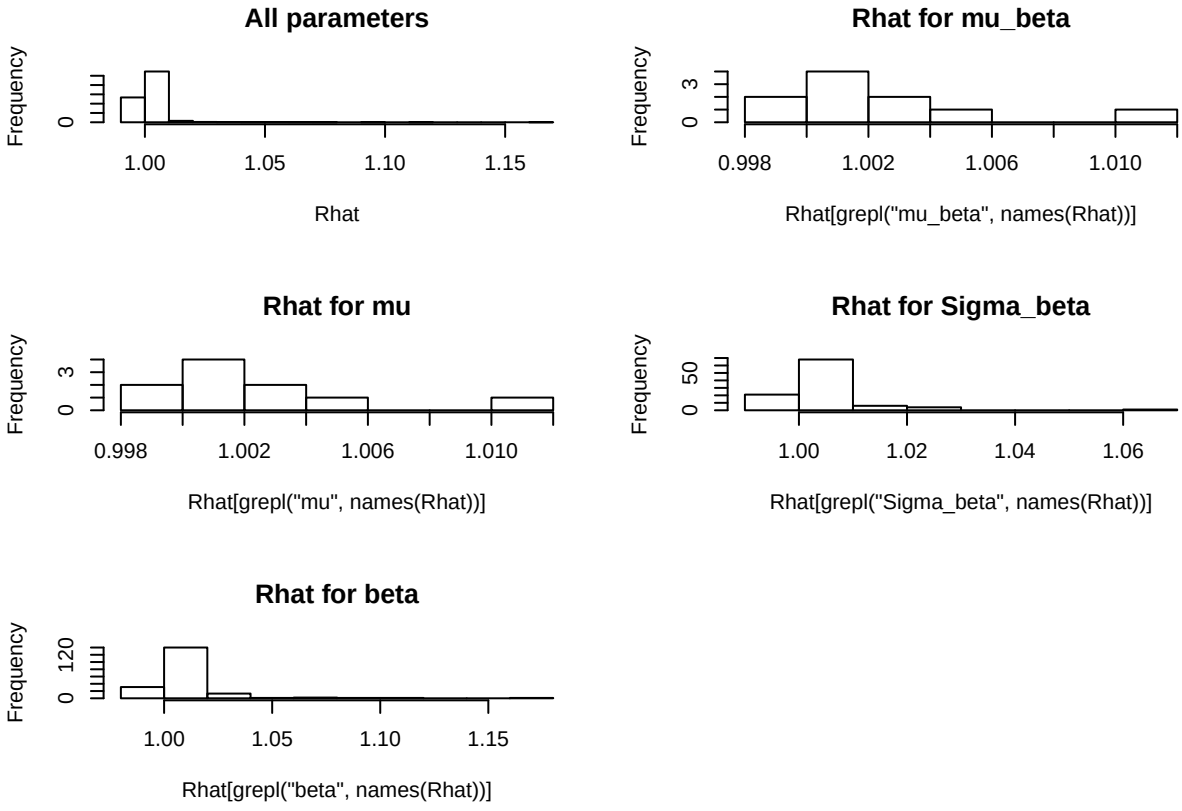
```
## define the model parameters for the GAM model
params <- list(
  n_adapt                    = 15000,
  n_mcmc                     = 150000,
  n_thin                     = 150,
  likelihood                 = "dirichlet-multinomial",
  function_type              = "basis",
  multiplicative_correlation = FALSE,
  additive_correlation       = FALSE,
  n_chains                   = 4,
  n_cores                    = 4,
  df                         = 10)

if (file.exists(paste0(save_directory,  "sim-mvgp-fit-gam.RData"))) {
  load(paste0(save_directory, "sim-mvgp-fit-gam.RData"))
} else {
  ## potentially long running MCMC code
  out_gam <- fit_compositional_data(
    y                  = dat$y,
    X                  = dat$X,
    params             = params,
    progress_directory = progress_directory,
    progress_file      = "sim-mvgp-fit-gam.txt")
  ## save the file
  save(out_gam, file = paste0(save_directory, "sim-mvgp-fit-gam.RData"))
}
```

S2.2.7 GAM convergence diagnostics

After fitting the model, the posterior samples are generated and MCMC convergence is assessed using the Gelman-Rubin $\hat{R}$ statistic. We see the distribution of $\hat{R}$ statistics is close to 1 with the largest $\hat{R} = 1.1631908 \lessapprox 1.1$ at an acceptable value (Gelman et al. [2013], pp.287).

```
## extract posterior samples
samples_gam <- extract_compositional_samples(out_gam)
mu_post <- samples_gam$mu
alpha_post <- samples_gam$alpha
beta_post <- samples_gam$beta
mu_beta_post <- samples_gam$mu_beta
Sigma_beta_post <- samples_gam$Sigma_beta


n_samples <- nrow(mu_post)

## Calculate Gelman-Rubin convergence statistic
Rhat <- make_gelman_rubin(out_gam)
layout(matrix(1:6, 3, 2))
hist(Rhat, main="All parameters")
hist(Rhat[grepl("mu", names(Rhat))], main = "Rhat for mu")
hist(Rhat[grepl("beta", names(Rhat))], main = "Rhat for beta")
hist(Rhat[grepl("mu_beta", names(Rhat))], main = "Rhat for mu_beta")
hist(Rhat[grepl("Sigma_beta", names(Rhat))], main = "Rhat for Sigma_beta")
Rhat[!is.finite(Rhat)] <- NA
max(unlist(na.omit(Rhat)))
```

