Worksheet 4

Foundations of Bayesian Methodology

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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 $\sigma^2 = 16$.

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

```r
# 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
```

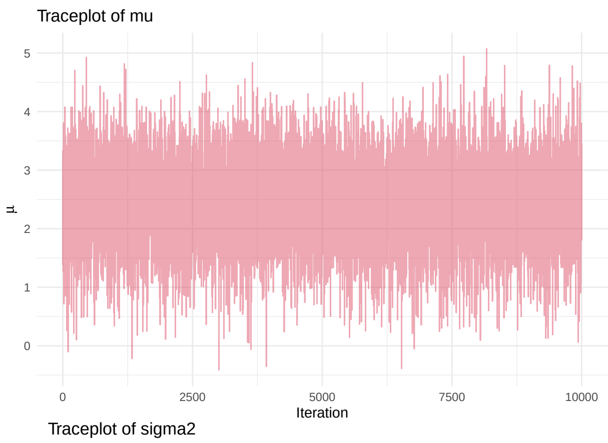
```
# n.iter samples after n.burnin taking every n.thin'th sample
dim(gibbs_samples)
```

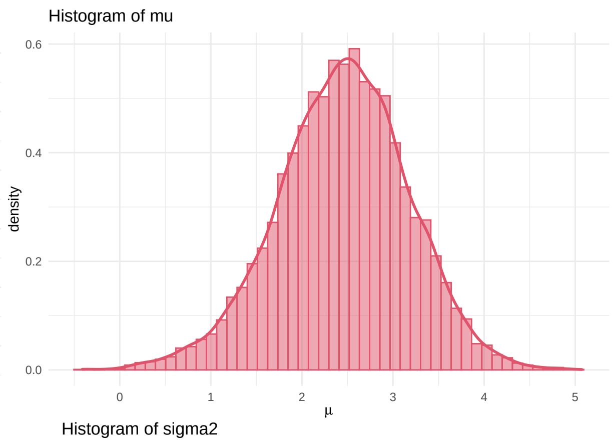
```
## [1] 10000     3
```

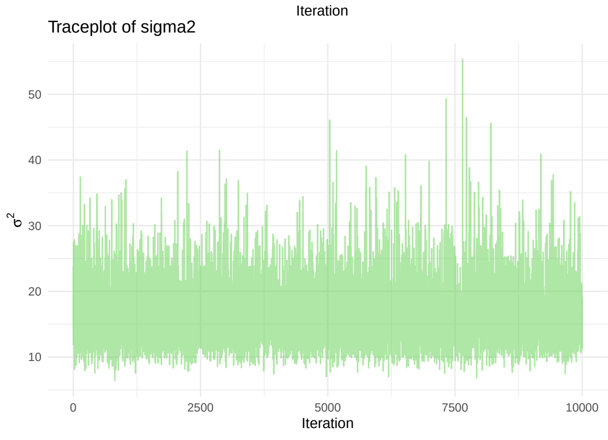
```
mu_gibbs_samples <- gibbs_samples[,"mu"]
sigma2_gibbs_samples <- gibbs_samples[,"sigma2"]
inv_sigma2_gibbs_samples <- gibbs_samples[,"inv_sigma2"]
```

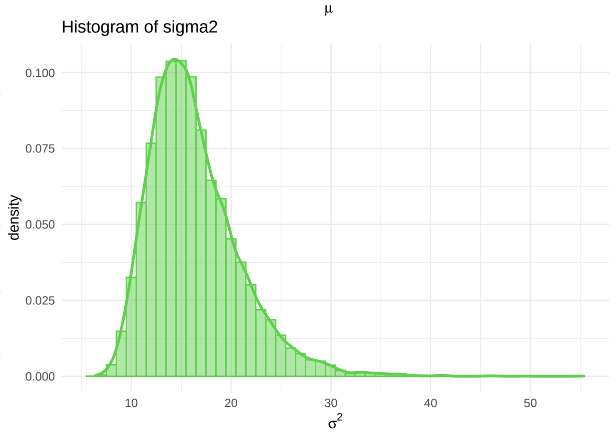
```
library(ggplot2)

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
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()
```

