Biostat276 Project 2

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2/16/2022

Contents

Bayesian Probit Regression

In `R` load the `package (survival)` and consider the analysis of the data-set `(infert)`. Ignoring dependence due to matching, consider a Bayesian analysis for a logistic regression model relating case status to: age, parity, education, spontaneous and induced. More precisely, assume case status y_i has density $y_i \sim_{ind} Bern(p_i)$, $p_i = \Phi(X_i'\beta)$, where $\Phi(\cdot)$ is the standard Gaussian cdf. Consider a prior $\beta \sim N(0, 10^2(X'X)^{-1})$. We are interested in $p(\beta|Y)$.

```
rm(list = ls())
library(ggplot2)
library(tidyverse)
```

```
## -- Attaching packages --------------------------------------- tidyverse 1.3.0 --

## v tibble  3.1.0     v dplyr   1.0.7
## v tidyr   1.1.3     v stringr 1.4.0
## v readr   1.4.0     v forcats 0.5.1
## v purrr   0.3.4

## -- Conflicts ------------------------------------------ tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
```

```
library(mvtnorm)
library(kableExtra)
```

```
##
## Attaching package: 'kableExtra'

## The following object is masked from 'package:dplyr':
##
##     group_rows
```

```
library(truncnorm)
library(profmem)
library(microbenchmark)
```

```r
# load the data
library(survival)
data("infert")

# change the data type of `education`
inferthw <- infert
inferthw$education <- as.numeric(inferthw$education) - 1
dat <- inferthw %>%
  dplyr::select(c("education", "age", "parity", "induced", "case",
                  "spontaneous"))
str(dat) # all variables are numeric
```

```
## 'data.frame':    248 obs. of  6 variables:
##  $ education  : num  0 0 0 0 1 1 1 1 1 1 ...
##  $ age        : num  26 42 39 34 35 36 23 32 21 28 ...
##  $ parity     : num  6 1 6 4 3 4 1 2 1 2 ...
##  $ induced    : num  1 1 2 2 1 2 0 0 0 0 ...
##  $ case       : num  1 1 1 1 1 1 1 1 1 1 ...
##  $ spontaneous: num  2 0 0 0 1 1 0 0 1 0 ...
```

Frequentist Method (Not related to the questions, just a try)

Before answering the questions, we can directly compute the MLE of the model parameters using `glm()` function with a probit link function.

```r
freq <- glm(case ~ age + parity + education + spontaneous + induced,
            data = dat, family = binomial(link = probit))
```

```r
# MLE estimator
freq$coefficients
```

```
## (Intercept)         age      parity   education spontaneous     induced 
## -0.91127035  0.02073028 -0.43967798 -0.28754507  1.16488031  0.71911970
```

```r
# Deviance
freq$deviance # the deviance is large
```

```
## [1] 259.6669
```

Question 1

(1) Describe and implement an adaptive Metropolis-Hastings algorithm designed to obtain a MC with stationary distribution $p(\beta|Y)$.

Solution: The full posterior distribution for the Bayesian binary probit model can be computed as follows:

$$\begin{aligned}
\pi(\beta|Y,X) &\propto \pi(\beta)\cdot\pi(Y,X|\beta) \\
&= \pi(\beta)\cdot\prod_{i=1}^{n} p(y_i, X_i|\beta) \\
&= \pi(\beta)\cdot\prod_{i=1}^{n}\Phi(X_i'\beta)^{y_i}[1-\Phi(X_i'\beta)]^{1-y_i} \\
&\propto \exp[-\frac{\beta'(X'X)\beta}{200}]\cdot\prod_{i=1}^{n}\Phi(X_i'\beta)^{y_i}[1-\Phi(X_i'\beta)]^{1-y_i}
\end{aligned}$$

It's obvious that $\pi(\beta)$ is not a conjugate prior by the fact that no conjugate prior $\pi(\beta)$ exists for the parameters of the probit regression model.

We compute the posterior distribution first:

```r
# Calculation of posterior
beta_prior <- 100 * solve(as.matrix(t(dat[, -5])) %*% as.matrix(dat[, -5]))

posterior <- function(beta) {
  pi <- pnorm(as.matrix(dat[, -5]) %*% t(beta))
  data <- data.frame(pi = pi, y = dat[, 5])
  post <- apply(data, 1, function(x) {ifelse(x[2] == 1, x[1], 1 - x[1])})
  post <- log(post) %>%
    sum(.) - 1/2 * beta %*% solve(beta_prior) %*% t(beta)
}
```

```r
# Adaptive Random Walk-Metropolis Hastings
mh.Q1 <- function(nsim = 10000, burn = 0.2, # chain parameters
                  delta = 0.75, c = 1,       # set c = 1 (c > 0)
                  seed = 1998) {
  # initialization----------------------------------
  set.seed(seed)
  nsim1 <- nsim * (1 + burn)
  burni <- nsim * burn

  beta_num <- dim(dat)[2] - 1

  beta <- matrix(data = rep(0, beta_num), nrow = 1)
  beta.ch <- matrix(data = NA, nrow = nsim, ncol = beta_num)
  betavar <- diag(beta_num) * (10^(-14)) # error term \epsilon
  deltaset <- rbinom(nsim1, 1, delta)
  # run chain----------------------------------------

  for (i in 1:nsim1) {
    # here we use adaptive MH for the first 2200 iterations
    if (i <= 2200) {
    # \Sigma^{\tilde}_t = \Sigma_t + \epsilon*I
    betavar <- (betavar * (i - 1) + t(beta) %*% beta)/i +
      diag(beta_num) * (10^(-14))
    delta_tm <- deltaset[i] # delta = 0.75 during adaptive
    } else {delta_tm <- 1} # delta is fixed after adaptive
    # use the last variance of beta from adaptive for the remaining iterations
    beta_tm1 <- rmvnorm(n = 1, mean = beta, sigma = c * betavar)
    beta_tm2 <- rmvnorm(n = 1, mean = beta, sigma = beta_prior)
    beta_tm <- beta_tm1 * delta_tm + beta_tm2 * (1 - delta_tm)

    P0 <- posterior(beta)
    P1 <- posterior(beta_tm)
    ratio <- P1 - P0
    if (log(runif(1)) < ratio) {
      beta <- beta_tm
    }
    # Store Chain after burn
    if (i > burni) {
      i1 <- i - burni
      beta.ch[i1, ] <- beta
      }
    }
  return(list(beta = beta.ch))
}

# Simulation
arw_mh <- mh.Q1(nsim = 10000, burn = 0.2, delta = 0.75, c = 1)
```

```r
# get the result
result_Q1 <- apply(arw_mh$beta, 2,
                   function(x) {quantile(x, c(0.025, 0.5, 0.975))}) %>%
  round(., 3) # 95% credible interval & median
colnames(result_Q1) <- colnames(dat)[-5]
```

