Simulation

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12/10/2024

Simulation Example

This is an R Markdown document for the paper

Bayesian Spatio-temporal Small Area Modeling: A Case Study of Estimating Late-Stage Melanoma Incidence in Texas.

Let $t \in [T]$ denote the discrete time of interest, and let $i \in [M]$ represent the geographical units (e.g., counties). For each diagnosed individual $j \in [n_{it}]$ within area i at time t, let y_{itj} denote the stage of melanoma. Specifically, $Y_{itj} = 1$ if the individual is in late-stage melanoma, and $Y_{itj} = 0$ if the individual is in the early stage. At each time t, for each individual j in area i, let $\mathbf{x}_{itj} \in \mathbb{R}^{p+1}$ denote the corresponding unit-level covariates, and let $\mathbf{z}_{it} \in \mathbb{R}^q$ denote the area-level covariates. Additionally, the population is categorized into different strata $\{1, 2, \ldots, H\}$ based on cross-tabulated demographic variables such as sex and race/ethnicity. We use $h_{itj} \in [H]$ and g_{itj} to represent the stratum and the age, respectively, of the individual j in area i at time t.

The proposed model takes the following form:

$$y_{itj} \mid p_{itj} \sim \text{Bernoulli}(p_{itj}),$$

$$\theta_{itj} := \text{logit}(p_{itj}) = \mathbf{x}_{itj}^\top \boldsymbol{\beta} + \mathbf{z}_{it}^\top \boldsymbol{\alpha} + G_{itj} + \delta_i + \epsilon_{it},$$

where ϵ_{it} is a latent spatiotemporal process, δ_i is a latent area-level effect, and G_{itj} represents the effect of an individual's age g_{itj}, given the corresponding stratum h_{ij} at time t. Our focus is on estimating the regression coefficients $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)^\top$, $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_q)^\top$, as well as the age effect G across different times and strata.

1. Data generation

```
library(sp)
library(nimble)
library(splines2)
# Read Texas county data
load('Data/polygons_list_bycounty.RData')  # county_list, polygons_list_bycounty
load('Data/Adj_mat.RData')
Adj_mat = as.matrix(Adj_mat) # 254*254
source('Functions//Basis_functions.R')
```

```
n_it = 10  # number of samples in each county at each time
T = 10
num_group = 3
M = dim(Adj_mat)[1]
n = n_it*M*T*num_group
q = 20
q0 = 2

L = 8
degree = 3
J = 8

# Generete covariates
set.seed(0)
Z = array(rnorm(T*M*q), dim = c(T, M, q))
DATA = expand.grid(stage = rep(1, n_it), group = seq(num_group), county = seq(M), dxyear = seq(T))
DATA$age = runif(n)

county_design = DATA$county
h_design = DATA$group
t_design = DATA$dxyear
H = length(unique(h_design))

# Basis function
internal_nodes = as.vector(quantile(DATA$age,
                            probs = seq(0,1,length.out=J-degree+1)[-c(1,J-degree+1)]))
Phi = Bspline.Basis(DATA$age, r = J, knots = internal_nodes, degree = degree)
MI = array(0, dim = c(T, M, L))
for(t in 1:T){
    MI[t,,] = MoransI.Basis(cbind(matrix(1, M, 1), Z[t,,]), r = L, A = Adj_mat)
}


# Generate coefficients
alpha = c(rep(1,q0),rep(0,q-q0))

xi = array(1, dim = c(H, T, J))
for (h in 1:H) {  xi[h,,] = h  }
B = 0.8*diag(J)
sigmasq_xi = 0.001
for (h in 1:H) { for (t in 2:T){ for(i_J in 1:J){
    xi[h, t, i_J] = rnorm(1,  inprod(B[i_J, 1:J], xi[h, t - 1, 1:J]), sd = sqrt(sigmasq_xi))
}}}

eta = matrix(1, T, L)
A = 0.8*diag(L)
sigmasq_eta = 0.001
for (t in 2:T){for(i_L in 1:L){
    eta[t, i_L] = rnorm(1, inprod(A[i_L, 1:L], eta[t - 1, 1:L]), sd = sqrt(sigmasq_eta) )
}}

delta = rep(0, M)
```

```r
# Generate response
DATA$prob = rep(0, n)
for(i in 1:n){
    DATA$prob[i] = ilogit(inprod(Z[t_design[i],county_design[i],1:q], alpha[1:q]) +
                      inprod(Phi[i,1:J], xi[h_design[i], t_design[i], 1:J]) +
                      inprod(MI[t_design[i],county_design[i],1:L], eta[t_design[i], 1:L]) +
                      delta[county_design[i]])
    DATA$stage[i] = rbinom(1, 1, p = DATA$prob[i])
}
y = DATA$stage

save(DATA, Z, alpha, Phi, xi, MI, eta, delta, file = 'Data/data.RData')
```