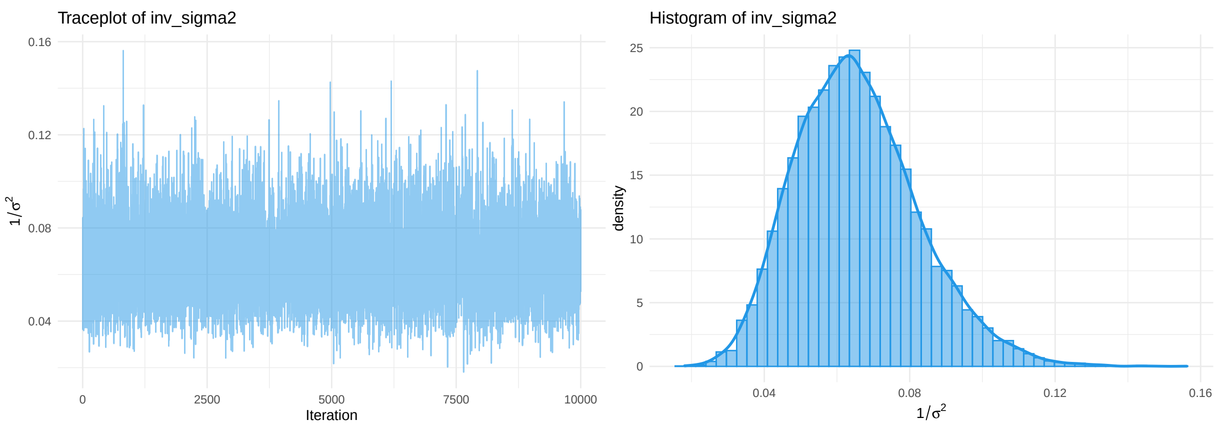
```r
## Histogram/Density of sigma2
ggplot(d.gibbs, aes(x=sigma2, y=..density..)) +
  geom_histogram(color=3, fill=3, alpha=0.5, bins=50) +
  geom_density(color=3, lwd=1) +
  labs(title="Histogram of sigma2", x=expression(sigma^2)) +
  theme_minimal()

## 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")
```

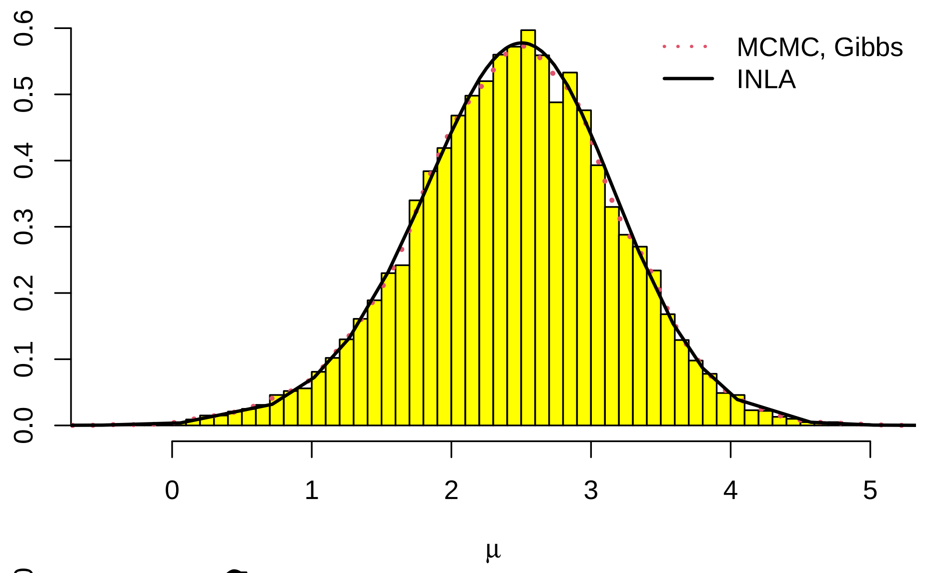
Table 1: Summary statistics of the marginal posteriors