Question 2

Describe and implement a data augmented (DA-MCMC) strategy targeting $p(\beta|y)$.

Solution: Here targeting $p(\beta, z|y)$ could be easier enough.

Let prior of $\beta : \beta \sim \mathcal{N}(0, \Sigma_\beta)$, i.e. $\Sigma_\beta = 10^2(X'X)^{-1})$

Let $Z_i|\beta \sim \mathcal{N}(X_i'\beta, 1)$ and define the sampling model conditionally as $Y_i|Z_i = I(Z_i > 0)$. Then we use the Gibbs Sampling:

For β :

$$
\begin{aligned}
p(\beta|Z_{1:n}, Y_{1:n}) &= p(\beta|Z_{1:n}) \\
&\propto \prod_{i=1}^{n} \exp[-\frac{-(z_i - X_i'\beta)^2}{2}] \cdot \exp(-\frac{\beta^T \Sigma_\beta^{-1} \beta}{2}) \\
&= \exp[-\frac{(Z - X\beta)'(Z - X\beta) + \beta'\Sigma_\beta^{-1}}{\beta} 2] \\
&\propto \exp[\frac{\beta'(X'X + \Sigma_\beta^{-1})\beta - 2\beta'X'Z}{2}]
\end{aligned}
$$

By completing the square, we realize that the density is proportional to a normal kernel, the posterior of β satisfies a normal distribution:

$$
p(\beta|Z_{1:n}, Y_{1:n}) \sim \mathcal{N}\{(X'X + \Sigma_\beta^{-1})^{-1}X'Z, (X'X + \Sigma_\beta^{-1})^{-1}\}
$$

For Z_i :

$$
\begin{aligned}
p(Z_i|Y_i, \beta) &\propto p(Y_i|Z_i) \cdot p(Z_i|\beta) \\
&= I(Z_i > 0) \cdot \exp[-\frac{-(z_i - X_i'\beta)^2}{2}] \quad (\text{if } y_i = 1) \\
&= I(Z_i \leq 0) \cdot \exp[-\frac{-(z_i - X_i'\beta)^2}{2}] \quad (\text{if } y_i = 0)
\end{aligned}
$$

The posterior of Z_i follows a **truncated normal distributon**, i.e.

$$p(Z_i|Y_i,\beta) = \begin{cases} \mathcal{TN}(X_i'\beta, 1, 0, +\infty) & \text{if } y_i = 1 \\ \mathcal{TN}(X_i'\beta, 1, -\infty, 0) & \text{if } y_i = 0 \end{cases}$$

```r
DA_Q2 <- function(nsim = 10000, burn = 0.2, # chain parameters
                  seed = 1998,
                  x = as.matrix(dat[-5]), # load the dataset
                  y = as.matrix(dat[5])) {
  # initialization---------------------------------
  set.seed(seed)
  nsim1 <- nsim * (1 + burn)
  burni <- nsim * burn

  beta_num <- dim(dat)[2] - 1

  beta <- matrix(data = rep(0, beta_num), nrow = 1)
  beta.ch <- matrix(data = NA, nrow = nsim, ncol = beta_num)

  # generate data z---------------------------------
  z <- rep(0, length(y))
  z.ch <- matrix(data = NA, nrow = nsim, ncol = length(y))

  interval <- cbind(ifelse(y == 1, 0, -Inf),
                    ifelse(y == 1, Inf, 0)
                    )

  # run chain---------------------------------------
  for (i in 1:nsim1) {
    # z
    z_comb <- cbind(x %*% t(beta),     # mean of z
                    1,                 # variance of z
                    interval)          # interval of z
    z <- apply(z_comb, 1, function(comb) {
      rtruncnorm(1, comb[1], sd = comb[2], a = comb[3], b = comb[4])
    })

    # beta
    beta_mean <- solve(t(x) %*% x + solve(beta_prior)) %*% t(x) %*% z
    beta_var <- solve(t(x) %*% x + solve(beta_prior))
    beta <- rmvnorm(1, mean = beta_mean, sigma = beta_var)

    # Store Chain after burn
    if (i > burni) {
      i1 <- i - burni
      beta.ch[i1, ] <- beta
    }
  }
  return(list(beta = beta.ch))
}

# Simulation
DA_Gibbs <- DA_Q2(nsim = 10000, burn = 0.2)
```

```
# get the result
result_Q2 <- apply(DA_Gibbs$beta, 2,
                   function(x) {quantile(x, c(0.025, 0.5, 0.975))}) %>%
  round(., 3) # 95% credible interval & median
colnames(result_Q2) <- colnames(dat)[-5]
```

Question 3

Describe and implement a parameter expanded - data augmentation (PX-DA MCMC) algorithm targeting $p(\beta|Y)$.