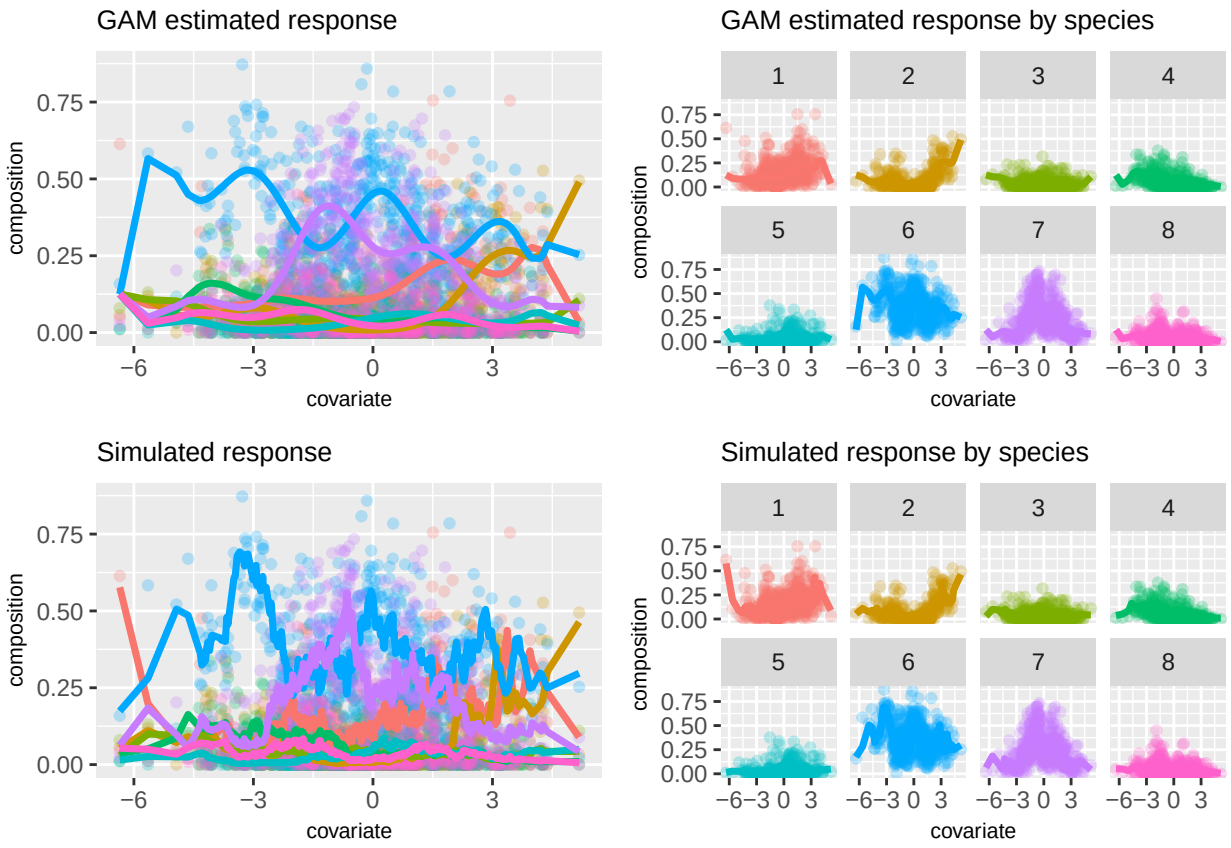
```
## [1] 1.163191
```



S2.2.8 GAM functional response estimation

We compare how well the GAM model reconstructs the simulated functional relationships below. The GAM model produces a smoother functional form than the MVGP model, but still reproduces the major functional features of the MVGP simulated data.

```
alpha_post_mean <- apply(alpha_post, c(2, 3), mean)

p_alpha_post_mean <- t(sapply(1:N, function(i) {
  alpha_post_mean[i, ] / sum(alpha_post_mean[i, ])
}))

fitPlotData <- data.frame(species=as.factor(rep(1:d, each=N)),
                          count=c(y_prop),
                          depth=rep(dat$X, times=d),
                          alpha=c(p_alpha_post_mean))

g1_gam_post <- ggplot(fitPlotData, aes(x=depth, y=count, color=species, group=species)) +
  geom_point(alpha=0.25) +
  theme(legend.position="none",
        title = element_text(size=8)) +
  ggtitle("GAM estimated response") +
  labs(x = "covariate", y="composition") +
  geom_line(aes(x=depth, y=alpha, col = species), fitPlotData, lwd=1.25)

g2_gam_post <- ggplot(fitPlotData, aes(x=depth, y=count, color=species, group=species)) +
  geom_point(alpha=0.25) +
  theme(legend.position="none",
        title = element_text(size=8)) +
  ggtitle("GAM estimated response by species") +
  labs(x = "covariate", y="composition") +
  geom_line(aes(x=depth, y=alpha, col = species), fitPlotData, lwd=1.25) +
  facet_wrap( ~ species, ncol = 4)
multiplot(g1_gam_post, g2_gam_post, gsim1, gsim2, cols=2)
```