2. Model Fitting

```r
nimbleOptions(MCMCusePredictiveDependenciesInCalculations = TRUE)

code <- nimbleCode({
  for(i in 1:n){
      y[i] ~ dbern(prob[i])
      prob[i] <- ilogit(inprod(Z[t_design[i],county_design[i],1:q], alpha[1:q]) +
                      inprod(Phi[i,1:J], xi[h_design[i], t_design[i], 1:J]) +
                      inprod(MI[t_design[i],county_design[i],1:L], eta[t_design[i], 1:L]) +
                      delta[county_design[i]])
  }


  # Age AR
  for (h in 1:H) {
    for(i_J in 1:J)  xi[h, 1, i_J] ~ dnorm(mu_xi[i_J], var = kappasq_1)
    for (t in 2:T){ for(i_J in 1:J){
          xi[h, t, i_J] ~ dnorm( inprod(B[i_J, 1:J], xi[h, t - 1, 1:J]), var = sigmasq_xi)
    }}
  }
  for(i_J in 1:J) mu_xi[i_J] ~ dnorm(0, var = kappasq_0)
  for(i_J in 1:J){
      B[i_J, i_J] ~ dnorm(1, var = kappasq_B)
      for(ii_J in (seq(from = 1, to = J)[-i_J])){  B[i_J, ii_J] ~ dnorm(0, var = kappasq_B) }
  }
  sigmasq_xi ~ dinvgamma(a_xi, b_xi)


  # Spatial AR
  for (t in 2:T){for(i_L in 1:L){
    eta[t, i_L] ~ dnorm( inprod(A[i_L, 1:L], eta[t - 1, 1:L]), var = sigmasq_eta)
  }}
  for(i_L in 1:L) eta[1, i_L] ~ dnorm(0, var = kappasq_2)
  for(i_L in 1:L){
      A[i_L, i_L] ~ dnorm(1, var = kappasq_A)
      for(ii_L in (seq(from = 1, to = L)[-i_L])){  A[i_L, ii_L] ~ dnorm(0, var = kappasq_A) }
  }
```

```
  sigmasq_eta ~ dinvgamma(a_eta, b_eta)

  # alpha S-and-S
  for (i_q in 1:q) {
    include[i_q] ~ dbern(0.5)  # Spike-and-slab prior
    alpha_latent[i_q] ~ dnorm(0, var = kappasq_alpha)
    alpha[i_q] <- alpha_latent[i_q] * include[i_q]
  }

  # prior for delta
  for(i in 1:M){
      delta[i] ~ dnorm(mu_delta, var = sigmasq_delta)
  }
  mu_delta ~ dnorm(0, var = 100)
  sigmasq_delta ~ dinvgamma(1, 1)


})

kappasq_alpha = 100
kappasq_0 = 100
kappasq_1 = 100
kappasq_B = 100
a_xi = 1
b_xi = 1
kappasq_2 = 100
kappasq_A = 100
a_eta = 1
b_eta = 1

constants <- list(
    n = n,
    T = T,
    M = M,
    q = q,
    J = J,
    L = L,
    H = H,
    h_design = h_design,
    t_design = t_design,
    county_design = county_design,
    Z = Z,
    Phi = Phi,
    MI = MI,
    kappasq_alpha = kappasq_alpha, # regression coeff
    kappasq_0 = kappasq_0, kappasq_1 = kappasq_1, kappasq_B = kappasq_B, a_xi = a_xi, b_xi = b_xi,
    kappasq_2 = kappasq_2, kappasq_A = kappasq_A, a_eta = a_eta, b_eta = b_eta
)

inits <- list(
    alpha_latent = rep(0, q), include = rep(1,q),
    xi = array(0, dim = c(H, T, J)), mu_xi = rep(0, J), sigmasq_xi = 1, B = diag(J),
    eta = matrix(0, T, L), sigmasq_eta = 1,  A = diag(L),
```

```
    mu_delta = 0, sigmasq_delta = 1, delta = rep(0, M)
)
data = list(
    y = y
)
model <- nimbleModel(code, constants = constants, data = data, inits = inits)