Solution: The Standard Probit Regression is:

$$Z_i|\beta \sim \mathcal{N}(X_i'\beta, 1), \quad Y_i|Z_i \sim I(Z_i > 0)$$

Now we do the parameter expansion:

$$\begin{aligned} W_i|\beta,\alpha &\sim \mathcal{N}(X_i'\beta\alpha, \alpha^2) \\ Y_i|W_i &= I(W_i > 0) \\ \alpha^2 &\sim InverseGamma(a, b) \end{aligned}$$

For β :

Then we calculate the full posterior distribution of β, σ^2 and w:

$$\begin{aligned} p(\beta|W_{1:n},\alpha) &\propto p(W_{1:n}|\alpha,\beta)\cdot p(\alpha,\beta) \\ &= p(W_{1:n}|\alpha,\beta)\cdot p(\alpha)p(\beta) \\ &\propto p(W_{1:n}|\alpha,\beta)\cdot p(\beta) \\ &\propto \prod_{i=1}^{n} \exp[-\frac{(w_i - X_i'\beta\alpha)^2}{2\alpha^2}]\cdot \exp(-\frac{\beta'\Sigma_\beta^{-1}\beta}{2}) \\ &= \exp[-\frac{(W-\alpha X\beta)'(W-\alpha X\beta)+\alpha^2\beta'\Sigma_\beta^{-1}\beta}{2\sigma^2}] \\ &\propto \exp(-\frac{\beta'(X'X+\Sigma_\beta^{-1})\beta - 2\frac{\beta'X'W}{\alpha}}{2}) \end{aligned}$$

By completing the square, we realize that the density is proportional to a normal kernel, the posterior of β satisfies a normal distribution:

$$p(\beta|W_{1:n},\alpha) \sim \mathcal{N}\{(X'X+\Sigma_\beta^{-1})^{-1}\frac{X'W}{\alpha}, (X'X+\Sigma_\beta^{-1})^{-1}\}$$

For α^2 :

$$\begin{aligned} p(\alpha^2|W,\beta) &\propto \propto p(W_i|\beta,\alpha^2)\cdot p(\alpha^2) \\ &\propto \prod_{i=1}^{n}\frac{1}{\alpha}\cdot\exp[-\frac{(w_i-X_i'\beta\alpha)^2}{2\alpha^2}]\cdot(\frac{1}{\alpha^2})^{a+1}\exp(-\frac{b}{\alpha^2}) \\ &= \exp[-\frac{\sum_{i=1}^{n}(w_i-X_i'\beta\alpha)^2+2b}{2\alpha^2}]\cdot(\frac{1}{\alpha^2})^{a+\frac{n}{2}+1} \qquad (1) \end{aligned}$$

For W_i :

$$\begin{aligned} p(W_i|Y_i,\alpha,\beta) &\propto p(Y_i|W_i)\cdot p(W_i|\alpha,\beta) \\ &= I(W_i>0)\cdot \exp[-\frac{-(w_i-X_i'\beta\alpha)^2}{2\alpha^2}] \quad (\text{if } y_i=1) \\ &= I(W_i\le 0)\cdot \exp[-\frac{-(w_i-X_i'\beta\alpha)^2}{2\alpha^2}] \quad (\text{if } y_i=0) \end{aligned}$$

The posterior of W_i follows a **truncated normal distributon**, i.e.

