Worksheet 04 Group 2

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```
library(tidyverse)
library(rjags)
library(coda)
library(bayesmeta)
library(pCalibrate)
library(glue)
```

Exercise 2

TODO

Exercise 3

1

Explain step by step in your own words what the code in 04MHSampler.R is doing.

Preparation:

- Cleaning the environment; storing the dosage values, centered dosage values, number of deaths, and total number of mice in vectors
- Defining the variance for the normal priors
- Creating a function that takes the intercept and slope (α and β) and x (dosage) as input and returns the inverse logit function of the log-odds $\alpha + \beta x$, i.e. it projects it onto a scale between 0 and 1 and returns the corresponding p, which is the probability of death.
- Setting a seed, defining the number of iterations; burn-in length; and thinning parameter
- Preparing two empty vectors to store the sampled alpha and betas; two vectors with 0's of the length "number of iterations times thinning parameter", to record whether the proposals were accepted (1) or not (0); initial start values for alpha and beta; the standard deviations for the proposal distributions of alpha and beta (tuning parameters); and a counter that will track the counts of the for-loop
- The for-loop is set up to go from –burninlength (negative) to the number of desired iterations times the thinning parameter. The current loop number is called i.

For-Loop:

1. At the beginning of each loop, the counter is updated by 1 (however it's not really needed)
2. A new proposal for alpha (alpha*) is sampled from the proposal distribution, which is a univariate normal distribution centered around the current alpha with a pre-defined standard deviation (tuning parameter).
3. The inverse-logit function transforms $\alpha^* + \beta x$ into probability of death pi on a scale from 0 to 1. X is a vector of dosages so it returns a vector of pi's. The pi's are then passed as parameters to the binomial distribution function to calculate the log-likelihood of the observed proportions of dead mice given the corresponding pi. The log-likelihood is then added to the log of the prior density for alpha*. The prior follows a normal distribution with mean 0 and an assumed variance. The sum of the log-likelihood and the log-prior is proportionate to the log-posterior.
4. Step 3 is done again but this time with the current/old alpha value, instead of alpha*.
5. IF the difference of the log-posterior for alpha* minus the log-posterior for the old alpha is larger than a random value sampled from a standard uniform distribution, alpha* gets accepted and is now considered the current alpha. If not, the current alpha keeps its value.
6. Only if burn-in period is finished, i.e. if i $\geqslant$ 1 (otherwise this step is skipped): the current element in the acceptance vector for alpha is changed to 1 if the proposed alpha* was accepted, otherwise it keeps the default value 0.
7. Still within the same iteration, steps 2-6 are now repeated but for the beta parameter (slope)
8. Only if burn-in period is finished, i.e. if i $\geqslant$ 1 (otherwise this step is skipped): the current alpha and beta samples are stored in their corresponding vector. They are stored whether the values got accepted or not. If the thinning parameter k is $\neq 1$, only every k'th sample is stored in the vector.
9. Only if burn-in period is finished, i.e. if i $\geqslant$ 1 (otherwise this step is skipped): the acceptance rates are printed for every 1000th iteration, to keep track of the algorithm. The acceptance rate is the current number of accepted alphas resp. betas post-burn-in-period divided by the current nr. of iterations i.

2

Comment on the differences in traceplots, auto-correlations (acf()) and cross-correlations depending on the tuning parameters' choice. What are the reasons for observed differences?

```
rm(list=ls())

## Metropolis-Hastings for logistic model
## Two independent normal proposals

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

# Assumption
# variance of normal priors
sigma2 <- 10^(4)

# 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

# number of MCMC iterations
n.iter <- 10000
# burnin length
n.burnin <- 4000
# thinning parameter
n.thin <- 1
#n.thin <- floor((n.iter-n.burnin)/500)

## Putting everything into a function to then call it for tuning parameters
## univariate random walk proposals ##
MCMC_MH <- function(s_alpha, s_beta){ # Input: SD's of proposal distributions

  set.seed(44566)
  alpha_samples <- c()
  beta_samples <- c()
  # number of accepted proposals
  alpha_yes <- rep.int(0, times = n.thin*n.iter)
  beta_yes <- rep.int(0, times = n.thin*n.iter)