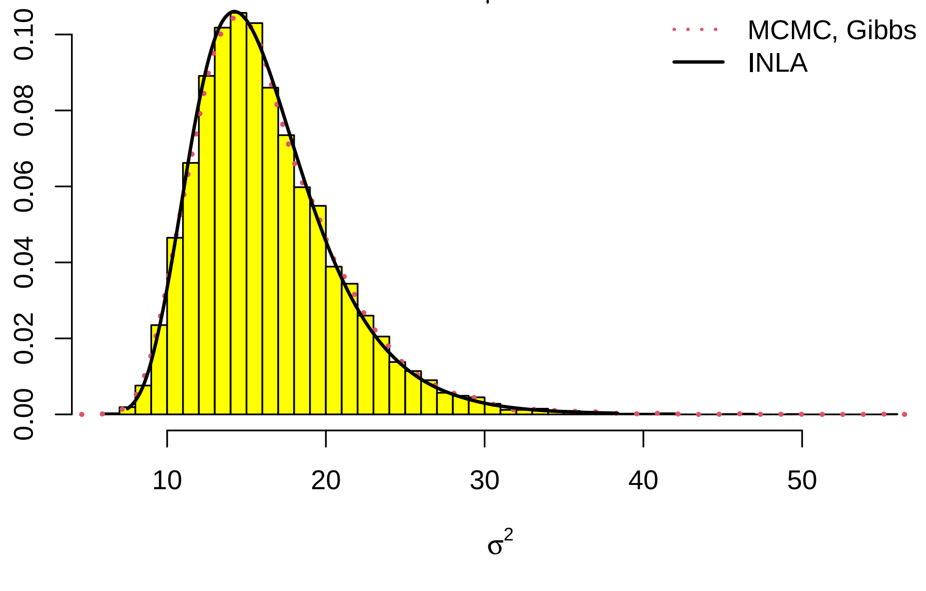
	Mean	SD	2.5%	Median	97.5%
mu	2.4479404	0.7206035	0.9436683	2.4692436	3.808022
sigma2	16.3331563	4.5483340	9.7333046	15.5669100	27.221752
inv_sigma2	0.0656163	0.0169525	0.0367353	0.0642388	0.102740

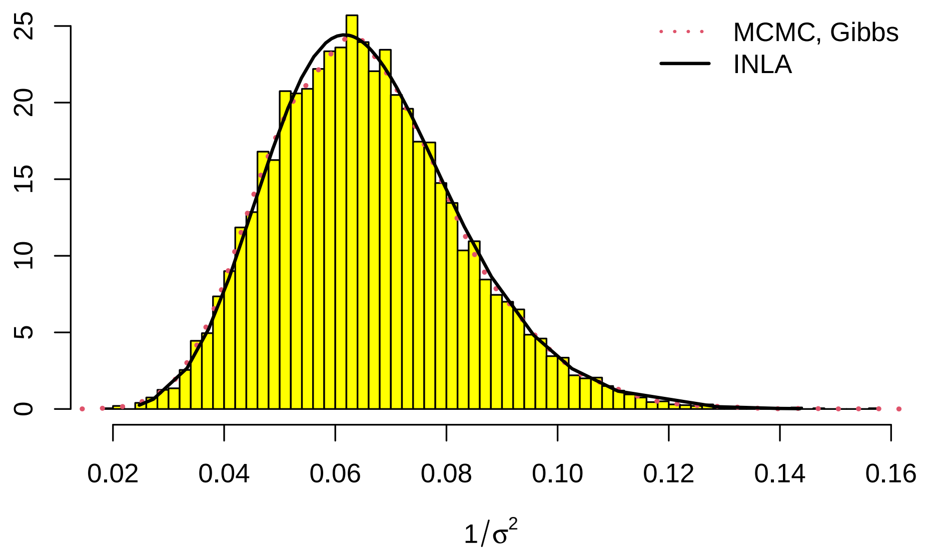
```r
# plots (compare with INLA)
# INLA is exact

# 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")
```