$$p(W_i|Y_i,\alpha,\beta)=\begin{cases}\mathcal{TN}(X_i'\beta\alpha,\alpha^2,0,+\infty) & \text{if } y_i=1\\ \mathcal{TN}(X_i'\beta\alpha,\alpha^2,-\infty,0) & \text{if } y_i=0\end{cases}$$

```r
alpha_post <- function(alpha_sq, w, x, beta,
                       a = 5,  # a, b are paras for sigma_sq ~ InverseGamma
                       b = 5) {
  f <- -(t(w - x %*% t(beta) * sqrt(alpha_sq)) %*%
               (w - x %*% t(beta) *sqrt(alpha_sq)) + 2*b)/(2 * alpha_sq) +
    (a + 1 + 248/2) * log(1/alpha_sq)
  return(f)
}
```

```r
PXDA_Q3 <- function(nsim = 10000, burn = 0.2, # chain parameter
                    seed = 1998,
                    x = as.matrix(dat[-5]),
                    y = as.matrix(dat[5]),
                    eta = 0.05) { # random walk jump size
  # initialization----------------------------------
  set.seed(seed)
  nsim1 <- nsim * (1 + burn)
  burni <- nsim * burn

  beta_num <- dim(dat)[2] - 1
  beta <- matrix(data = rep(0, beta_num), nrow = 1)
  beta.ch <- matrix(data = NA, nrow = nsim, ncol = beta_num)
  alpha_sq <- 1
  alpha_sq.ch <- vector()

  # generate data w---------------------------------
  w <- rep(1, length(y))
  w.ch <- matrix(data = NA, nrow = nsim, ncol = length(y))


  interval <- cbind(ifelse(y == 1, 0, -Inf),
                    ifelse(y == 1, Inf, 0)
                    )

  # run chain--------------------------------------
  for (i in 1:nsim1) {
    # beta
    bmean <- solve(t(x) %*% x + solve(beta_prior)) %*% t(x) %*% w/sqrt(alpha_sq)
    bvar <- solve(t(x) %*% x + solve(beta_prior))
    beta <- rmvnorm(1, mean = bmean, sigma = bvar)
    # w_i
    w_comb <- cbind(x %*% t(beta) * sqrt(alpha_sq),              # mean of w
                              sqrt(rep(alpha_sq, length(y))),    # variance of w
                              interval)                          # interval of w
    w <- apply(w_comb, 1, function(comb) {
      rtruncnorm(1, comb[1], sd = comb[2], a = comb[3], b = comb[4])
    })

    # alpha_sq :Using RW-MH: alpha_sq* | alpha_sq ~ N(alpha_sq, eta)
    alpha_sq_tm <- rnorm(1, alpha_sq, eta)
    P0 <- alpha_post(alpha_sq, w = w, x = x, beta = beta)
    P1 <- alpha_post(alpha_sq_tm, w = w, x = x, beta = beta)
    ratio <- P1 - P0

    if (log(runif(1)) < ratio) {
      alpha_sq <- alpha_sq_tm
    }


    # Store Chain after burn
    if (i > burni) {
      i1 <- i - burni
      beta.ch[i1, ] <- beta
      alpha_sq.ch[i1] <- alpha_sq
      w.ch[i1, ] <- w
    }
  }
  return(list(beta = beta.ch, alpha_sq =  alpha_sq.ch))
}

# Simulation
PXDA <- PXDA_Q3(nsim = 10000, burn = 0.2)
```

```
# get the result
result_Q3 <- apply(PXDA$beta, 2,
                   function(x) {quantile(x, c(0.025, 0.5, 0.975))}) %>%
  round(., 3) # 95% credible interval & median
colnames(result_Q3) <- colnames(dat)[-5]
```

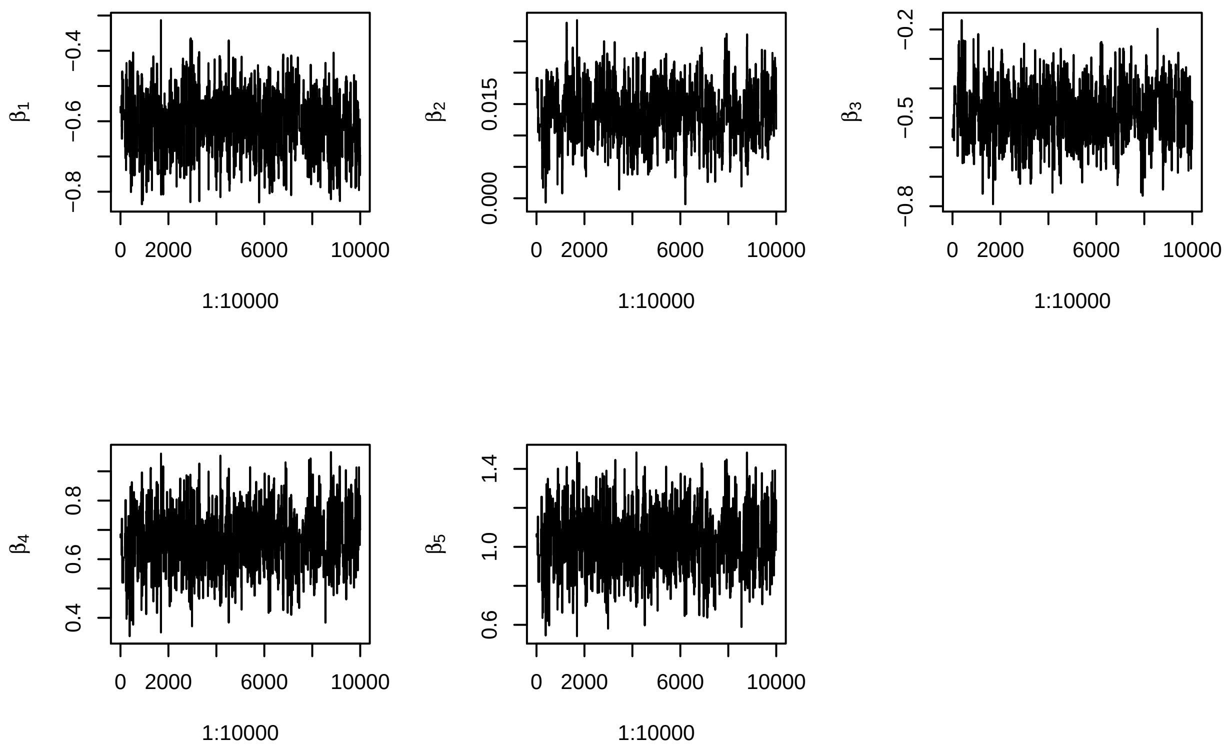
Question 4

Assess mixing and convergence of the chains induced by the competing transition schemes implemented in 1,2 and 3. Comment on potential trade-offs involving: coding complexity, storage and cpu time.