  # starting values
  alpha <- 0
```

```
beta <- 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
    if (i > 0){
      alpha_yes[i] <- 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
    if (i > 0){
      beta_yes[i] <- 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 > 0) && i%%1000 ==0){ ### skipping this
    # print the acceptance rates on the fly
```

```
      # cat(c(i, sum(alpha_yes)/i, sum(beta_yes)/i), "\n")
      #}
  }


  ## Plot results:

  # Traceplots
  print(glue("Traceplots:\n"))
  par(mfrow = c(1,2),mar = c(8, 5, 8, 1))
  plot(alpha_samples, type = "l", ylab = "Alpha", xlab = "Iteration")
  plot(beta_samples, type = "l", ylab = "Beta", xlab = "Iteration")

  # Autocorrelation plots
  print(glue("Autocorrelation and Cross-Correlation:"))
  par(mfrow = c(1,3), mar = c(8, 4, 12, 1), oma = c(1,1,3,1) )
  acf(alpha_samples, ylab = "ACF for alpha", main = "")
  acf(beta_samples, ylab = "ACF for beta", main = "")

  # Crosscorrelation
  ccf(alpha_samples, beta_samples, ylab = "Cross Correlation", main = "")

  # Acceptance Rates
  acceptance_alpha <- sum(alpha_yes)/(n.iter*n.thin)
  acceptance_beta <- sum(beta_yes)/(n.iter*n.thin)
  print(glue("Acceptance rate alpha: {acceptance_alpha} "))
  print(glue("Acceptance rate beta: {acceptance_beta} "))

  # Return MCMC and acceptance rate for alpha and beta
  return( list(alpha_samples, beta_samples, acceptance_alpha, acceptance_beta ) )

}
```

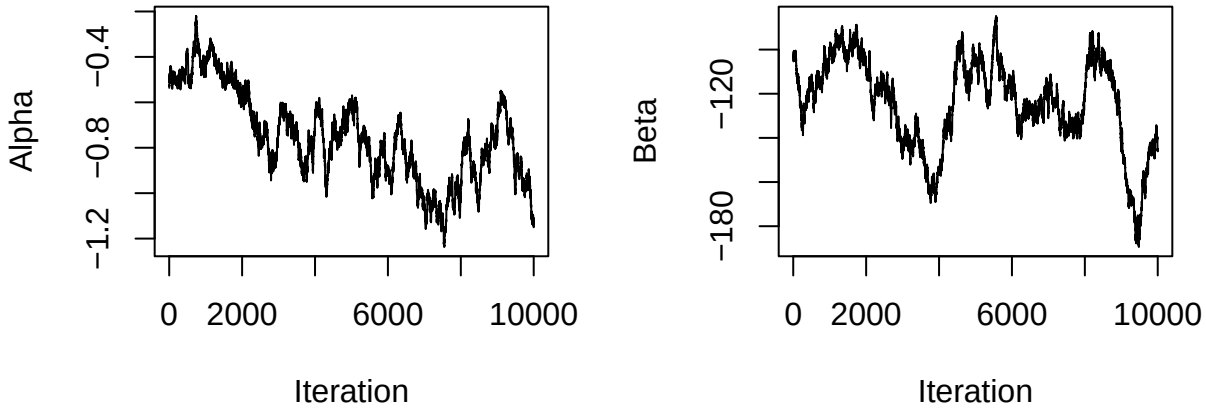
Now calling the function MCMC_MH to show the results:

```
# Defining 3 different sets of tuning parameters
s_alpha <- c(0.01, 1, 50)
s_beta <- c(1, 100, 5000 )
```

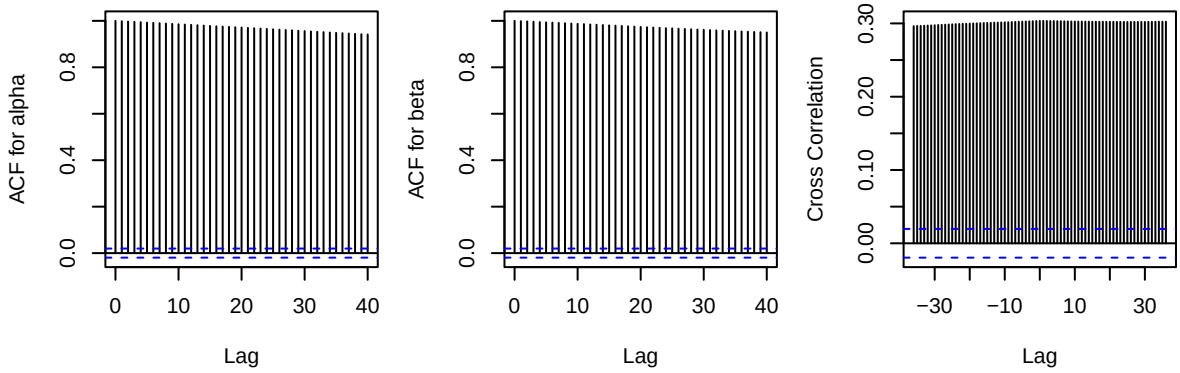
Results for low tuning parameters (0.01, 1):

```
MCMC_1_result <- MCMC_MH(s_alpha[1], s_beta[1])
```

```
## Traceplots:
```




```
## Autocorrelation and Cross-Correlation:
```



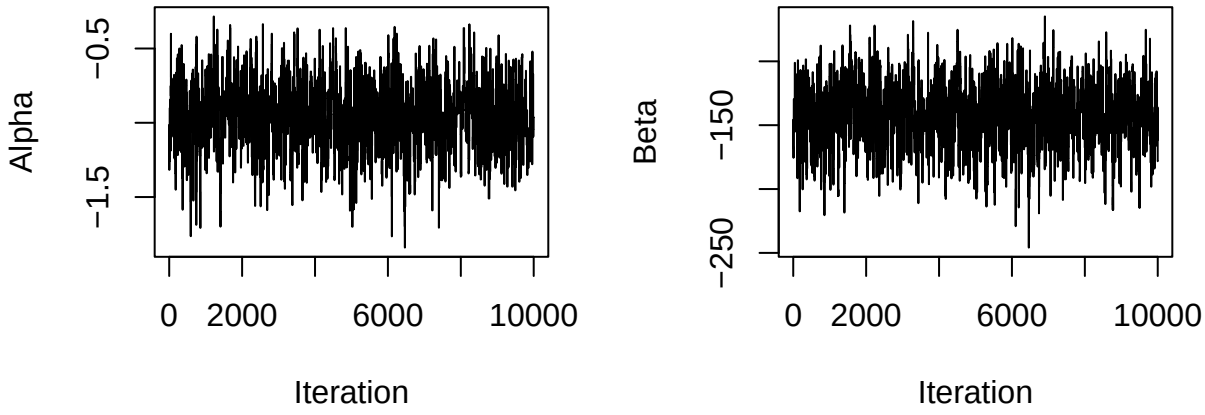