initInfo <- model$initializeInfo()
uninitializedNodes <- initInfo$uninitializedNodes
warnings <- initInfo$warnings
errors <- initInfo$errors
cat("\nWarnings:\n")
print(warnings)
cat("\nErrors:\n")
print(errors)


# Set up the MCMC configuration
mcmcConf <- configureMCMC(model)
mcmcConf$setMonitors('alpha_latent', 'alpha', 'xi', 'eta',
                     'include', 'delta', 'mu_delta', 'sigmasq_delta')
# Build and compile the MCMC
mcmc <- buildMCMC(mcmcConf)
Cmodel <- compileNimble(model)
Cmcmc <- compileNimble(mcmc, project = model)

n_batches <- 200
batch_size <- 200
n_batches_save = 40
num_thin <- 20
mcmc.out = runMCMC(Cmcmc, niter=batch_size*n_batches,
        nburnin=batch_size*(n_batches - n_batches_save),
        thin=num_thin, nchains=1, setSeed = TRUE, progressBar = TRUE)
# ===== Samplers =====
# RW sampler (594)
#   - eta[]  (80 elements)
#   - alpha_latent[]  (20 elements)
#   - xi[]  (240 elements)
#   - delta[]  (254 elements)
# conjugate sampler (140)
#   - mu_xi[]  (8 elements)
#   - B[]  (64 elements)
#   - sigmasq_xi
#   - A[]  (64 elements)
#   - sigmasq_eta
#   - mu_delta
#   - sigmasq_delta
# binary sampler (20)
#   - include[]  (20 elements)
# thin = 1: alpha, alpha_latent, delta, eta, include, mu_delta, sigmasq_delta, xi

samples_save = as.matrix(mcmc.out)
```

```r
# Calculate WAIC
waic_results = calculateWAIC(Cmcmc)
save(samples_save, waic_results, file = 'Data/MCMCsamples.RData')


## Prediction
## -----------## -----------## -----------## -----------## -----------## -----------
load(file = 'Data/MCMCsamples.RData')
num_save = batch_size * n_batches_save / num_thin
age_range = c(10,100)

# Designs for prediction
age_grid = seq(from = 20, to = 90, by = 5)
age_grid = (age_grid - age_range[1]) / (diff(age_range))
num_G = length(age_grid)
phi_grid = Bspline.Basis(age_grid, r = J, knots = internal_nodes, degree = degree)

# Posterior prediction
posterior_params = as.data.frame(samples_save)

# Extracting alpha vector
alpha <- as.matrix(posterior_params[,grep("^alpha", colnames(posterior_params))])

# Extracting 3-d array xi
xi <- array(0, dim = c(num_save, H, T, J))
for(h in 1:H) {
  for(t in 1:T) {
    for(j in 1:J) {
      xi[, h, t, j] <- as.matrix(posterior_params[,paste0("xi[", h,", ", t, ", ", j, "]")])
    }
  }
}

# Extracting matrix eta
eta <- array(0, dim = c(num_save, T, L))
for(t in 1:T) {
  for(l in 1:L) {
    eta[, t, l] <- as.matrix(posterior_params[,paste0("eta[", t, ", ", l, "]")])
  }
}

# Extracting delta
delta <- as.matrix(posterior_params[,grep("^delta", colnames(posterior_params))])

# county-level prediction
prob_summary_M_H_T_Age_MCMC = array(0, dim = c(num_save, M,H,T,num_G))