Solution:

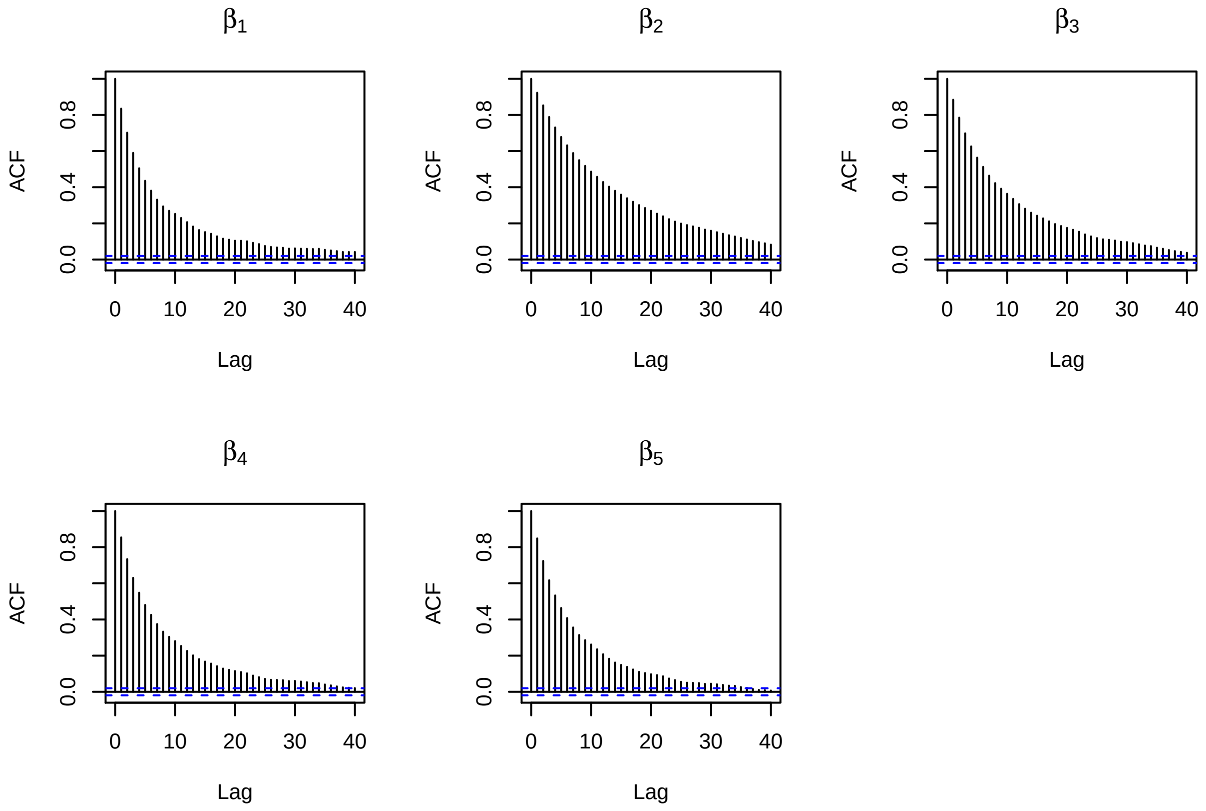
```
# Plots
# Adaptive Random Walk Metropolis Hasting
  # Convergence Checking
par(mfrow = c(2, 3))
for (i in 1:5) {
  plot(1:10000, arw_mh$beta[, i], type = "l",
       ylab = substitute(beta[x], list(x = i)))
}
```

```r
  # Autocorrelation plot
par(mfrow = c(2, 3))
```



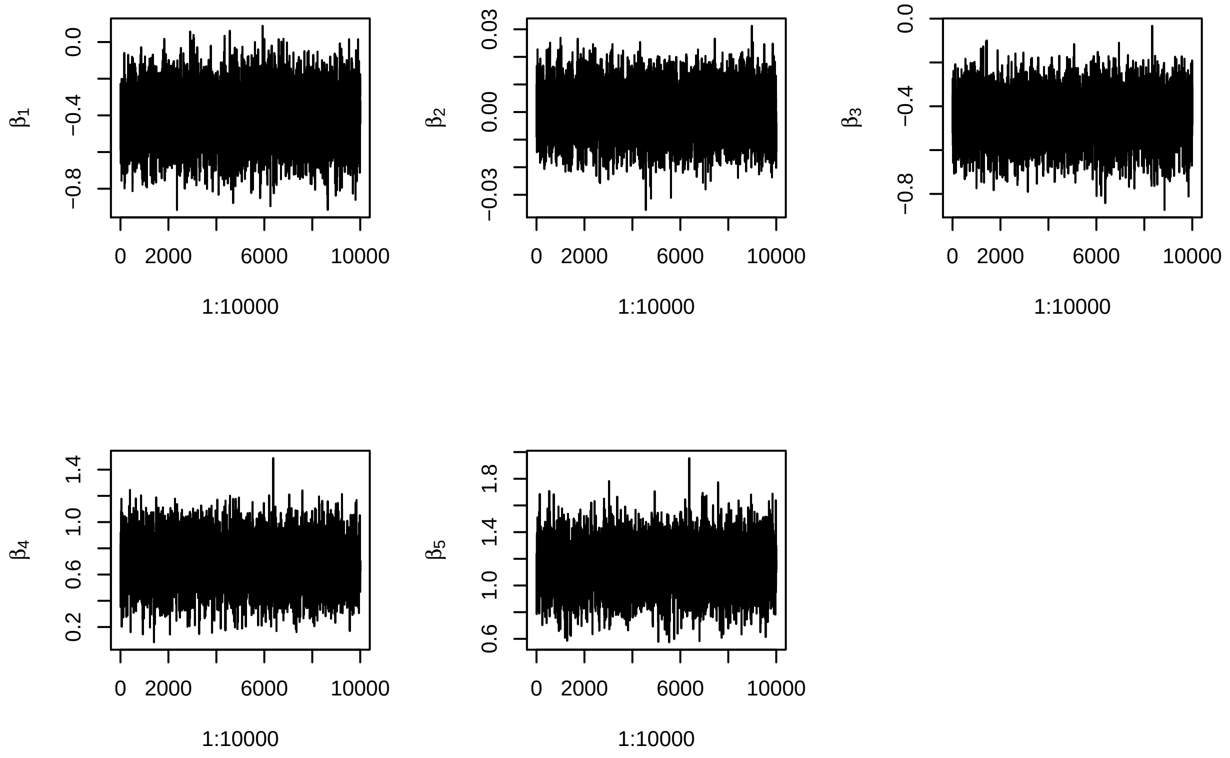
```r
for (i in 1:5) {
  acf(arw_mh$beta[, i], main = substitute(beta[x], list(x = i)))
} # autocorrelation plots look good (beta_2 is kind of worse but acceptable)


# Data Augmentation
  # convergence checking
par(mfrow = c(2, 3))
```



