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:

- Store the dosage values, centered dosage values, number of deaths, and total number of mice in vectors
- Creating a function that takes the intercept and slope (α and β) and x (dosage) as input and returns the inverse logit function of $\alpha + \beta x$, i.e. it projects it onto a logistic scale between 0 and 1 to return the corresponding p, which is the probability of death.
- Defining number of iterations; burn-in length; thinning parameter; and standard deviations for the normal proposals
- Preparing empty vectors to store the sampled alpha and betas; a variable to record the number of accepted proposals; initial start values for alpha and beta; and a counter that will track the counts of the for-loop
- The for-loop is set up to go from –burninlength to the number of desired iterations

For-Loop:

1. At the beginning of each loop, the counter is updated by 1.
2. A new proposal for the intercept (alpha*) is sampled from the proposal distribution, which is a univariate normal distribution centered around the current alpha with a pre-defined standard deviation.
3. The inverse-logit function transforms $\alpha^* + \beta x$ into probability of death on a scale from 0 to 1. X is a vector of dosages so it returns a vector of p's. The p's are then passed as parameters to the binomial distribution function to calculate the log-likelihood of the observed proportions of dead mice given their corresponding p. The log-likelihood is then added to the log of the prior of α^*, which follows a normal distribution with mean 0 and an assumed standard deviation. The sum of the log-likelihood and the log-prior is proportionate to the log-posterior.
4. The same is done again but this time with the current/old alpha value, instead of the proposed alpha.
5. IF the difference between the two posteriors is larger than a random value sampled from a standard uniform distribution, the proposed alpha gets accepted and is now considered the current alpha, and the counter of the number of accepted alphas is raised by 1.
6. Steps 2-5 are now repeated for the beta parameter
7. As long as the counter is still $\leqslant 0$ (burn-in period), steps 1-6 are repeated.
8. At i = 1, the actual iterations begin, and the current alpha value is added to the vector of alpha samples, regardless of whether it's a newly accepted proposal or the same as in the previous iteration. If the thinning parameter t is $\neq 1$, only every t'th sample is stored in the vector.
9. Every 1000th count, the acceptance rates are printed, i.e. the number of accepted alphas and betas divided by the number of counts.

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())

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

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

# the covariate values (dose)
# x_original <- c(0.0028, 0.0056, 0.0112, 0.0225, 0.0450)
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(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)

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


## 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

# 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)
```

```r
## univariate random walk proposals ##
MCMC_MH <- function(s_alpha, s_beta){

  set.seed(44566)
  alpha_samples <- c()
  beta_samples <- c()
  # number of accepted proposals
  alpha_yes <- 0
  beta_yes <- 0

  # 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
      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")
    }
  }


## 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
  print(glue("Acceptance rate alpha: {formatC(alpha_yes/count, 3)} "))
  print(glue("Acceptance rate beta: {formatC(beta_yes/count, 3)} "))

  # Return MCMC and acceptance rate for alpha and beta
  return( list(alpha_samples, beta_samples, alpha_yes/count, beta_yes/count) )
}
```

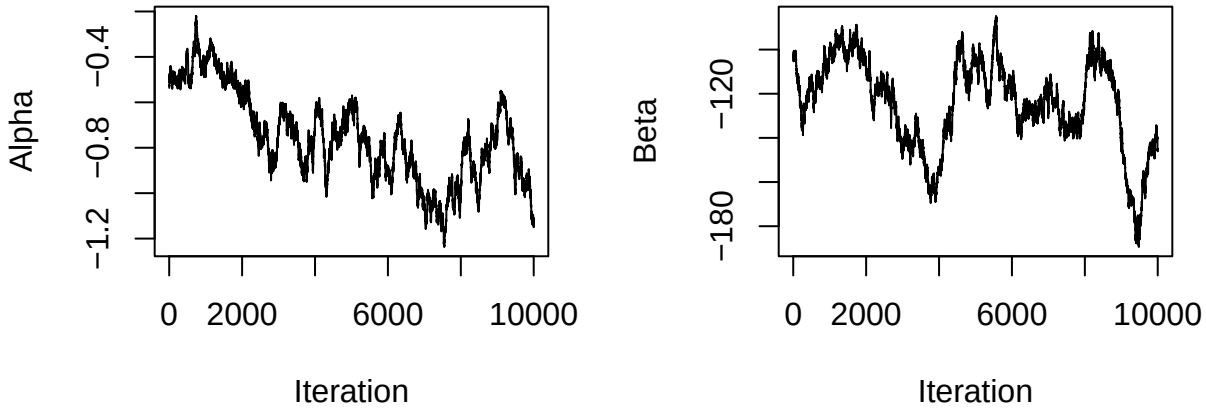
Now calling the function MCMC_MH to show the results:

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

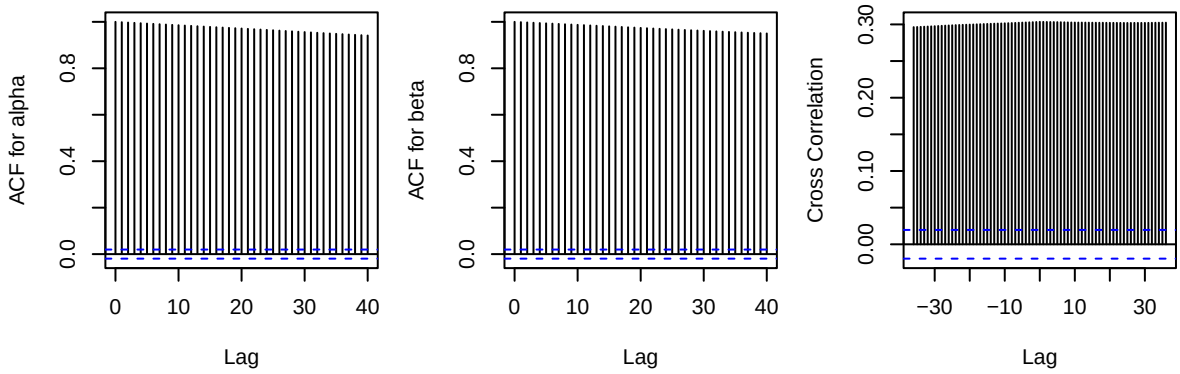
Results for low tuning parameters (0.01, 1):

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

