Worksheet 4

Foundations of Bayesian Methodology

Wenje Tu   Lea Bührer   Jerome Sepin   Zhixuan Li
Elia-Leonid Mastropietro   Jonas Raphael Füglistaler   Nico Schümperli

Spring Semester 2022

Exercise 2 (Gibbs sampler)

2(a)

$$
\begin{aligned}
p(x) &= \exp\left(-\frac{1}{2}(ax^2 - 2bx)\right) \\
&= \exp\left(-\frac{a}{2}\left\{x^2 - 2\frac{b}{a}x\right\}\right) \\
&= \exp\left(-\frac{a}{2}\left\{x^2 - 2\frac{b}{a}x + \left(\frac{b}{a}\right)^2 - \left(\frac{b}{a}\right)^2\right\}\right) \\
&= \exp\left(-\frac{a}{2}\left(x - \frac{b}{a}\right)^2 + \frac{b^2}{2a}\right) \\
&= \underbrace{\exp\left(\frac{b^2}{2a}\right)}_{\text{costant}} \exp\left(-\frac{a}{2}\left(x - \frac{b}{a}\right)^2\right)
\end{aligned}
$$

Distribution function of $p(x)$:

$$
\begin{aligned}
f(x) &= \frac{p(x)}{\int_{-\infty}^{\infty} p(x)dx} \\
&= \frac{\exp\left(\frac{b^2}{2a}\right)\exp\left(-\frac{a}{2}\left(x-\frac{b}{a}\right)^2\right)}{\int_{-\infty}^{\infty}\exp\left(\frac{b^2}{2a}\right)\exp\left(-\frac{a}{2}\left(x-\frac{b}{a}\right)^2\right)dx} \\
&= \frac{\exp\left(-\frac{a}{2}\left(x-\frac{b}{a}\right)^2\right)}{\int_{-\infty}^{\infty}\exp\left(-\frac{a}{2}\left(x-\frac{b}{a}\right)^2\right)dx} \\
&= \frac{\exp\left(-\frac{a}{2}\left(x-\frac{b}{a}\right)^2\right)}{\sqrt{\frac{2\pi}{a}}\underbrace{\int_{-\infty}^{\infty}\sqrt{\frac{a}{2\pi}}\exp\left(-\frac{a}{2}\left(x-\frac{b}{a}\right)^2\right)dx}_{\text{integrates to 1}}} \\
&= \sqrt{\frac{a}{2\pi}}\exp\left(-\frac{a}{2}\left(x-\frac{b}{a}\right)^2\right)
\end{aligned}
$$

$$
X \sim \mathrm{N}\left(\frac{b}{a}, \frac{1}{a}\right)
$$

2(b)

Generate data: a random normal sample by assuming `set.seed(44566)`, $n = 30$, $\mu = 4$ and $\sigma^2 = 16$.

```
# Generate data
set.seed(44566)
mu <- 4
sigma2 <- 16
n <- 30
y <- rnorm(n=n, mean=mu, sd=sqrt(sigma2))
```

```
# Define the parameters of the prior distributions
mu0 <- -3
sigma2_0 <- 4
a0 <- 1.6
b0 <- 0.4

####################
## Gibbs sampler (1 chain)
####################

# initialisation
set.seed(44566)

n.iter <- 10000
n.burnin <- 4000
n.thin <- 1
#n.thin <- floor((n.iter-n.burnin)/500)
n.chains <- 1
parameters <- c("mu", "sigma2", "inv_sigma2")
n.parameters <- length(parameters)

n.tot <- n.burnin + n.iter*n.thin

gibbs_samples <- matrix(NA, nrow = n.iter, ncol = n.parameters)
colnames(gibbs_samples) <- parameters

mu.sim <- rep(NA, length = n.tot)
sigma2.sim <- rep(NA, length = n.tot)
inv.sigma2.sim <- rep(NA, length = n.tot)

# Set the initial value
sigma2.sim[1] <- 1/runif(n.chains)

# set the counter
k <- 1

#Run the for loop (only one chain)
for(i in 2:(n.burnin+n.iter*n.thin)){

  mu.sim[i] <- rnorm(1,
                     mean = (sum(y)/sigma2.sim[i-1] + mu0/sigma2_0) /
                       (n/sigma2.sim[i-1] + 1/sigma2_0),
                     sd = sqrt(1/(n/sigma2.sim[i-1] + 1/sigma2_0)))

  sigma2.sim[i] <- 1/rgamma(1, shape = n/2 + a0,
                            scale = 1 / (sum((y-mu.sim[i])^2)/2 + b0))

  inv.sigma2.sim[i] <- 1/sigma2.sim[i]
  # after the burnin save every n.thin'th sample
  if((i > n.burnin) && (i%%n.thin == 0)){
    gibbs_samples[k,] <- c(mu.sim[i], sigma2.sim[i], inv.sigma2.sim[i])
    k <- k + 1
  }

  if(i%%1000 == 0){
    # report on the fly in which iteration the chain is
    cat(i, "\n")
  }

}
```

```
## 1000
## 2000
## 3000
## 4000
## 5000
## 6000
## 7000
## 8000
## 9000
## 10000
## 11000
## 12000
## 13000
## 14000
```