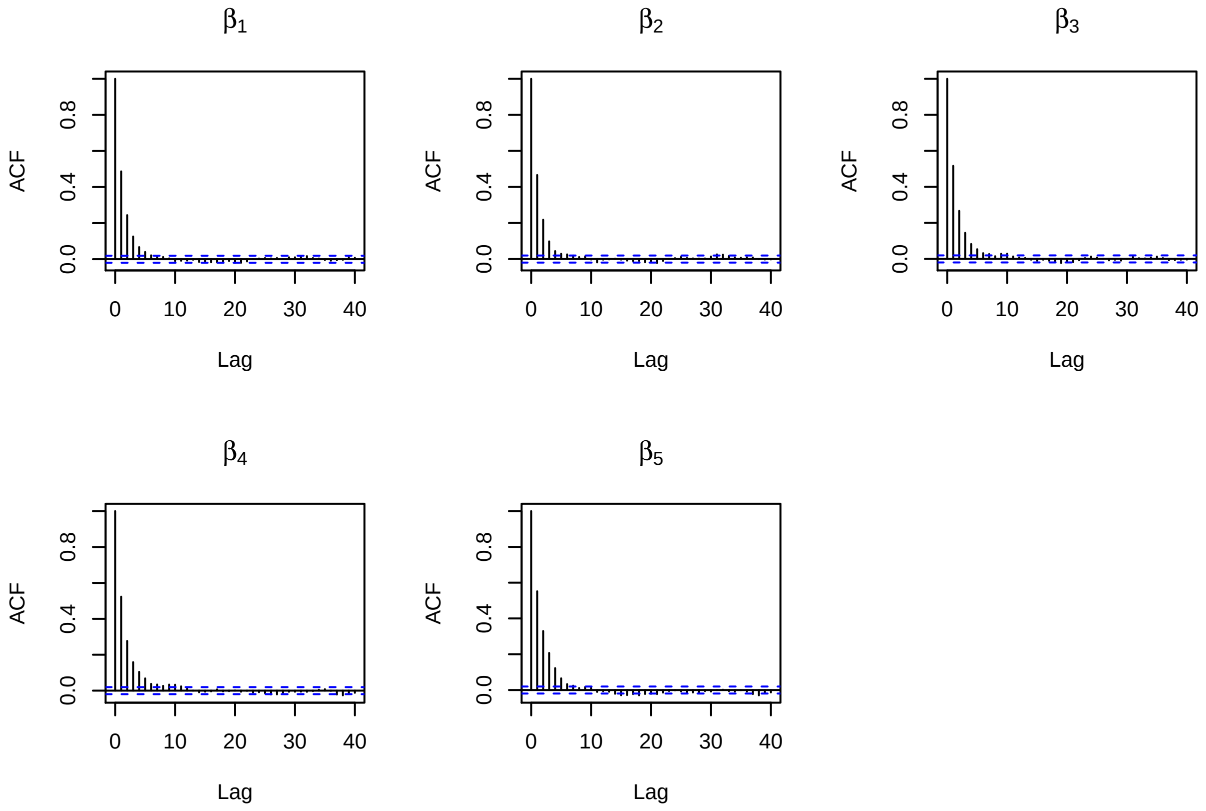
```
for (i in 1:5) {
  plot(1:10000, DA_Gibbs$beta[, i], type = "l",
       ylab = substitute(beta[x], list(x = i)))
}

  # Autocorrelation plot
par(mfrow = c(2, 3))
```