S2.2.9 Generate GAM predictions

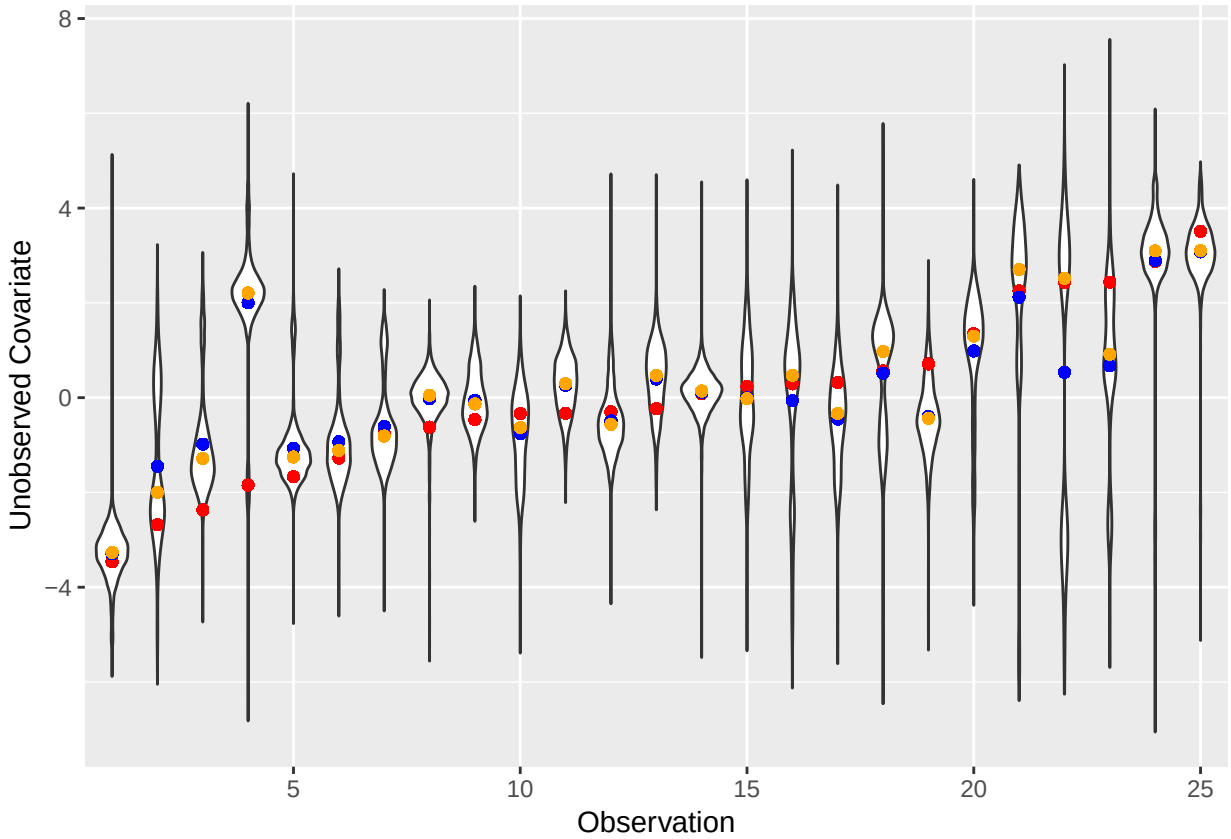
Using the elliptical slice sampler [Murray et al., 2010], we generate posterior predictions for the unobserved covariates using the posterior samples estimated from the GAM calibration model. These estimates can be generated either jointly with the calibration model or estimated using a two-stage approach as presented here. We have found, there is little practical difference in model performance between joint and two-stage estimation and follow the convention in the transfer function literature of using two-stage estimation.

```
## Note, there might be some initial warnings about ESS shrunk to the
##    current position for the first few iterations. This is not a
##    major concern as long as the warnings don't continue.
if (file.exists(paste0(save_directory, "sim-mvgp-predict-gam.RData"))) {
  load(paste0(save_directory, "sim-mvgp-predict-gam.RData"))
} else {
  pred_gam <- predict_compositional_data(
    dat$y_pred,
    dat$X,
    params,
    samples_gam,
    progress_directory,
    "sim-mvgp-predict-gam.txt")
  save(pred_gam, file = paste0(save_directory, "sim-mvgp-predict-gam.RData"))
}
```

S2.2.10 Plot GAM predictions

The predictions for 25 randomly chosen missing covariate observations are shown below. The simulated covariate values are shown as red dots and the posterior distribution shown as a violin plot where the width of the violin is proportional to the posterior density. The posterior mean is shown in blue and the posterior median is shown in orange. In general, the posterior distributions are doing a good job of estimating the unobserved covariate. Notice that there is still multi-modality in the posterior estimates.

```
## plot the same 25 observations as the MVGP model
n_samples <- length(pred_gam$X[, 1])

sim_gam_df <- data.frame(
  Covariate   = c(pred_gam$X[, idx[plot_idx]]),
  Mean        = rep(apply(pred_gam$X[, idx[plot_idx]], 2, mean), each = n_samples),
  Median      = rep(apply(pred_gam$X[, idx[plot_idx]], 2, median), each = n_samples),
  Observation = factor(rep(1:n_plot, each = n_samples )),
  truth       = rep(dat$X_pred[idx[plot_idx]], each = n_samples))

ggplot(sim_gam_df, aes(Observation, Covariate)) +
  geom_violin(position="identity") +
  geom_point(aes(Observation, truth), color="red") +
  geom_point(aes(Observation, Mean), color="blue") +
  geom_point(aes(Observation, Median), color="orange") +
  scale_x_discrete(breaks=seq(5, n_plot, 5)) +
  labs(x="Observation", y="Unobserved Covariate")
```