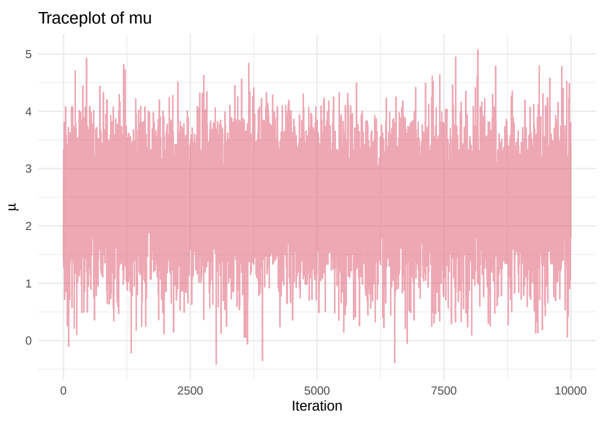
```
# n.iter samples after n.burnin taking every n.thin'th sample
dim(gibbs_samples)
```

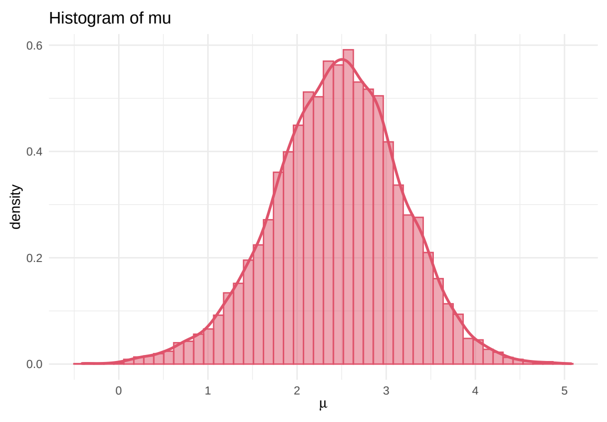
```
## [1] 10000     3
```

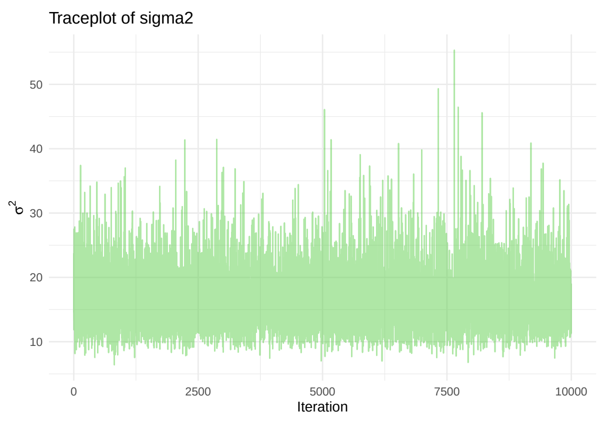
```
mu_gibbs_samples <- gibbs_samples[,"mu"]
sigma2_gibbs_samples <- gibbs_samples[,"sigma2"]
inv_sigma2_gibbs_samples <- gibbs_samples[,"inv_sigma2"]
```

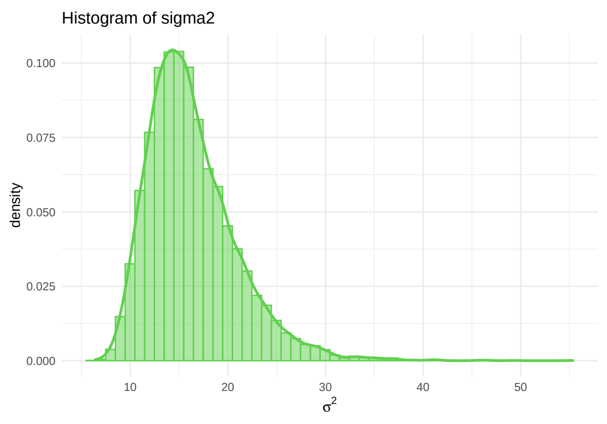
```
library(ggplot2)

d.gibbs <- data.frame(gibbs_samples)

## Traceplot of mu
ggplot(d.gibbs, aes(x=1:nrow(d.gibbs), y=mu)) +
  geom_line(color=2, alpha=0.5) +
  labs(title="Traceplot of mu", x="Iteration", y=expression(mu)) +
  theme_minimal()

## Histogram/Density of mu
ggplot(d.gibbs, aes(x=mu, y=..density..)) +
  geom_histogram(color=2, fill=2, alpha=0.5, bins=50) +
  geom_density(color=2, lwd=1) +
  labs(title="Histogram of mu", x=expression(mu)) +
  theme_minimal()

## Traceplot of sigma2
```