MCMC, Gibbs
INLA
0
5
10
15
20
25
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
$1/\sigma^2$

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

3.1

The aim of the Metropolis-Hastings algorithm is to generate a collection of states (here parameters α, β) that describe our target distribution, which is the logistic regression $f(\alpha, \beta|\boldsymbol{y}, \boldsymbol{n}, \boldsymbol{x})$. Via a Markov process, the state (the parameters) should converge to a stationary state which is the desired target distribution.

The algorithm starts with the so called condition of detailed balance and means simply that each transition, for example $\alpha \to \alpha'$, is reversible and happens with the same probability. More specifically this means the probability to be in state α and transitioning to state α' is equal to the probability to be in state α' and transitioning to state α.

$$\underbrace{P(\alpha'|\alpha)}_{\text{Transitioning to state } \alpha' \text{ given one is in } \alpha} \cdot \underbrace{f(\alpha, \beta|\boldsymbol{y}, \boldsymbol{n}, \boldsymbol{x})}_{\text{P to be in state } \alpha} = P(\alpha|\alpha')f(\alpha', \beta|\boldsymbol{y}, \boldsymbol{n}, \boldsymbol{x})$$

Which can be rewritten as:

$$\frac{P(\alpha'|\alpha)}{P(\alpha|\alpha')} = \frac{f(\alpha', \beta|\boldsymbol{y}, \boldsymbol{n}, \boldsymbol{x})}{f(\alpha, \beta|\boldsymbol{y}, \boldsymbol{n}, \boldsymbol{x})}$$

For simplicity we focus her on one transition, namely $P(\alpha'|\alpha)$ but the same procedures also hold for the back-transition $P(\alpha|\alpha')$. Now, the transition $P(\alpha'|\alpha)$ has to be split into two steps. The first one is to "propose" the next value (α') and the second one is to accept this proposal or not. The proposal distribution $q(\alpha'|\alpha)$ is in our case a normal distribution, so $\alpha' \sim \mathcal{N}(\alpha, \sigma_\alpha^2)$ and this means that the proposed value α' is depending on the current value α but the spread is defined by a tuning parameter σ_α^2 which kind of defines the update step. The acceptance distribution $A(\alpha', \alpha)$ does not have to be defined here as we will see. We can now rewrite:

$$\begin{aligned}\frac{A(\alpha', \alpha) \cdot q(\alpha'|\alpha)}{A(\alpha, \alpha') \cdot q(\alpha|\alpha')} &= \frac{f(\alpha', \beta|\boldsymbol{y}, \boldsymbol{n}, \boldsymbol{x})}{f(\alpha, \beta|\boldsymbol{y}, \boldsymbol{n}, \boldsymbol{x})} \\ \frac{A(\alpha', \alpha)}{A(\alpha, \alpha')} &= \frac{f(\alpha', \beta|\boldsymbol{y}, \boldsymbol{n}, \boldsymbol{x}) \cdot q(\alpha|\alpha')}{f(\alpha, \beta|\boldsymbol{y}, \boldsymbol{n}, \boldsymbol{x}) \cdot q(\alpha'|\alpha)}\end{aligned}$$

In case of the Metropolis-Hastings algorithm the acceptance ratio $\frac{A(\alpha', \alpha)}{A(\alpha, \alpha')}$ can be written as A^α and it is forced to be lower or equal to 1 by definition. When we achieve an acceptance ratio larger than 1, which is theoretically possible, we will assume an acceptance ratio of 1, meaning that we will change from the current state α to the proposed state α' with a probability of 100%.

$$A^\alpha = \min\left(1, \frac{f(\alpha', \beta|\boldsymbol{y}, \boldsymbol{n}, \boldsymbol{x}) \cdot q(\alpha|\alpha')}{f(\alpha, \beta|\boldsymbol{y}, \boldsymbol{n}, \boldsymbol{x}) \cdot q(\alpha'|\alpha)}\right)$$