S2.3 Fitting the BUMMER model

The `BayesComposition` package has an option for fitting the BUMMER model. We fit the model for 200,000 MCMC iterations, discarding the first 50,000 iterations with adaptive Metropolis-Hastings proposals as burn in and thinning every 150 iterations. The model is run for 4 chains resulting in 4000 posterior samples.

```
## define the model parameters for the BUMMER model
params <- list(
  n_adapt                    = 50000,
  n_mcmc                     = 150000,
  n_thin                     = 150,
  likelihood                 = "dirichlet-multinomial",
  function_type              = "bummer",
  n_chains                   = 4,
  n_cores                    = 4)

if (file.exists(paste0(save_directory,  "sim-mvgp-fit-bummer.RData"))) {
  load(paste0(save_directory, "sim-mvgp-fit-bummer.RData"))
} else {
  ## potentially long running MCMC code
  out_bummer <- fit_compositional_data(
    y                  = dat$y,
    X                  = dat$X,
    params             = params,
    progress_directory = progress_directory,
    progress_file      = "sim-mvgp-fit-bummer.txt")
  ## save the file
  save(out_bummer, file = paste0(save_directory, "sim-mvgp-fit-bummer.RData"))
}
```

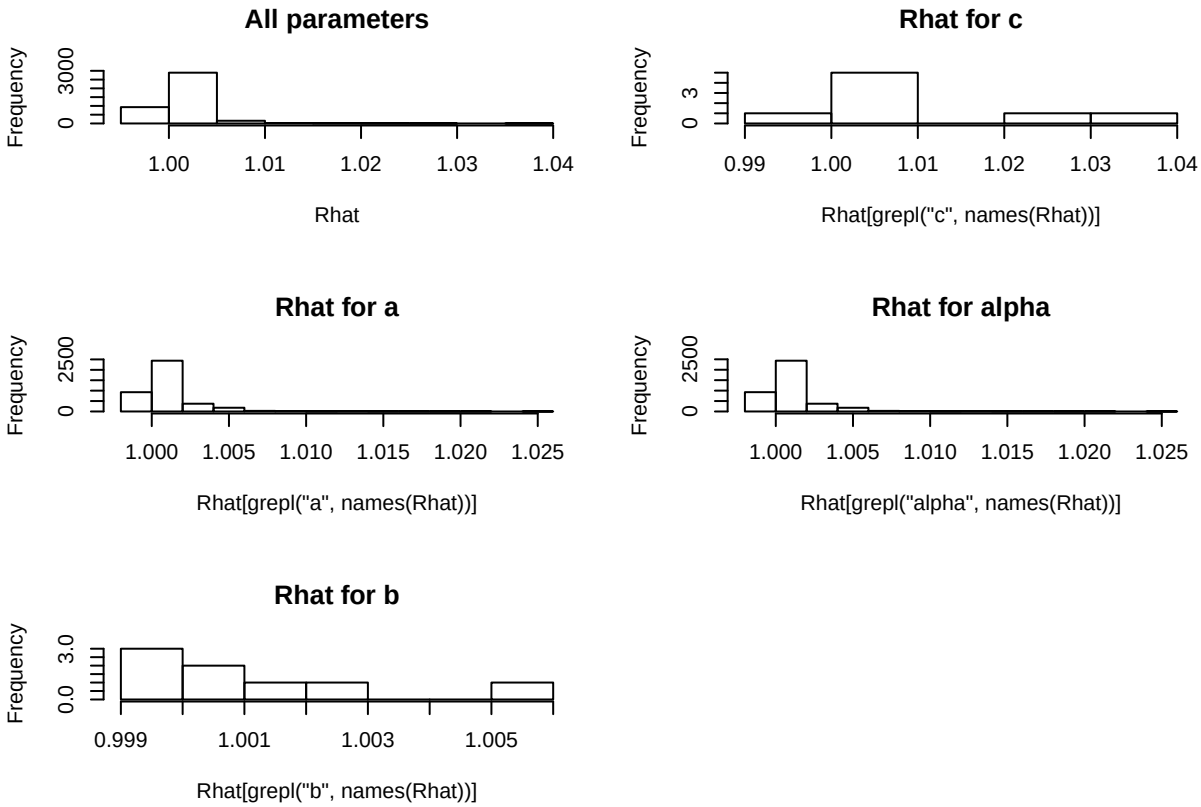
S2.3.1 BUMMER convergence diagnostics

After fitting the model, the posterior samples are generated and MCMC convergence is assessed using the Gelman-Rubin $\hat{R}$ statistic. We see the distribution of $\hat{R}$ statistics is close to 1 with the largest $\hat{R} = 1.0367496 \leq 1.1$ at an acceptable value (Gelman et al. [2013], pp.287).

```
## extract posterior samples
samples_bummer <- extract_compositional_samples(out_bummer)
a_post <- samples_bummer$a
b_post <- samples_bummer$b
c_post <- samples_bummer$c
alpha_post <- samples_bummer$alpha

n_samples <- nrow(a_post)

## Calculate Gelman-Rubin convergence statistic
Rhat <- make_gelman_rubin(out_bummer)
layout(matrix(1:6, 3, 2))
hist(Rhat, main="All parameters")
hist(Rhat[grepl("a", names(Rhat))], main = "Rhat for a")
hist(Rhat[grepl("b", names(Rhat))], main = "Rhat for b")
hist(Rhat[grepl("c", names(Rhat))], main = "Rhat for c")
hist(Rhat[grepl("alpha", names(Rhat))], main = "Rhat for alpha")
```

```
Rhat[!is.finite(Rhat)] <- NA
max(unlist(na.omit(Rhat)))
```

```
## [1] 1.03675
```