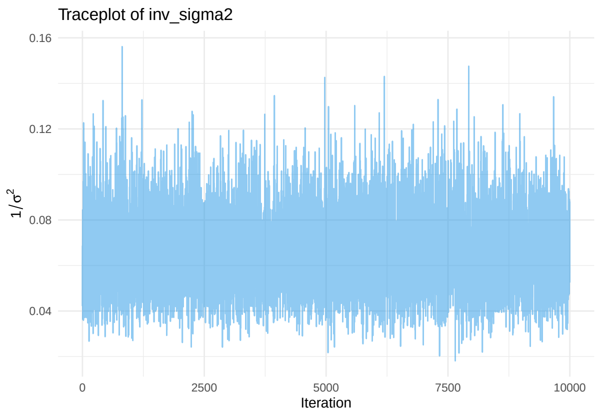
```r
ggplot(d.gibbs, aes(x=1:nrow(d.gibbs), y=sigma2)) +
  geom_line(color=3, alpha=0.5) +
  labs(title="Traceplot of sigma2", x="Iteration", y=expression(sigma^2)) +
  theme_minimal()

## Histogram/Density of sigma2
ggplot(d.gibbs, aes(x=sigma2, y=..density..)) +
  geom_histogram(color=3, fill=3, alpha=0.5, bins=50) +
  geom_density(color=3, lwd=1) +
  labs(title="Histogram of sigma2", x=expression(sigma^2)) +
  theme_minimal()

## Traceplot of inv_sigma2
ggplot(d.gibbs, aes(x=1:nrow(d.gibbs), y=inv_sigma2)) +
  geom_line(color=4, alpha=0.5) +
  labs(title="Traceplot of inv_sigma2", x="Iteration", y=expression(1/sigma^2)) +
  theme_minimal()

## Histogram/Density of inv_sigma2
ggplot(d.gibbs, aes(x=inv_sigma2, y=..density..)) +
  geom_histogram(color=4, fill=4, alpha=0.5, bins=50) +
  geom_density(color=4, lwd=1) +
  labs(title="Histogram of inv_sigma2", x=expression(1/sigma^2)) +
  theme_minimal()
```

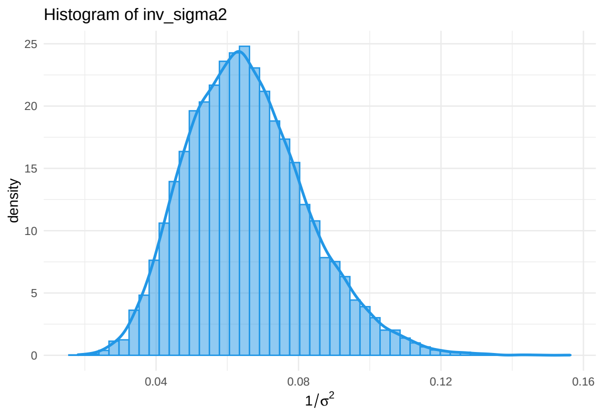












```r
d.summary <- t(
  rbind(
    colMeans(d.gibbs),
    sapply(d.gibbs, function(x) sd(x)),
    sapply(d.gibbs, function(x) quantile(x, probs=c(0.025, 0.5, 0.975)))
  )
)

d.summary <- data.frame(d.summary)
colnames(d.summary) <- c("Mean", "SD", "2.5%", "Median", "97.5%")

knitr::kable(d.summary, align="c", caption="Summary statistics of the marginal posteriors")
```

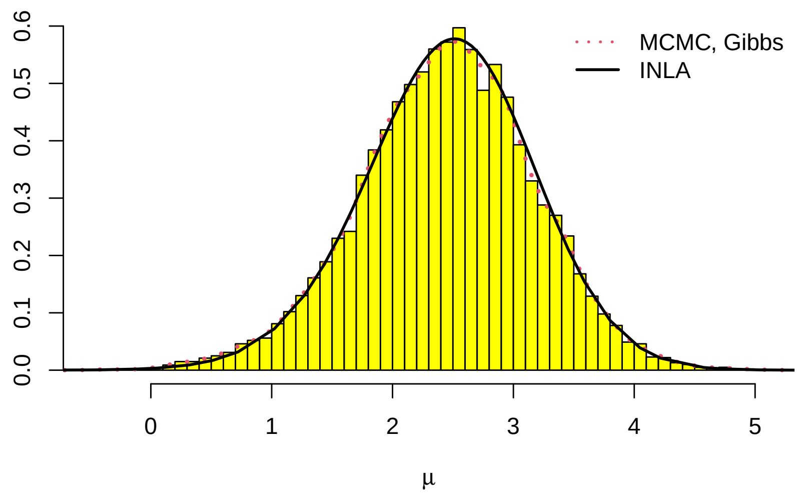
Table 1: Summary statistics of the marginal posteriors