prob_summary_M_H_T_Age = array(0, dim = c(M,H,T,num_G))
prob_summary_M_H_T_Age_upper = array(0, dim = c(M,H,T,num_G))
prob_summary_M_H_T_Age_lower = array(0, dim = c(M,H,T,num_G))

# Make prediction
for(i in 1:M){
    temp_i = delta[, i, drop = FALSE]
```

```
    for (t in 1:T){
        temp_it =  temp_i + alpha[, 1:q]%*% as.vector(Z[t,i,1:q]) +
                                eta[, t, 1:L]%*%as.vector(MI[t,i,1:L])
        for(h in 1:H){for(i_age in 1:num_G){
            prob_summary_M_H_T_Age_MCMC[,i,h,t,i_age] =
                            as.vector(temp_it + xi[, h, t, 1:J]%*% as.vector(phi_grid[i_age, 1:J]))
        }}
    }
}
prob_summary_M_H_T_Age_MCMC = ilogit( prob_summary_M_H_T_Age_MCMC )
prob_summary_M_H_T_Age <- apply(prob_summary_M_H_T_Age_MCMC, c(2, 3, 4, 5), mean)
prob_summary_M_H_T_Age_upper <- apply(prob_summary_M_H_T_Age_MCMC,
                                            c(2, 3, 4, 5), quantile, probs = c(0.95))
prob_summary_M_H_T_Age_lower <- apply(prob_summary_M_H_T_Age_MCMC,
                                            c(2, 3, 4, 5), quantile, probs = c(0.05))
prob_summary_M_H_T_Age_average_mcmc <- apply(prob_summary_M_H_T_Age_MCMC, 1, mean)

# Make prediction to all individuals
Phi_Data = Bspline.Basis(DATA$age, r = J, knots = internal_nodes, degree = degree)
prob_summary_individuals_MCMC = matrix(0, num_save, n)
prob_summary_individuals = rep(0, n)
prob_summary_individuals_upper = rep(0, n)
prob_summary_individuals_lower = rep(0, n)
for(i_individual in 1:n){
    i = county_design[i_individual]
    t = t_design[i_individual]
    h = h_design[i_individual]
    prob_summary_individuals_MCMC[,i_individual] = delta[, i, drop = FALSE] +
                        alpha[, 1:q]%*% as.vector(Z[t,i,1:q]) + eta[, t, 1:L]%*%as.vector(MI[t,i,1:L])
                        as.vector(xi[, h, t, 1:J]%*% as.vector(Phi_Data[i_individual, 1:J]))
}

prob_summary_individuals_MCMC = ilogit( prob_summary_individuals_MCMC )
prob_summary_individuals <- apply(prob_summary_individuals_MCMC, 2, mean)
prob_summary_individuals_upper <- apply(prob_summary_individuals_MCMC, 2, quantile, probs = c(0.95))
prob_summary_individuals_lower <- apply(prob_summary_individuals_MCMC, 2, quantile, probs = c(0.05))
prob_summary_individuals_average_mcmc = apply(prob_summary_individuals_MCMC, 1, mean)

save(prob_summary_M_H_T_Age, prob_summary_M_H_T_Age_upper,
     prob_summary_M_H_T_Age_lower, prob_summary_M_H_T_Age_average_mcmc,
     prob_summary_individuals, prob_summary_individuals_upper,
     prob_summary_individuals_lower, prob_summary_individuals_average_mcmc,
     file = 'Data/Posterior_summary_ALL.RData')
```