```
## Acceptance rate alpha: 0.9771
## Acceptance rate beta: 0.9816
```

The tuning parameters are the SDs of the proposal distributions for alpha and beta. With small tuning parameters, the proposal distributions are narrow. The new alpha and beta values are likely to be very close to the previous alpha and beta values, the exploration of the parameter space is done in small steps, so there is high autocorrelation and cross-correlation over many lags. The sampler doesn't take any "big risks" and so the acceptance rate is very high, but it doesn't explore the parameter space well. Also it can drift off and then it takes a lot of iterations to get back again to the region of high posterior density. It's not stationary.

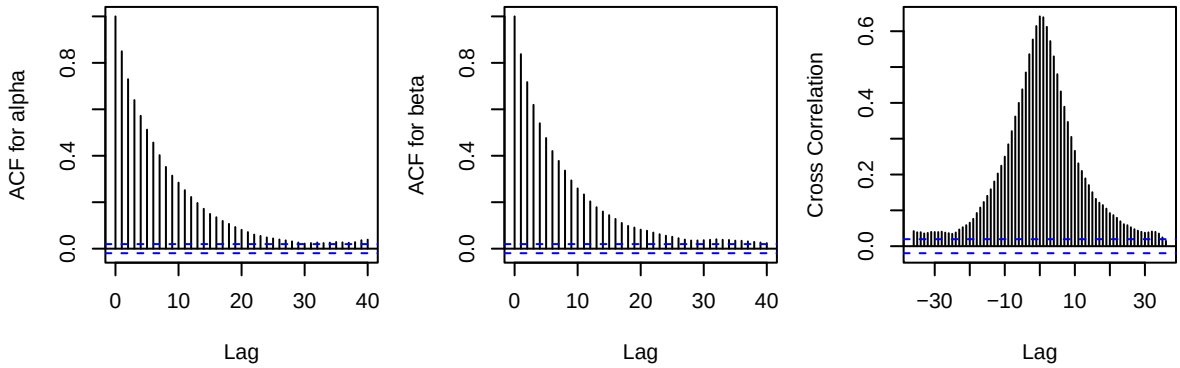
Results for medium tuning parameters (1, 100):

```
MCMC_2_result <- MCMC_MH(s_alpha[2], s_beta[2])
```

```
## Traceplots:
```




```
## Autocorrelation and Cross-Correlation:
```



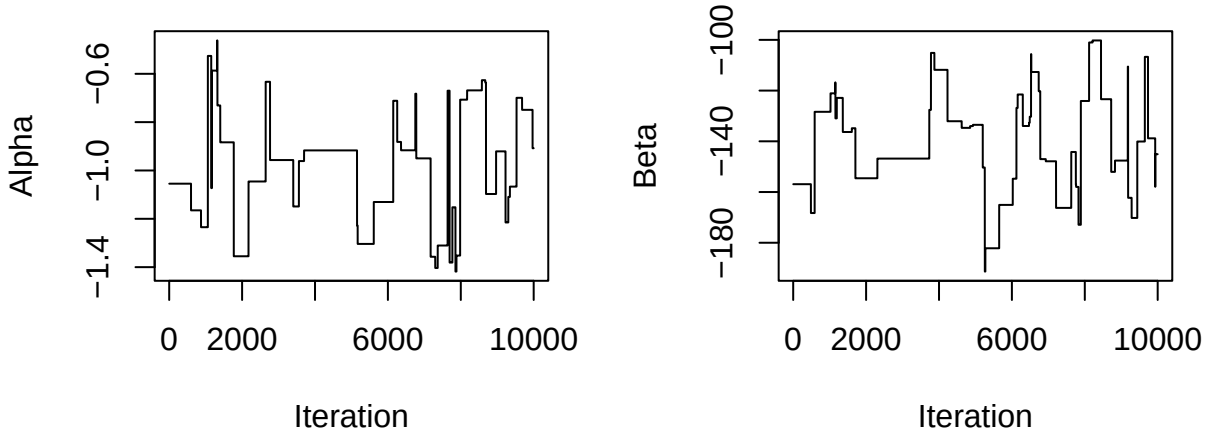