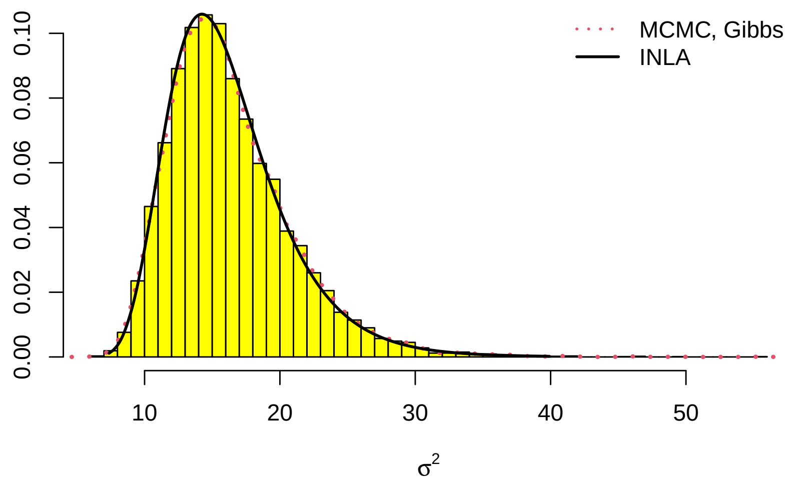
	Mean	SD	2.5%	Median	97.5%
mu	2.4479404	0.7206035	0.9436683	2.4692436	3.808022
sigma2	16.3331563	4.5483340	9.7333046	15.5669100	27.221752
inv_sigma2	0.0656163	0.0169525	0.0367353	0.0642388	0.102740

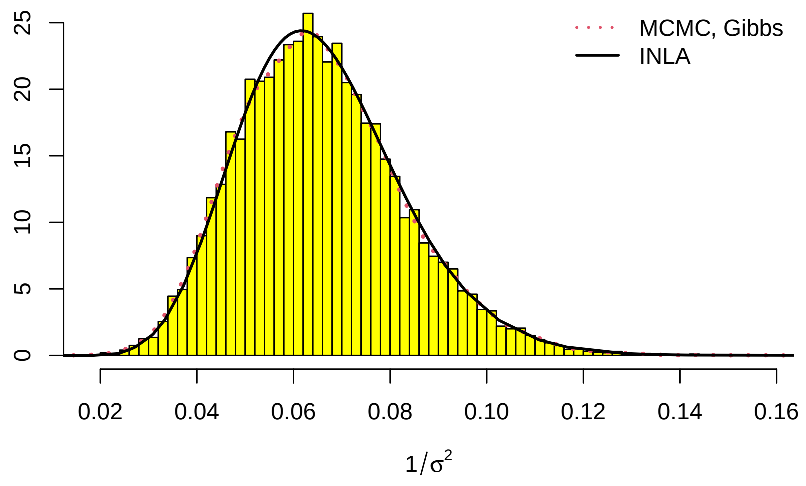
```r
# plots (compare with INLA)
# INLA is exact

# Question: How long should we run the MCMC Gibbs chain to get close to the exact INLA approximation
# Run for 10 min, for 30 min, for 1h...

library(INLA)
library(MASS)

formula <- y ~ 1
inla.output <- inla(formula,data=data.frame(y=y),
                    control.family = list(hyper =
                                            list(prec = list(prior="loggamma",param=c(a0,b0)))),
                    control.fixed = list(mean.intercept=mu0, prec.intercept=1/sigma2_0))
```

```r
par(mfrow=c(1,1))
# plot for mean
rg <- range(inla.output$marginals.fixed$"(Intercept)"[,2])
truehist(mu_gibbs_samples, prob=TRUE, col="yellow", xlab=expression(mu))
lines(density(mu_gibbs_samples),lty=3,lwd=3, col=2)
lines(inla.output$marginals.fixed$"(Intercept)",lwd=2)
```

```
legend("topright",c("MCMC, Gibbs","INLA"),lty=c(3,1),lwd=c(2,2),col=c(2,1),cex=1.0,bty="n")

# plot for variance
m_var <-inla.tmarginal(function(x) 1/x, inla.output$marginals.hyperpar[[1]])
truehist(sigma2_gibbs_samples, prob=TRUE, col="yellow", xlab=expression(sigma^2))
lines(density(sigma2_gibbs_samples),lty=3,lwd=3, col=2)
lines(m_var,lwd=2)
legend("topright",c("MCMC, Gibbs","INLA"),lty=c(3,1),lwd=c(2,2),col=c(2,1),cex=1.0,bty="n")

# plot for precision
truehist(inv_sigma2_gibbs_samples, prob=TRUE, col="yellow", xlab=expression(1/sigma^2))
lines(density(inv_sigma2_gibbs_samples),lty=3,lwd=3, col=2)
lines(inla.output$marginals.hyperpar[[1]],lwd=2)
legend("topright",c("MCMC, Gibbs","INLA"),lty=c(3,1),lwd=c(2,2),col=c(2,1),cex=1.0,bty="n")
```







Exercise 3 (Metropolis-Hastings sampler for a logistic regression)