Estimated Late-Stage Probability

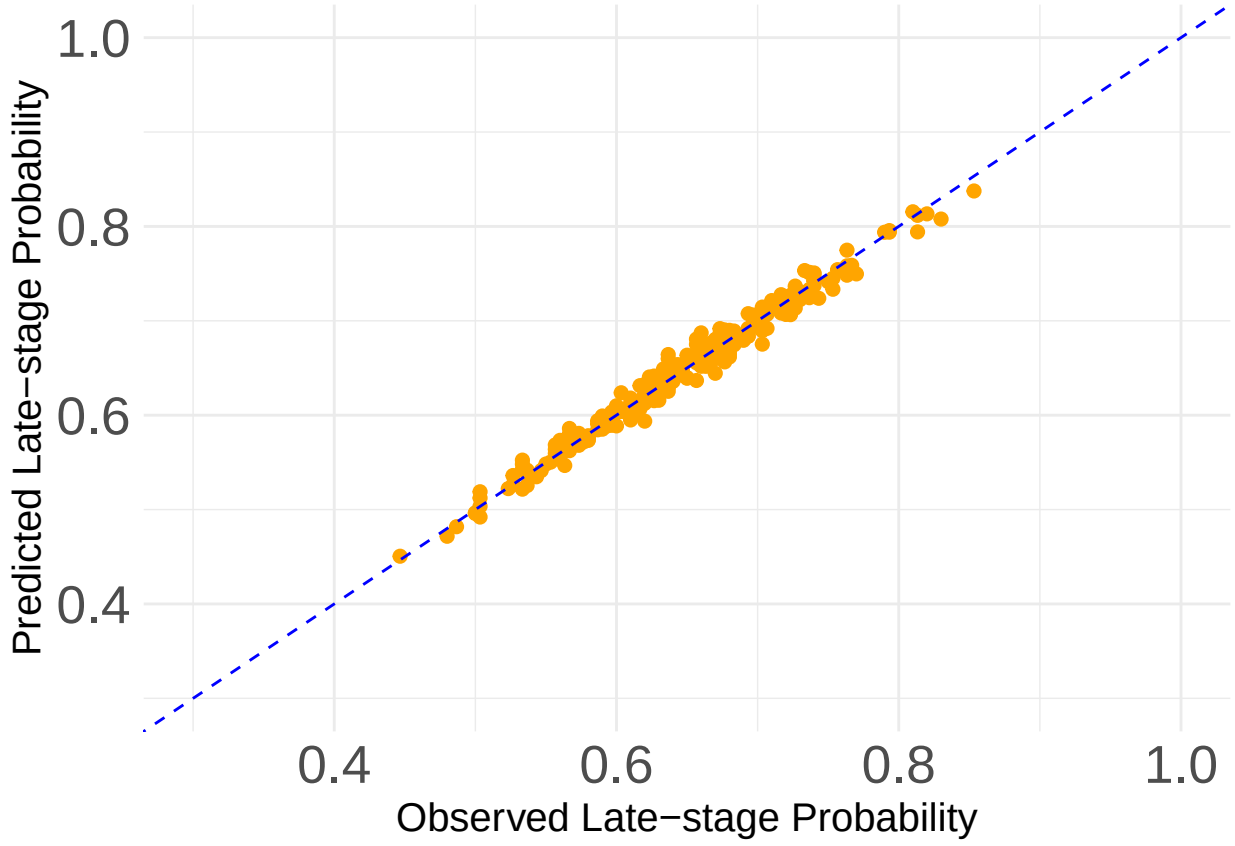
To investigate the estimation performance of the proposed model, we calculate the late-stage probabilities for all individuals in the dataset and then average these probabilities for each county. We also calculate the "observed" county-level late-stage probability as the late-stage proportion for each county.

A comparison of the observed and predicted late-stage probabilities is depicted in the following code chunk. We find that the predictions match the observed values well.

```r
library(tidyverse)
```

```
## -- Attaching core tidyverse packages ------------------------------------------------------------
## v dplyr     1.1.4     v readr     2.1.5
## v forcats   1.0.0     v stringr   1.5.1
## v ggplot2   3.5.1     v tibble    3.2.1
## v lubridate 1.9.3     v tidyr     1.3.1
## v purrr     1.0.2
## -- Conflicts ------------------------------------------------------------------------------------
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
## i Use the conflicted package (<http://conflicted.r-lib.org/>) to force all conflicts to become errors
```