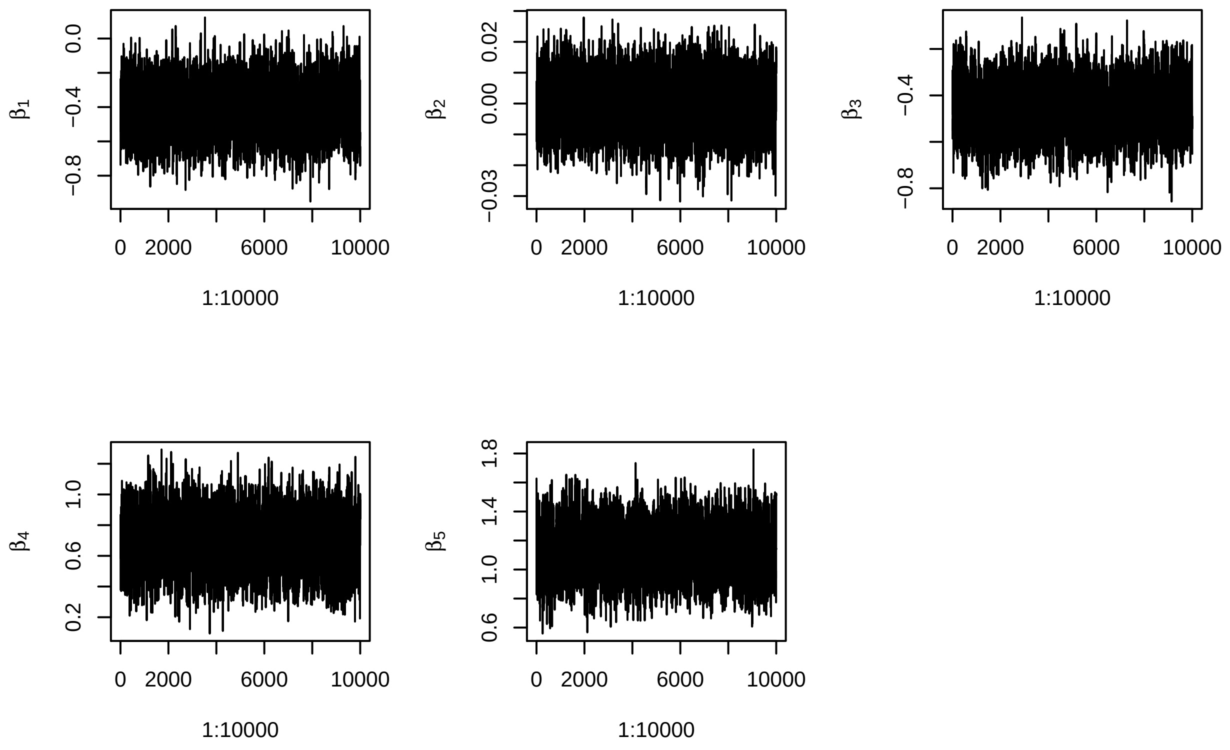
```
for (i in 1:5) {
  acf(DA_Gibbs$beta[, i], main = substitute(beta[x], list(x = i)))
} # autocorrelation plots look good (beta_2 is kind of worse but acceptable)


# PX-DA
  # convergence checking
par(mfrow = c(2, 3))
```

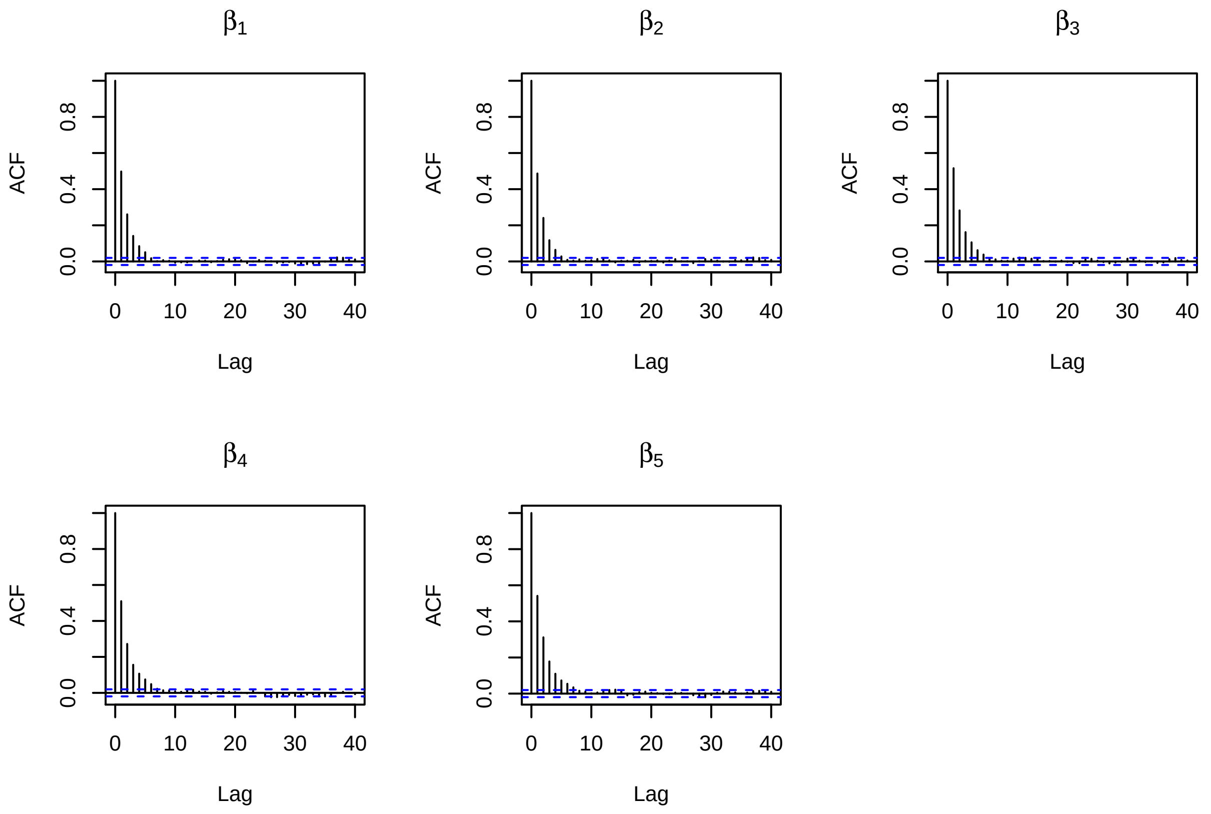


```
for (i in 1:5) {
  plot(1:10000, PXDA$beta[, i], type = "l",
       ylab = substitute(beta[x], list(x = i)))
}

  # Autocorrelation plot
par(mfrow = c(2, 3))
```



```r
for (i in 1:5) {
  acf(PXDA$beta[, i], main = substitute(beta[x], list(x = i)))
} # autocorrelation plots look good (beta_2 is kind of worse but acceptable)
```



```
# Combined table
result_Q4 <- rbind(result_Q1, result_Q2, result_Q3) %>% as.data.frame(.)
result_comb <- matrix(data = NA, nrow = 3, ncol = 5)
colnames(result_Q4) <- colnames(dat[-5])

for (i in 1:5) {
  for (j in 1:3) {
    result_comb[j, i] <- paste0(result_Q4[3*j - 1, i], "(",
                                result_Q4[3*j - 2, i], ",",
                                result_Q4[3*j, i], ")")
  }
}
colnames(result_comb) <- colnames(dat[-5])
```

```
result_comb %>%
  kbl(caption = "Summary Table of Coefficients with 95% CI") %>%
  kable_classic(full_width = F, html_font = "Cambria", position = "center",
                latex_options = "HOLD_position")
```