3.1

Explain Metropolis-Hastings sampler

3.2

```
MH.sampler <- function(x,         # covariate values
                       y,         # number of mice deaths
                       n,         # total number of mice
                       sigma2 = 10^(4), # variance of normal priors
                       n.iter = 10000,  # number of MCMC iterations
                       n.burnin = 4000, # burnin length
                       n.thin = 1,        # thinning parameter
                       alpha = 0,       # starting point
                       beta = 0,        # starting point
                       s_alpha = 1,     # SD for normal proposal
                       s_beta = 60      # SD for normal proposal
                       ) {

  ####################
  ## Bayesian analysis
  ####################

  # inverse logit: logit^(-1)(alpha + beta*x)
  mypi <- function(alpha, beta, x){
    tmp <- exp(alpha + beta*x)
    pi <- tmp/(1+tmp)
    return(pi)
  }



  #####################################
  ## Step 1: R: (univariate proposal) Metropolis MCMC settings
  #####################################
```

```r
alpha_samples <- c()
beta_samples <- c()
# number of accepted proposals
alpha_yes <- 0
beta_yes <- 0

# counter
count <- 0

# start the MCMC algorithm (the first iteration after the burn-in is 1)
for(i in -n.burnin:(n.iter*n.thin)){
  count <- count + 1

  ## update alpha
  # generate a new proposal for alpha
  alpha_star <- rnorm(1, alpha, sd=s_alpha)

  # NOTE: it is more stable to calculate everything on the log scale
  enum <- sum(dbinom(y, size=n, prob=mypi(alpha_star, beta, x), log=TRUE)) +
    dnorm(alpha_star, mean=0, sd=sqrt(sigma2), log=TRUE)
  denom <- sum(dbinom(y, size=n, prob=mypi(alpha, beta, x), log=TRUE))  +
    dnorm(alpha, mean=0, sd=sqrt(sigma2), log=TRUE)

  # log accetpance rate (since we use a random walk proposal there is no
  #   proposal ratio in the acceptance probability)
  logacc <- enum - denom
  if(log(runif(1)) <= logacc){
    # accept the proposed value
    alpha <- alpha_star
    alpha_yes <- alpha_yes + 1
  }

  ## update beta
  # generate a new proposal for beta
  beta_star <- rnorm(1, beta, sd=s_beta)

  enum <- sum(dbinom(y, size=n, prob=mypi(alpha, beta_star, x), log=TRUE)) +
    dnorm(beta_star, mean=0, sd=sqrt(sigma2), log=TRUE)
  denom<- sum(dbinom(y, size=n, prob=mypi(alpha, beta, x), log=TRUE)) +
    dnorm(beta, mean=0, sd=sqrt(sigma2), log=TRUE)
  # log accetpance rate
  logacc <- enum - denom

  if(log(runif(1)) <= logacc){
    # accept the proposed value
    beta <- beta_star
    beta_yes <- beta_yes + 1
  }

  # after the burnin save every kth sample
  if((i > 0) && (i%%n.thin == 0)){
    alpha_samples <- c(alpha_samples, alpha)
    beta_samples <- c(beta_samples, beta)
  }
  if(i%%1000 ==0){
    # print the acceptance rates on the fly
    cat(c(i, alpha_yes/count, beta_yes/count), "\n")
    }
  }
  return(list(alpha_samples=alpha_samples,
              beta_samples=beta_samples))
}
```

```
x_original <- c(0.0028, 0.0028, 0.0056, 0.0112, 0.0225, 0.0450)
# the centered covariate values (centered dose)
x <- x_original - mean(x_original)
# number of mice deaths
# y <- c(35, 21, 9, 6, 1)
y <- c(26, 9, 21, 9, 6, 1)
# total number of mice
# n <- c(40, 40, 40, 40, 40)
n <- c(28, 12, 40, 40, 40, 40)
```

```
d.mice <- data.frame(
  x_original, y, n, x, y/n
)
colnames(d.mice) <- c("$x$", "$y$", "$n$", "centered $x$", "$p$")
knitr::kable(d.mice, align="c", caption="Mice data from Collett (2003)")
```

Table 2: Mice data from Collett (2003)