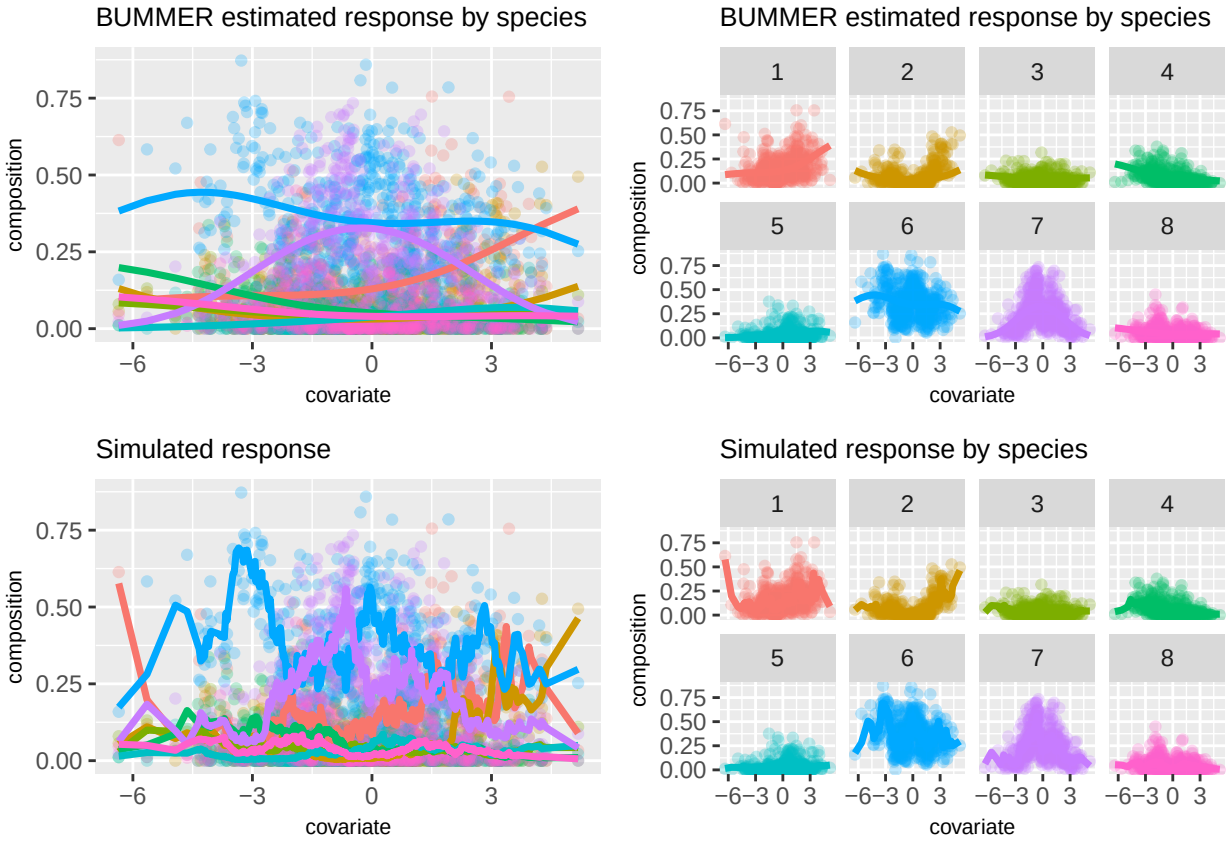


S2.3.2 BUMMER functional response estimation

We compare how well the BUMMER model reconstructs the simulated functional relationships below. The BUMMER model produces a much smoother functional form than the MVGP and GAM models and fails to capture the functional responses of the simulated MVGP data. The BUMMER model can only reliably estimate the mean absolute abundance averaged over the covariate space and fails to reconstruct the simulated functional response.

```
alpha_post_mean <- apply(alpha_post, c(2, 3), mean)

p_alpha_post_mean <- t(sapply(1:N, function(i) {
  alpha_post_mean[i, ] / sum(alpha_post_mean[i, ])
}))

fitPlotData <- data.frame(species=as.factor(rep(1:d, each=N)),
                          count=c(y_prop),
                          depth=rep(dat$X, times=d),
                          alpha=c(p_alpha_post_mean))

g1_gam_post <- ggplot(fitPlotData, aes(x=depth, y=count, color=species, group=species)) +
  geom_point(alpha=0.25) +
  theme(legend.position="none",
        title = element_text(size=8)) +
```

```
  ggtitle("BUMMER estimated response by species") +
  labs(x = "covariate", y="composition") +
  geom_line(aes(x=depth, y=alpha, col = species), fitPlotData, lwd=1.25)

g2_gam_post <- ggplot(fitPlotData, aes(x=depth, y=count, color=species, group=species)) +
  geom_point(alpha=0.25) +
  theme(legend.position="none",
        title = element_text(size=8)) +
  ggtitle("BUMMER estimated response by species") +
  labs(x = "covariate", y="composition") +
  geom_line(aes(x=depth, y=alpha, col = species), fitPlotData, lwd=1.25) +
  facet_wrap( ~ species, ncol = 4)
multiplot(g1_gam_post, g2_gam_post, gsim1, gsim2, cols=2)
```



S2.3.3 Generate BUMMER predictions

Using the elliptical slice sampler [Murray et al., 2010], we generate posterior predictions for the unobserved covariates using the posterior samples estimated from the BUMMER calibration model. These estimates can be generated either jointly with the calibration model or estimated using a two-stage approach as presented here. We have found, there is little practical difference in model performance between joint and two-stage estimation and follow the convention in the transfer function literature of using two-stage estimation.