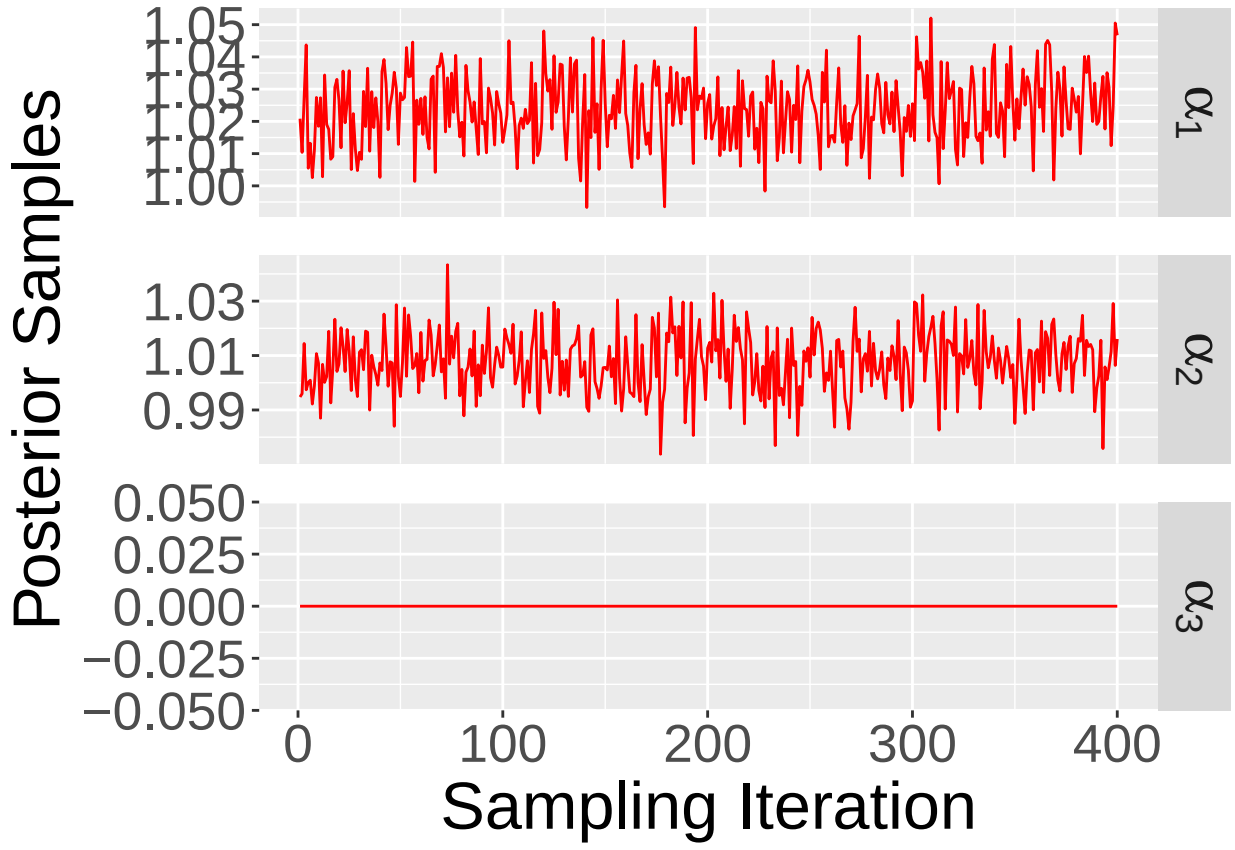
```r
load(file = 'Data/data.RData')
load(file = 'Data/Posterior_summary_ALL.RData')
DATA_temp = DATA
DATA_temp$stage_pred = prob_summary_individuals
DATA_summary = DATA_temp %>% group_by(county) %>%
            summarize(prob_obs = mean(stage, na.rm = TRUE), prob_pred= mean(stage_pred, na.rm = TRUE))

ggplot(DATA_summary, aes(x = prob_obs, y = prob_pred)) +
  geom_point(size = 2, color = 'orange') +
  geom_abline(intercept = 0, slope = 1, color = "blue", linetype = "dashed") +
  labs(x = "Observed Late-stage Probability", y = "Predicted Late-stage Probability") +
  xlim(0.3, 1) + ylim(0.3, 1) +
  theme_minimal() +
  theme(axis.title = element_text(size = 15), axis.text = element_text(size = 20),
        legend.position = NULL
          )
```




```
ggsave(file = 'Data/Prob_Overall_compare.pdf', width = 8, height = 6)
```

Finally, we present the trace plots for the estimates of the regression coefficients α_1, α_2, and α_3.

```
load(file = 'Data/MCMCsamples.RData')
posterior_params = as.data.frame(samples_save)
mcmc_samples = posterior_params[,c('alpha[1]','alpha[2]','alpha[3]')]
df = data.frame(iter = seq(dim(mcmc_samples)[1]), value = as.vector(as.matrix(mcmc_samples)),
                variable = rep( c('alpha[1]','alpha[2]','alpha[3]'),
                                each = dim(mcmc_samples)[1]   ))
ggplot(df) + geom_path(aes(x = iter, y = value), color = 'red') +
             facet_grid(variable ~ ., scales = 'free_y', labeller = label_parsed) +
             labs(x = 'Sampling Iteration', y =  "Posterior Samples")+
             theme(legend.key.size = unit(1, 'cm'),
                   legend.title = element_text(size=20),legend.text = element_text(size=15)) +
             theme(axis.text=element_text(size=20),axis.title=element_text(size=25)) +
             theme(strip.text=element_text(size=20)) +
             theme(panel.spacing = unit(1, 'lines'))
```




```
ggsave(filename = 'Data/Traceplot.pdf', width = 10, height = 10)
```