Now, if we get a proposed value α' that is more probable then the current value α this means that the acceptance ratio A^α is higher than 1 and we should always accept this value. On the other hand, if we get a proposed value that is less likely we should sometimes accept it. This is achieved by adding a stochastic component in form of a random sample from the uniform distribution. If the acceptance ratio is higher then the random sample we still accept this point. If it is lower we reject and stick with the current value α.

```r
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
                       alpha_yes_history = rep(0,n.burnin + n.iter*n.thin),
                        beta_yes_history = rep(0,n.burnin + n.iter*n.thin)
                       ) {

  ####################
  ## 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
  #####################################

  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
      alpha_yes_history[count] <- 1
      beta_yes_history[count] <- 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
      print(cbind("i"=as.integer(i), "acc.rate alpha"=alpha_yes/count,
                  "acc.rate beta"=beta_yes/count))
    }
  }
  #output:
  output <- list("alpha_samples"=alpha_samples, "beta_samples"=beta_samples,
                 "alpha_yes"=alpha_yes, "beta_yes"=beta_yes,
                 "alpha_yes_history"= alpha_yes_history,
                 "beta_yes_history"= beta_yes_history)
return(output)
}
```

```r
x_original <- c(0.0028, 0.0028, 0.0056, 0.0112, 0.0225, 0.0450)
# the centered covariate values (centered dose) from the Mice data from Collett
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)
```

```r
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)

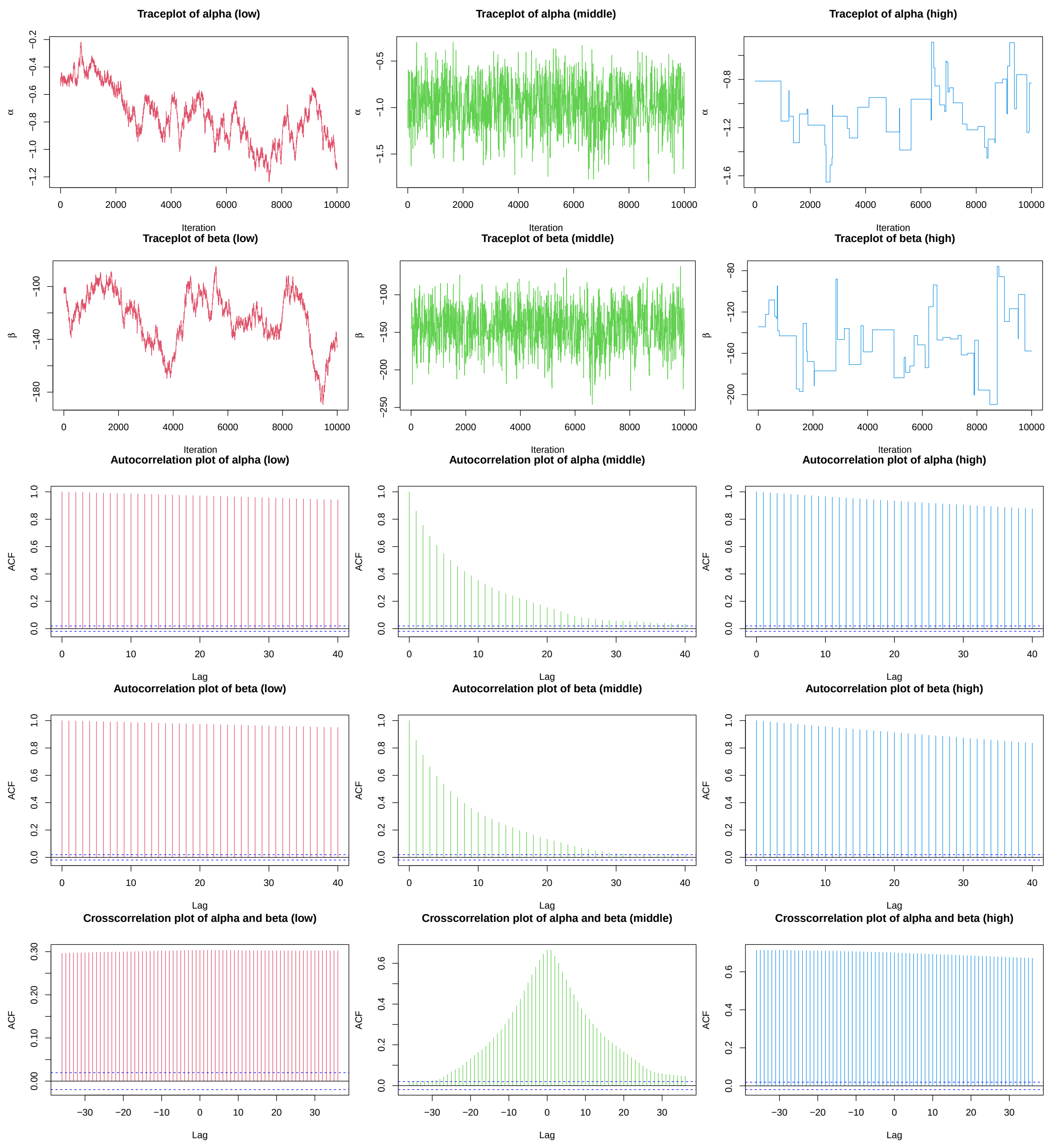
$x$	$y$	$n$	centered $x$	$p$
0.0028	26	28	-0.0121833	0.9285714
0.0028	9	12	-0.0121833	0.7500000
0.0056	21	40	-0.0093833	0.5250000
0.0112	9	40	-0.0037833	0.2250000
0.0225	6	40	0.0075167	0.1500000
0.0450	1	40	0.0300167	0.0250000

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

3.2