Table 1: Summary Table of Coefficients with 95% CI

education	age	parity	induced	spontaneous
-0.613(-0.76,-0.457)	0.014(0.005,0.022)	-0.484(-0.662,-0.319)	0.667(0.48,0.85)	1.033(0.751,1.319)
-0.416(-0.678,-0.148)	0(-0.016,0.016)	-0.456(-0.656,-0.26)	0.695(0.372,1.022)	1.141(0.829,1.463)
-0.411(-0.679,-0.139)	0(-0.016,0.016)	-0.451(-0.652,-0.251)	0.687(0.372,1.013)	1.13(0.815,1.452)

```
# Calculate storage
storage_arwmh <- profmem(mh.Q1(nsim = 10000, burn = 0.2, delta = 0.75, c = 1))
storage_da <- profmem(DA_Q2(nsim = 10000, burn = 0.2))
storage_pxda <- profmem(PXDA_Q3(nsim = 10000, burn = 0.2))
```

```
storage <- data.frame(Method = c("Adaptive RW-MH", "DA", "PX-DA"),
                      Storage = c(storage_arwmh$bytes %>% sum(na.rm = TRUE),
                                  storage_da$bytes %>% sum(na.rm = TRUE),
                                  storage_pxda$bytes %>% sum(na.rm = TRUE)))

storage %>%
  kbl(caption = "Summary Table of Memory Use") %>%
  kable_classic(full_width = F, html_font = "Cambria", position = "center",
                latex_options = "HOLD_position")
```

Table 1: Summary Table of Memory Use

Method	Storage
Adaptive RW-MH	1095448376
DA	8527881720
PX-DA	8791800984

```
# CPU Time
  # Adaptive Random-Walk Metropolis Hasting
```

```r
time.arw.mh <- matrix(data = NA, nrow = 5, ncol = 5)
for (i in 1:5) {
 time.arw.mh[i, ] <- system.time(mh.Q1(nsim = 10000, burn = 0.2,
                                        delta = 0.75, c = 1))
}

  # Data Augmentation
time.da <- matrix(data = NA, nrow = 5, ncol = 5)
for (i in 1:5) {
  time.da[i, ] <- system.time(DA_Q2(nsim = 10000, burn = 0.2))
}

  # Parameter Expansions with Data Augmentation
time.pxda <- matrix(data = NA, nrow = 5, ncol = 5)
for (i in 1:5) {
 time.pxda[i, ] <-system.time(PXDA_Q3(nsim = 10000, burn = 0.2))
}
```

```r
cpu_time <- rbind(colMeans(time.arw.mh), colMeans(time.da), colMeans(time.pxda))
colnames(cpu_time) <- c("user", "system", "elapsed",
                        "user_child", "system_child")
cpu_time %>%
  kbl(caption = "Summary Table of CPU time") %>%
  kable_classic(full_width = F, html_font = "Cambria", position = "center",
              latex_options = "HOLD_position")
```

Table 2: Summary Table of CPU time

user	system	elapsed	user_child	system_child
57.0222	0.5662	57.7370	0	0
46.7652	1.1966	48.1222	0	0
47.8000	1.2436	49.2414	0	0

According to the result, `Adaptive Metropolis Hasting` uses the least storage, while `Data Augmentation` and `PX-DA` takes similar storage . As for running time, `Data Augmentation` is a little bit more efficient than `PX-DA` and both of them are much more efficient than `Adaptive Metropolis Hasting`. For the convergence condition, `Data Augmentation` and `PX-DA` are better than `Adaptive Metropolis Hasting`, and β_4 obtained by `PX-DA` converged faster than `Data Augmentation`.

In conclusion, `Adaptive Metropolis Hasting` takes the least storage, `Data Augmentation` is the most efficient method, and `PX-DA` has the best convergence of the Markov Chains.