```
## Acceptance rate alpha: 0.2147
## Acceptance rate beta: 0.2295
```

With optimal SDs for the proposal distributions, the sampler has a good balance between exploration of the parameter space and acceptance rate. The traceplot is stationary. The sampler moves rapidly across the whole parameter space without getting stuck, leading to the characteristic caterpillar shape, and autocorrelation and cross-correlation quickly decaying to zero.

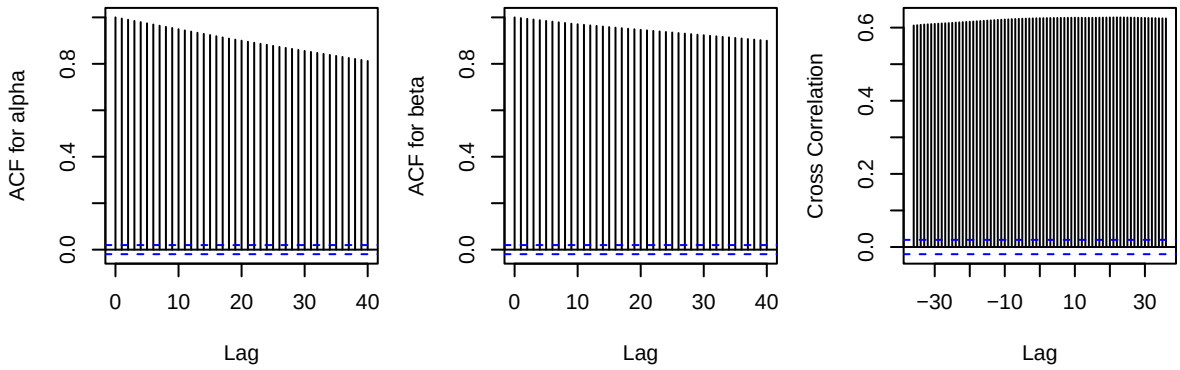
Results for high tuning parameters (50, 5000):

```
MCMC_3_result <- MCMC_MH(s_alpha[3], s_beta[3])
```

```
## Traceplots:
```




```
## Autocorrelation and Cross-Correlation:
```




```
## Acceptance rate alpha: 0.0043
## Acceptance rate beta: 0.0051
```

Here the SDs of the proposal distributions are large, leading to "adventurous" exploration, so the sampler often proposes parameter values far outside in the parameter space, under which the data is unlikely, leading to low acceptance rates. Due to low acceptance rates, the chain is often stuck at the same value over several iterations, leading to these skyline-like traceplots with constant values over several iterations and thus high autocorrelation over many lags. Only sporadically there's a big jump when the sampler proposes a value that is accepted by chance. There is also high cross-correlation over many lags because the samples stay constant over many iterations.

3

Under which condition the optimal acceptance rate of about 0.2-0.4 ("rule of thumb") is attained?

With medium tuning parameters (1, 100), the acceptance rates are optimal:
Acceptance rate alpha: 0.2147 Acceptance rate beta: 0.2295

4

Provide summaries (mean, sd, 0.025, 0.5, 0.975 quantiles) of the marginal posteriors for alpha and beta for the middle choice of tuning parameters.

```
alphas_2 <- unlist(MCMC_2_result[1])

glue("Mean alpha: {formatC(mean(alphas_2), 5)} ")
glue("SD alpha: {formatC(sd(alphas_2), 5)} ")
glue("Quantiles:")
quantile(alphas_2, c(0.025, 0.5, 0.975) )
```

```
## Mean alpha: -0.94995
## SD alpha: 0.22527
## Quantiles:
##       2.5%        50%      97.5%
## -1.3975759 -0.9352910 -0.5340364
```

```
betas_2 <- unlist(MCMC_2_result[2])