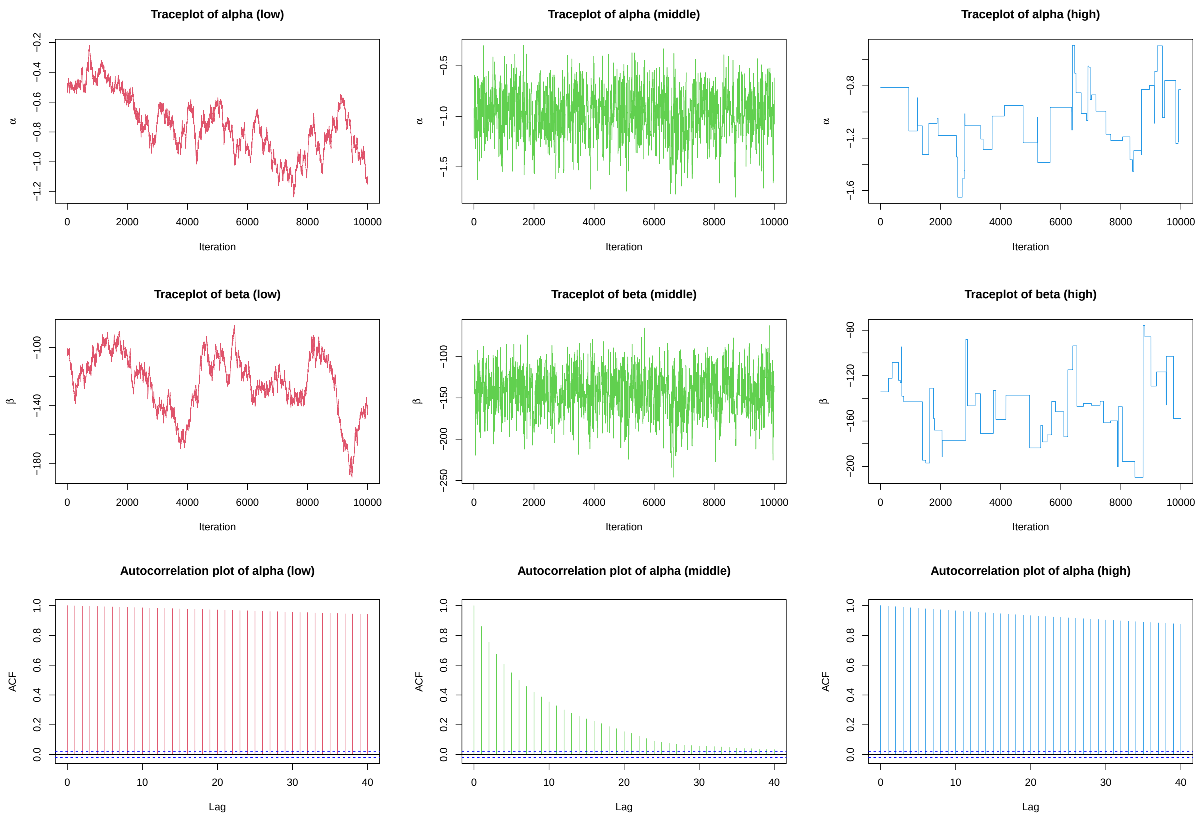
$x$	$y$	$n$	centered $x$	$p$
0.0028	26	28	-0.0121833	0.9285714
0.0028	9	12	-0.0121833	0.7500000
0.0056	21	40	-0.0093833	0.5250000
0.0112	9	40	-0.0037833	0.2250000
0.0225	6	40	0.0075167	0.1500000
0.0450	1	40	0.0300167	0.0250000

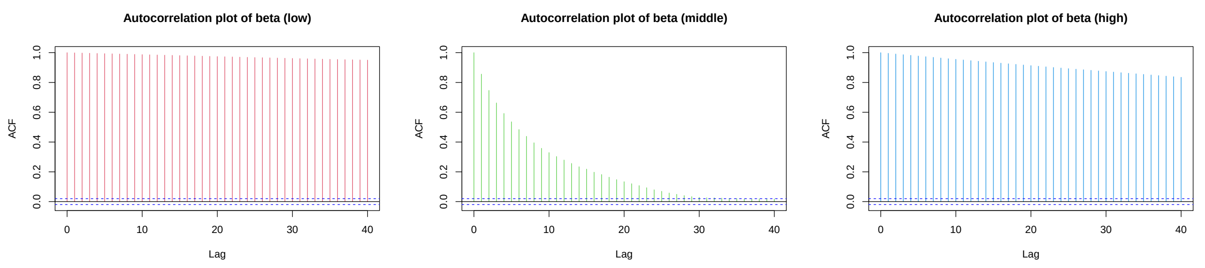
```
low <- c(0.01, 1)
middle <- c(1, 100)
high <- c(50, 5000)

set.seed(44566)
cat("\n---------Low values---------\n")
low.sampler <- MH.sampler(x=x, y=y, n=n, s_alpha=low[1], s_beta=low[2])

cat("\n---------Middle values---------\n")
middle.sampler <- MH.sampler(x=x, y=y, n=n, s_alpha=middle[1], s_beta=middle[2])

cat("\n---------High values---------\n")
high.sampler <- MH.sampler(x=x, y=y, n=n, s_alpha=high[1], s_beta=high[2])
```