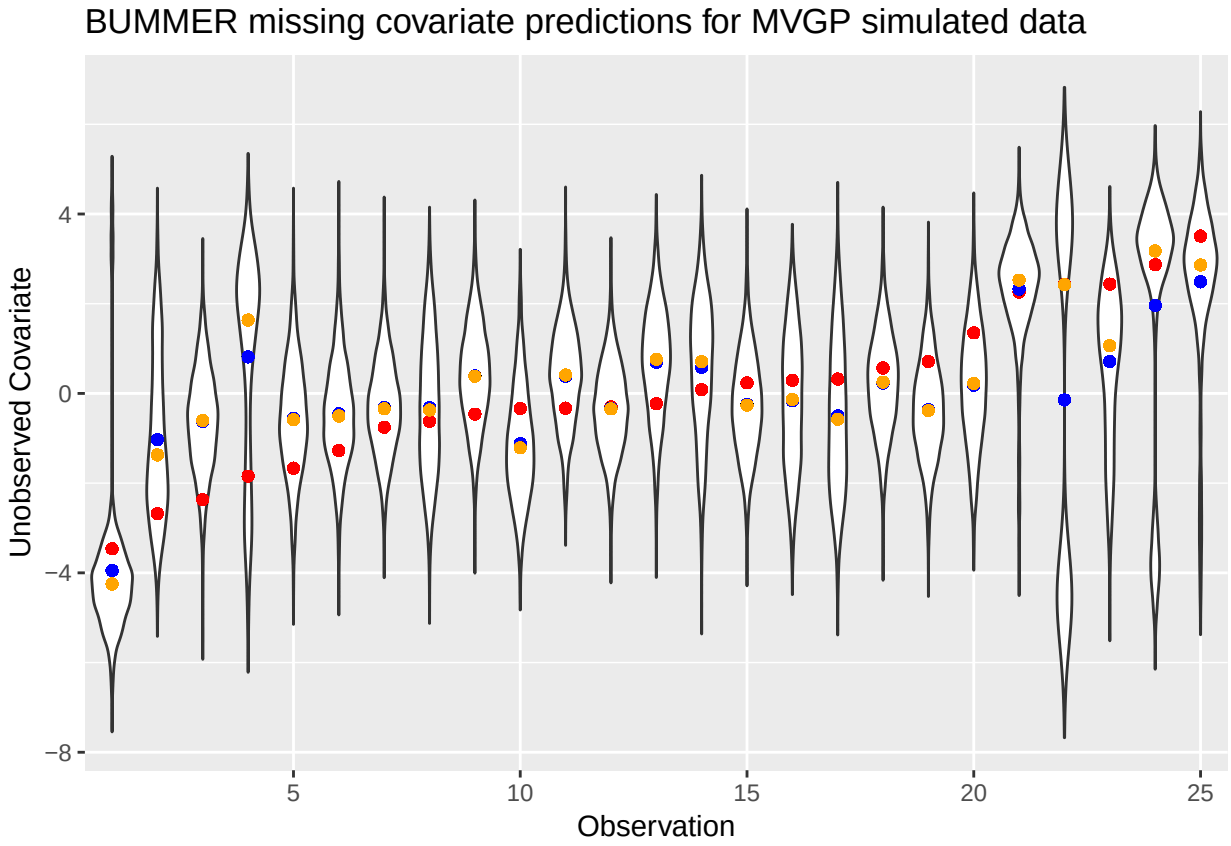
```
## Note, there might be some initial warnings about ESS shrunk to the
##    current position for the first few iterations. This is not a
##    major concern as long as the warnings don't continue.
if (file.exists(paste0(save_directory, "sim-mvgp-predict-bummer.RData"))) {
```

```
  load(paste0(save_directory, "sim-mvgp-predict-bummer.RData"))
} else {
  pred_bummer <- predict_compositional_data(
    dat$y_pred,
    dat$X,
    params,
    samples_bummer,
    progress_directory,
    "sim-mvgp-predict-bummer.txt")
  save(pred_bummer, file = paste0(save_directory, "sim-mvgp-predict-bummer.RData"))
}
```