```
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, col=2,
    main="Crosscorrelation plot of alpha and beta (low)")
ccf(alpha_middle, beta_middle, col=3,
    main="Crosscorrelation plot of alpha and beta (middle)")
ccf(alpha_high, beta_high, col=4,
    main="Crosscorrelation plot of alpha and beta (high)")
```



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

With high tuning parameters s_alpha and s_beta which are in form of the standard deviations of the proposal distribution $\theta' \sim \mathcal{N}(\theta_i, \sigma_\theta^2)$ the proposed value gets easier or harder accepted. If the standard devation is high, the proposed value is hardly accepted (low acceptance rate). This can also be seen in the traceplots for high α and β values, where horizontal lines are obtained, which indicates a low acceptance rate and a "stucking" of the algorithm at the same value. Additionally, the autocorrelation (ACF) and crosscorrelation (CCF) plots for high α an β values show a high correlation between the steps. This comes from the fact that we obtain a small acceptance rate and therefore a large probability of staying with the same value for some time.

If the standard deviation is too low, the acceptance rate is high but each updating step only converges rather slowly which means the updated value is very very similar to the value before. This also means for the ACF and CCF plots that the correlation is rather high because the iterative values, although they are not the same, are still very similar leading to a high correlation.

3.3

```
par(mfrow = c(1,2))
plot(cumsum(low.sampler$alpha_yes_history)/
       c(1:length(cumsum(low.sampler$alpha_yes_history))) ,
     type = "l",main = "",ylab = "Acceptance Rate",xlab = "Iteration",
     ylim=c(0,1))
polygon(x = c(0,0,14000,14000), y=c( 0.2,0.4,0.4,0.2) ,col="pink")
lines(cumsum(middle.sampler$alpha_yes_history)/
        c(1:length(cumsum(middle.sampler$alpha_yes_history))),col = "red")
lines(cumsum(high.sampler$alpha_yes_history)/
        c(1:length(cumsum(high.sampler$alpha_yes_history))),col = "blue")
abline(v = 4000,lty = 3, col ="gray")
legend("center", col = c("black","red","blue"),lty = 1,
       legend = c("low: 0.01","middle: 1","high: 50"),
       title = expression(alpha), cex = 0.6,bg="white")