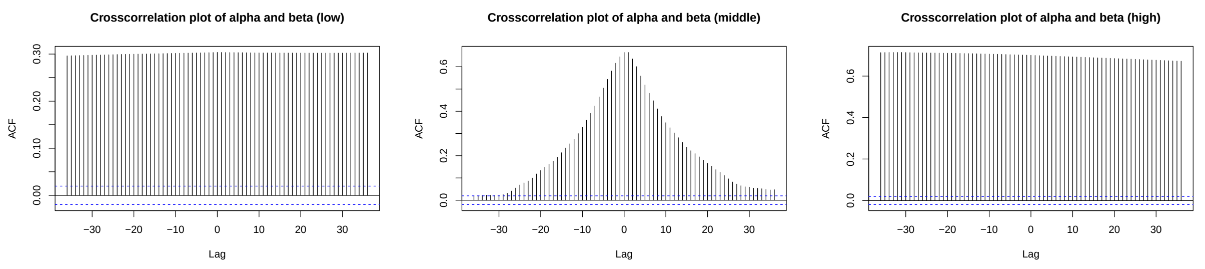
```
##
## ---------Low values---------
## -4000 1 0
## -3000 0.9440559 0.9090909
## -2000 0.966017 0.9355322
## -1000 0.9723426 0.9510163
## 0 0.9740065 0.9562609
## 1000 0.9696061 0.9638072
## 2000 0.9691718 0.9671721
## 3000 0.9714327 0.9705756
## 4000 0.9715036 0.9703787
## 5000 0.9726697 0.9706699
## 6000 0.9740026 0.9720028
## 7000 0.975275 0.9740933
## 8000 0.9753354 0.9750021
## 9000 0.9760018 0.9746173
## 10000 0.976216 0.974359
##
## ---------Middle values---------
## -4000 0 0
## -3000 0.2297702 0.2327672
## -2000 0.2278861 0.2358821
## -1000 0.2172609 0.2372542
## 0 0.2124469 0.2386903
## 1000 0.2167566 0.2343531
## 2000 0.2132978 0.2287952
## 3000 0.2141123 0.2286816
## 4000 0.2144732 0.2294713
## 5000 0.213754 0.229419
## 6000 0.2141786 0.230377
## 7000 0.216344 0.2305245
## 8000 0.2147321 0.2301475
## 9000 0.2136759 0.229367
## 10000 0.2134133 0.2302693
##
## ---------High values---------
## -4000 0 0
## -3000 0.003996004 0.004995005
## -2000 0.004497751 0.005497251
## -1000 0.004331889 0.005331556
## 0 0.003999 0.004248938
## 1000 0.00339932 0.00479904
## 2000 0.003832695 0.004832528
## 3000 0.004142265 0.004713612
## 4000 0.0039995 0.004624422
## 5000 0.003777358 0.004332852
## 6000 0.00369963 0.00439956
## 7000 0.004272339 0.004454141
## 8000 0.004249646 0.004582951
## 9000 0.004461195 0.004538112
## 10000 0.004713949 0.004571102
```

When the tuning parameters of the proposals are set to middle $(1, 100)$, the optimal acceptance rate is attained.

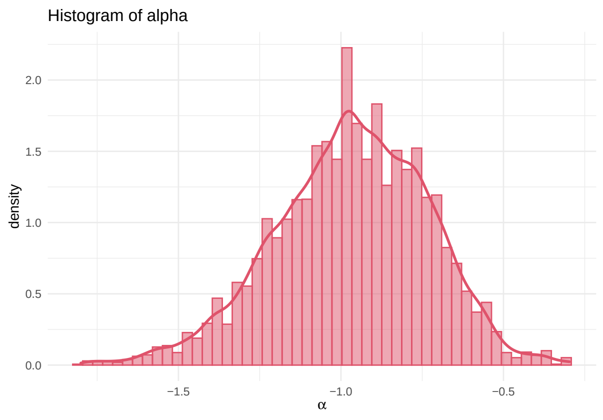
```r
alpha_low <- low.sampler$alpha_samples
beta_low <- low.sampler$beta_samples

alpha_middle <- middle.sampler$alpha_samples
beta_middle <- middle.sampler$beta_samples

alpha_high <- high.sampler$alpha_samples
beta_high <- high.sampler$beta_samples

plot(x=1:length(alpha_low), y=alpha_low, type="l", col=2,
     xlab="Iteration", ylab=expression(alpha), main="Traceplot of alpha (low)")
plot(x=1:length(alpha_middle), y=alpha_middle, type="l", col=3,
     xlab="Iteration", ylab=expression(alpha), main="Traceplot of alpha (middle)")
plot(x=1:length(alpha_high), y=alpha_high, type="l", col=4,
     xlab="Iteration", ylab=expression(alpha), main="Traceplot of alpha (high)")

plot(x=1:length(beta_low), y=beta_low, type="l", col=2,
     xlab="Iteration", ylab=expression(beta), main="Traceplot of beta (low)")
plot(x=1:length(beta_middle), y=beta_middle, type="l", col=3,
     xlab="Iteration", ylab=expression(beta), main="Traceplot of beta (middle)")
plot(x=1:length(beta_high), y=beta_high, type="l", col=4,
     xlab="Iteration", ylab=expression(beta), main="Traceplot of beta (high)")

acf(alpha_low, col=2, main="Autocorrelation plot of alpha (low)")
acf(alpha_middle, col=3, main="Autocorrelation plot of alpha (middle)")
acf(alpha_high, col=4, main="Autocorrelation plot of alpha (high)")

acf(beta_low, col=2, main="Autocorrelation plot of beta (low)")
acf(beta_middle, col=3, main="Autocorrelation plot of beta (middle)")
acf(beta_high, col=4, main="Autocorrelation plot of beta (high)")

ccf(alpha_low, beta_low, main="Crosscorrelation plot of alpha and beta (low)")
ccf(alpha_middle, beta_middle, main="Crosscorrelation plot of alpha and beta (middle)")
ccf(alpha_high, beta_high, main="Crosscorrelation plot of alpha and beta (high)")
```