glue("Mean beta: {formatC(mean(betas_2), 5)} ")
glue("SD beta: {formatC(sd(betas_2), 5)} ")
glue("Quantiles:")
quantile(betas_2, c(0.025, 0.5, 0.975) )
```

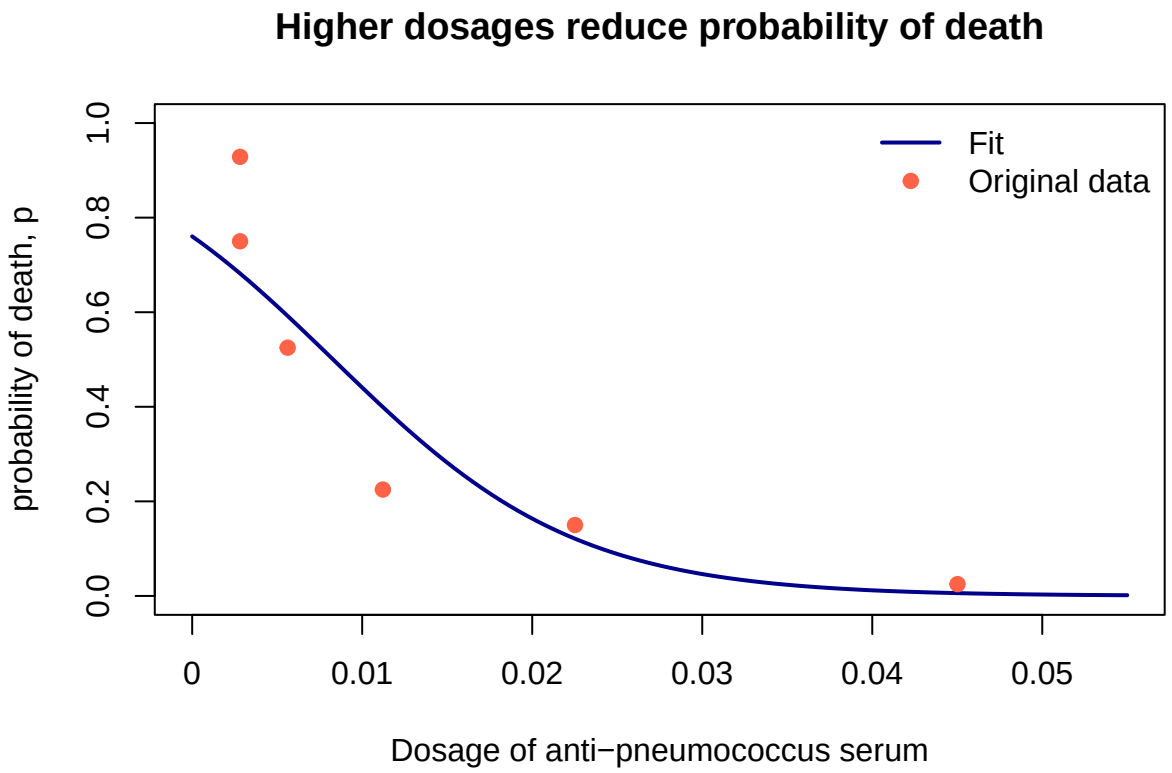
```
## Mean beta: -141.18
## SD beta: 24.388
## Quantiles:
##       2.5%        50%      97.5%
## -192.37525 -139.35901  -98.32787
```

5

Plot the logistic curve for median posterior values of α and β together with data and interpret the result.

```
median_alpha <- median(alphas_2)
median_beta <- median(betas_2)

curve( mypi(median_alpha, median_beta, x), from = -0.015, to = 0.04, ylim = c(0,1),
       xlab = "Dosage of anti-pneumococcus serum",
       ylab = "probability of death, p", xaxt = 'n', col = "darkblue", lwd = 2,
       main = "Higher dosages reduce probability of death" )
# Converting the dosages back to the uncentered, original values
breaks <- seq(-0.015, 0.04, by = 0.01)
axis(1, at = breaks, labels = as.character(round(breaks + mean(x_original), 2)) )
points(x, y/n, pch = 19, col = "tomato")
legend("topright", legend = c( "Fit", "Original data"),
       bty = "n", col = c("darkblue", "tomato"), lty = c(1,NA), pch = c(NA,19), lwd = c(2,NA) )
```



The resulting median beta is -139.359 and median alpha is -0.935.The modelled logistic curve is a good fit for the data, but it might slightly underestimate p for very low dosages. High dosages lead to lower probability of death, which is reflected in the negative beta value, and p is basically zero for dosages higher than 0.045. Of course, if the dosage would be too high, this might again be fatal, but this was not modelled here. For 1 unit increase in dosage x, the odds of death change by a factor of $exp(\beta)$, but since 1 unit is not really the scale that we're interested in, we could say that for an increase in dosage by 0.01, the odds of death change by a factor of $exp(\beta * 0.01) = 0.248$.