S2.3.4 Plot BUMMER predictions

The predictions for 25 randomly chosen missing covariate observations are shown below. The simulated covariate values are shown as red dots and the posterior distribution shown as a violin plot where the width of the violin is proportional to the posterior density. The posterior mean is shown in blue and the posterior median is shown in orange. In general, the posterior distributions are doing a good job of estimating the unobserved covariate. Even in the BUMMER model there is still some evidence of multi-modality.

```
## plot the same 25 observations as the MVGP model
n_samples <- length(pred_gam$X[, 1])

sim_bummer_df <- data.frame(
  Covariate   = c(pred_bummer$X[, idx[plot_idx]]),
  Mean        = rep(apply(pred_bummer$X[, idx[plot_idx]], 2, mean), each = n_samples),
  Median      = rep(apply(pred_bummer$X[, idx[plot_idx]], 2, median), each = n_samples),
  Observation = factor(rep(1:n_plot, each = n_samples )),
  truth       = rep(dat$X_pred[idx[plot_idx]], each = n_samples))

ggplot(sim_bummer_df, aes(Observation, Covariate)) +
  geom_violin(position="identity") +
  geom_point(aes(Observation, truth), color="red") +
  geom_point(aes(Observation, Mean), color="blue") +
  geom_point(aes(Observation, Median), color="orange") +
  scale_x_discrete(breaks=seq(5, n_plot, 5)) +
  labs(x="Observation", y="Unobserved Covariate") +
  ggtitle("BUMMER missing covariate predictions for MVGP simulated data")
```



S2.4 Fitting the transfer function models to the simulated data

Below we fit the transfer function models MAT, WA, and MLRC to the simulated data and evaluate the scoring statistics for each model.

```
if (file.exists(paste0(save_directory, "sim-mvgp-all-predictions.RData"))) {
  load(paste0(save_directory, "sim-mvgp-all-predictions.RData"))
} else {
X_train <- dat$X
X_test <- dat$X_pred
y_train <- dat$y
y_train_prop <- y_train
y_test <- dat$y_pred
y_test_prop <- y_test

## convert from counts to proportions
for (i in 1:N) {
  y_train_prop[i, ] <- y_train_prop[i, ] / sum(y_train_prop[i, ])
}
for (i in 1:N_pred) {
  y_test_prop[i, ] <- y_test_prop[i, ] / sum(y_test_prop[i, ])
}
colnames(y_train_prop) <- letters[1:d]
colnames(y_test_prop) <- letters[1:d]

##
```

```
## evaluate predictive ability for MVGP
##

CRPS_MVGP <- makeCRPS(pred$X, X_test, n_samples)
MSPE_MVGP <- (apply(pred$X, 2, mean) - X_test)^2
MAE_MVGP <- abs(apply(pred$X, 2, median) -  X_test)
X_025 <- apply(pred$X, 2, quantile, prob = 0.025)
X_975 <- apply(pred$X, 2, quantile, prob = 0.975)
coverage_MVGP <- (X_test >= X_025) & (X_test <= X_975)

##
## evaluate predictive ability for GAM
##

CRPS_GAM <- makeCRPS(pred_gam$X, X_test, n_samples)
MSPE_GAM <- (apply(pred_gam$X, 2, mean) - X_test)^2
MAE_GAM <- abs(apply(pred_gam$X, 2, median) -  X_test)
X_025 <- apply(pred_gam$X, 2, quantile, prob = 0.025)
X_975 <- apply(pred_gam$X, 2, quantile, prob = 0.975)
coverage_GAM <- (X_test >= X_025) & (X_test <= X_975)

##
## evaluate predictive ability for MVGP
##

CRPS_BUMMER <- makeCRPS(pred_bummer$X, X_test, n_samples)
MSPE_BUMMER <- (apply(pred_bummer$X, 2, mean) - X_test)^2
MAE_BUMMER <- abs(apply(pred_bummer$X, 2, median) -  X_test)
X_025 <- apply(pred_bummer$X, 2, quantile, prob = 0.025)
X_975 <- apply(pred_bummer$X, 2, quantile, prob = 0.975)
coverage_BUMMER <- (X_test >= X_025) & (X_test <= X_975)

##
## evaluate predictive ability for WA
##

## WA reconstruction - subset to deal with all zero occurrence species
zeros_idx <- which(colSums(y_train_prop) == 0)
if (length(zeros_idx) > 0) {
  modWA <- rioja::WA(y_train_prop[, - zeros_idx], X_train)
  predWA <- predict(modWA, y_test_prop[, - zeros_idx], sse=TRUE, nboot=1000)
} else {
  ## no data to subset
  modWA <- rioja::WA(y_train_prop, X_train)
  predWA <- predict(modWA, y_test_prop, sse=TRUE, nboot=1000)
}

CRPS_WA <- abs(predWA$fit[, 1] - X_test)
MAE_WA <- abs(predWA$fit[, 1] - X_test)
MSPE_WA <- (predWA$fit[, 1] - X_test)^2
coverage_WA <-
  (X_test >= (predWA$fit[, 1] -
        2 * sqrt(predWA$v1.boot[, 1]^2 + predWA$v2.boot[1]^2))) &
```

```
  (X_test <= (predWA$fit[, 1] +
                2 * sqrt(predWA$v1.boot[, 1]^2 + predWA$v2.boot[1]^2)))


##
## evaluate predictive ability for MLRC
##

## MLRC reconstruction - subset to deal with all zero occurrence species
zeros_idx <- which(colSums(y_train_prop) == 0)
if (length(zeros_idx) > 0) {
  modMLRC <- rioja::MLRC(y_train_prop[, - zeros_idx], X_train)
  predMLRC <- predict(modMLRC, y_test_prop[, - zeros_idx],
                      sse=TRUE, nboot=1000)
} else {
  modMLRC <- rioja::MLRC(y_train_prop, X_train)
  predMLRC <- predict(modMLRC, y_test_prop, sse=TRUE, nboot=1000)
}
CRPS_MLRC <- abs(predMLRC$fit[, 1] - X_test)
MSPE_MLRC <- (predMLRC$fit[, 1] - X_test)^2
MAE_MLRC <- abs(predMLRC$fit[, 1] - X_test)
coverage_MLRC <-
  (X_test >= (predMLRC$fit[, 1] -
                2 * sqrt(predMLRC$v1.boot[, 1]^2 + predMLRC$v2.boot[1]^2))) &
  (X_test <= (predMLRC$fit[, 1] +
                2 * sqrt(predMLRC$v1.boot[, 1]^2 + predMLRC$v2.boot[1]^2)))


##
## evaluate predictive ability for MAT
##

## Modern analogue technique
modMAT <- rioja::MAT(as.data.frame(y_train_prop), X_train, lean = FALSE)
predMAT <- predict(modMAT, as.data.frame(y_test_prop), sse=TRUE, n.boot=1000)
CRPS_MAT <- abs(predMAT$fit[, 1] - X_test)
MSPE_MAT <- (predMAT$fit[, 1] - X_test)^2
MAE_MAT <- abs(predMAT$fit[, 1] - X_test)

coverage_MAT <-
  (X_test >= ( predMAT$fit.boot[, 2] -
                 2 * sqrt(predMAT$v1.boot[, 2]^2+ predMAT$v2.boot[2])) &
     (X_test <= (predMAT$fit.boot[, 2] +
                   2*  sqrt(predMAT$v1.boot[, 2]^2+ predMAT$v2.boot[2]))))

save(
  CRPS_MVGP, MSPE_MVGP, MAE_MVGP, coverage_MVGP,
  CRPS_GAM, MSPE_GAM, MAE_GAM, coverage_GAM,
  CRPS_BUMMER, MSPE_BUMMER, MAE_BUMMER, coverage_BUMMER,
  modWA, predWA, CRPS_WA, MAE_WA, MSPE_WA, coverage_WA,
  modMLRC, predMLRC, CRPS_MLRC, MSPE_MLRC, MAE_MLRC, coverage_MLRC,
  modMAT, predMAT, CRPS_MAT, MSPE_MAT, MAE_MAT, coverage_MAT,
    file = paste0(save_directory, "sim-mvgp-all-predictions.RData"))
```

```
}
```