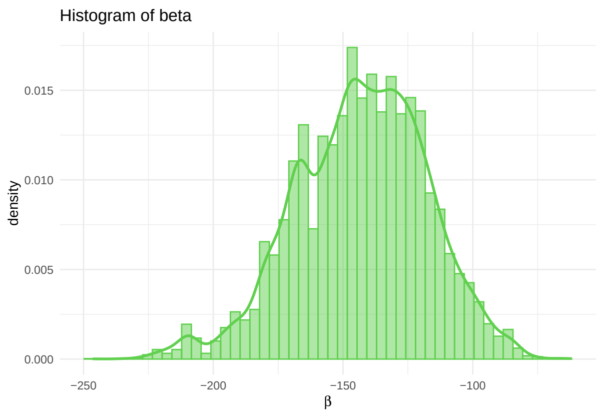






```r
d.MH <- data.frame(
  alpha = alpha_middle,
  beta  = beta_middle
)

ggplot(d.MH, aes(x=alpha, y=..density..)) +
  geom_histogram(color=2, fill=2, alpha=0.5, bins=50) +
  geom_density(color=2, lwd=1) +
  labs(title="Histogram of alpha", x=expression(alpha)) +
  theme_minimal()

ggplot(d.MH, aes(x=beta, y=..density..)) +
  geom_histogram(color=3, fill=3, alpha=0.5, bins=50) +
  geom_density(color=3, lwd=1) +
  labs(title="Histogram of beta", x=expression(beta)) +
  theme_minimal()
```





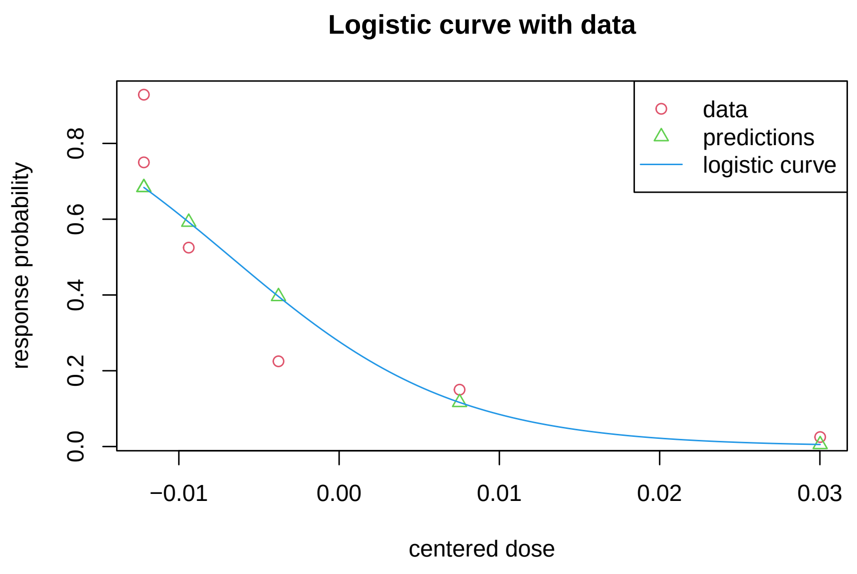
```r
d.summary <- t(
  rbind(
    colMeans(d.MH),
    sapply(d.MH, function(x) sd(x)),
    sapply(d.MH, function(x) quantile(x, probs=c(0.025, 0.5, 0.975)))
  )
)
```

```
d.summary <- data.frame(d.summary)
colnames(d.summary) <- c("Mean", "SD", "2.5%", "Median", "97.5%")

knitr::kable(d.summary, align="c",
             caption="Summary statistics of marginal posteriors (middle choice)")
```

Table 3: Summary statistics of marginal posteriors (middle choice)

	Mean	SD	2.5%	Median	97.5%
alpha	-0.9673889	0.2352573	-1.461707	-0.9592253	-0.5537754
beta	-143.0714300	25.3517136	-196.708001	-142.0147341	-96.3710245

```
med.alpha <- d.summary$Median[1]
med.beta <- d.summary$Median[2]

# inverse logit: logit^(-1)(alpha + beta*x)
mypi <- function(alpha, beta, x){
  tmp <- exp(alpha + beta*x)
  pi <- tmp/(1+tmp)
  return(pi)
}

x.grid <- seq(min(x), max(x), length.out=100)
y.pred <- mypi(alpha=med.alpha, beta=med.beta, x=x.grid)

plot(x=x, y=y/n, col=2, xlab="centered dose", ylab="response probability",
     main="Logistic curve with data")
points(x=x, y=mypi(alpha=med.alpha, beta=med.beta, x=x), col=3, pch=2)
lines(y.pred ~ x.grid, col=4)
legend("topright", legend=c("data", "predictions", "logistic curve"),
       col=2:4, lty=c(NA, NA, 1), pch=c(1, 2, NA))
```


Logistic curve with data
data
predictions
logistic curve
response probability
centered dose