plot(cumsum(low.sampler$beta_yes_history)/
       c(1:length(cumsum(low.sampler$beta_yes_history))) ,
     type = "l",main = "",ylab = "Acceptance Rate",xlab = "Iteration",
     ylim=c(0,1))
polygon( x = c(0,0,14000,14000), y=c( 0.2,0.4,0.4,0.2) ,col="pink")
lines(cumsum(middle.sampler$beta_yes_history)/
        c(1:length(cumsum(middle.sampler$beta_yes_history))),col = "red")
lines(cumsum(high.sampler$beta_yes_history)/
        c(1:length(cumsum(high.sampler$beta_yes_history))),col = "blue")
abline(v = 4000,lty = 3, col ="gray")
legend("center", col = c("black","red","blue"),lty = 1,
       legend = c("low: 0.01","middle: 1","high: 50"),
       title = expression(beta), cex = 0.6,bg="white")
```

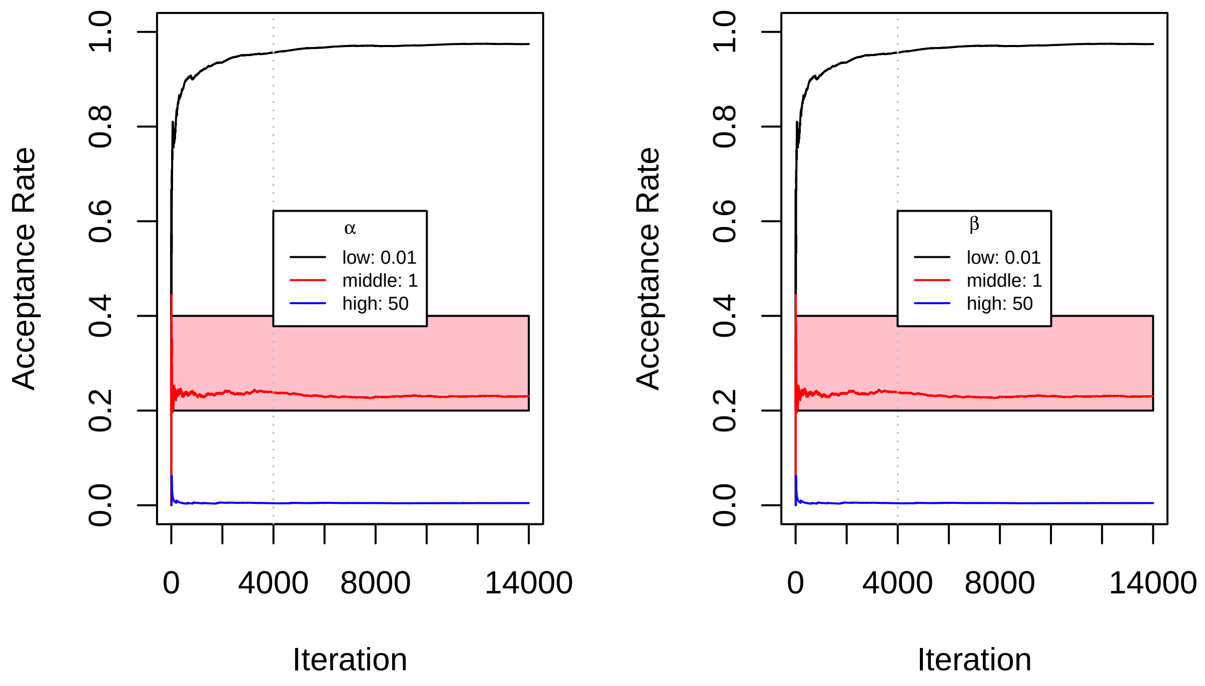
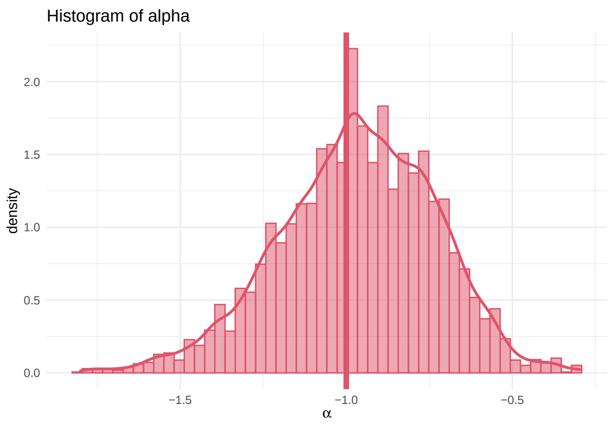


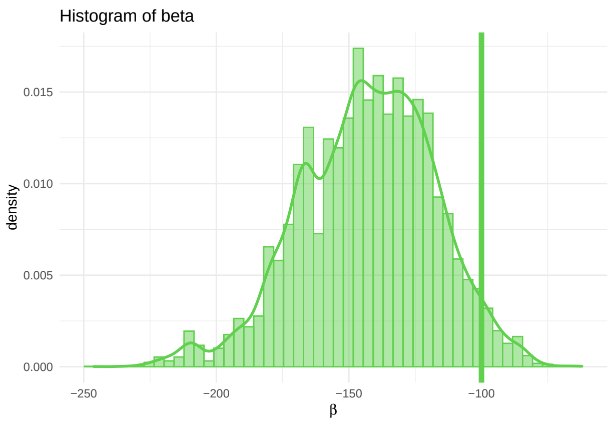
Figure 1: Acceptance rate versus number of iterations.

According to the "Rule of thumb" the optimal acceptance rate is between 0.2 and 0.4. SO the optimal tuning parameters of the proposal distributions in this case are obtained when the α proposal distribution has a standard deviation of 1 and the β proposal distribution has a standard deviation of 100.

Approach with Histograms:

```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()+
  geom_vline(xintercept =-1, color=2, lwd=2)

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()+
  geom_vline(xintercept =-100, color=3, lwd=2)
```





3.4

The following table illustrates the summary statistics of the marginal posteriors for α and β for the middle choice of tuning parameters $(=(\alpha = 1, \beta = 100))$.

```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

3.5

```
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="")
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))
```

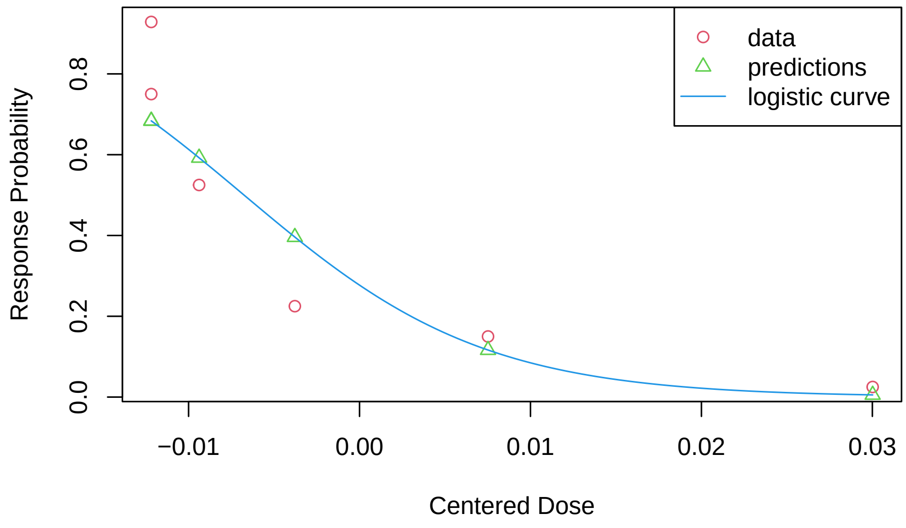


Figure 2: Logistic Curve plotted together with mice Data from Collett [1]

References:

[1] Collett, D. (2003). Modelling Binary Data. Second Edition. Chapman & Hall/CRC.