S2.4.1 Prediction results

Finally, we generate the results from the simulation study. The results below show that for data simulated from the MVGP model, the MVGP model generates the best predictions across all metrics. The GAM model produces the next best predictions with BUMMER performing worse than MVGP and GAM across all metrics. The transfer function methods perform worse than MVGP and GAM with MAT performing similarly to BUMMER.

```
CRPS_out <- cbind(CRPS_MVGP, CRPS_GAM, CRPS_BUMMER,
                  CRPS_WA, CRPS_MAT, CRPS_MLRC)
MSPE_out <- cbind(MSPE_MVGP, MSPE_GAM, MSPE_BUMMER,
                  MSPE_WA, MSPE_MAT, MSPE_MLRC)
MAE_out <- cbind(MAE_MVGP, MAE_GAM, MAE_BUMMER,
                 MAE_WA, MAE_MAT, MAE_MLRC)
coverage_out <- cbind(coverage_MVGP, coverage_GAM, coverage_BUMMER,
                      coverage_WA, coverage_MAT, coverage_MLRC)
colnames(CRPS_out) <- c("MVGP", "GAM", "BUMMER", "WA", "MAT", "MLRC")
colnames(MAE_out) <- c("MVGP", "GAM", "BUMMER", "WA", "MAT", "MLRC")
colnames(MSPE_out) <- c("MVGP", "GAM", "BUMMER", "WA", "MAT", "MLRC")
colnames(coverage_out) <- c("MVGP", "GAM", "BUMMER", "WA", "MAT", "MLRC")

CRPS <- data.frame(t(apply(CRPS_out, 2, mean)))
MSPE <- data.frame(t(apply(MSPE_out, 2, mean)))
MAE <- data.frame(t(apply(MAE_out, 2, mean)))
coverage <- data.frame(100/(N_pred)*t(apply(coverage_out, 2, sum)))

sim_results <- t(rbind(CRPS, MSPE, MAE, coverage))
colnames(sim_results) <- c("CRPS", "MSPE", "MAE", "95% CI coverage")
## print the results for table 2
# print(xtable(sim_results, digits=4), file="~/mvgp/results/sim-dm.tex",
#       floating=FALSE)
kable(sim_results)
```

	CRPS	MSPE	MAE	95% CI coverage
MVGP	0.5161966	1.263711	0.6793399	96.0
GAM	0.5393735	1.337201	0.7112596	96.5
BUMMER	0.7197881	1.793720	1.0056881	96.0
WA	1.0962305	1.946718	1.0962305	96.0
MAT	0.9412925	1.681372	0.9412925	95.0
MLRC	1.3244593	3.305458	1.3244593	95.0

References

Andrew Gelman, Hal S Stern, John B Carlin, David B Dunson, Aki Vehtari, and Donald B Rubin. *Bayesian Data Analysis*. Chapman and Hall/CRC, 2013.

Iain Murray, Ryan Prescott Adams, and David J. C. MacKay. Elliptical slice sampling. In *AISTATS*, volume 13, pages 541–548, 2010.

Gareth O. Roberts and Jeffrey S. Rosenthal. Examples of adaptive MCMC. *Journal of Computational and Graphical Statistics*, 18(2):349–367, 2009.

Hao Zhang. Inconsistent estimation and asymptotically equal interpolations in model-based geostatistics. *Journal of the American Statistical Association*, 99(465):250–261, 2004.