```
## Traceplots:
```




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



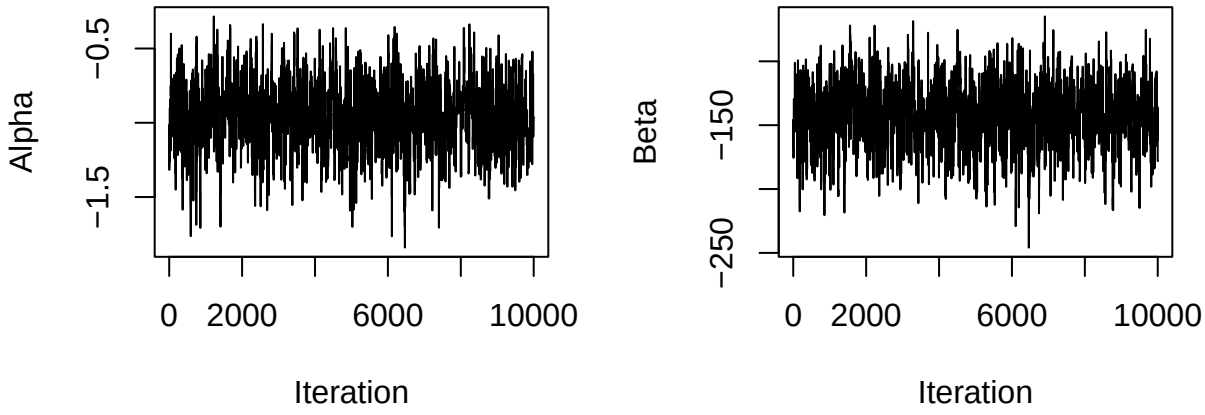

```
## Acceptance rate alpha: 0.976
## Acceptance rate beta: 0.974
```

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.

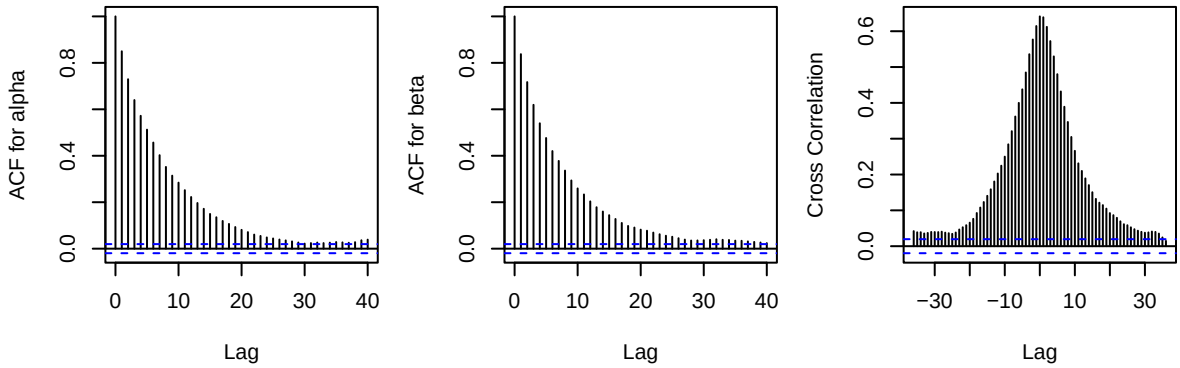
Results for medium tuning parameters (1, 100):

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

```
## Traceplots:
```




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



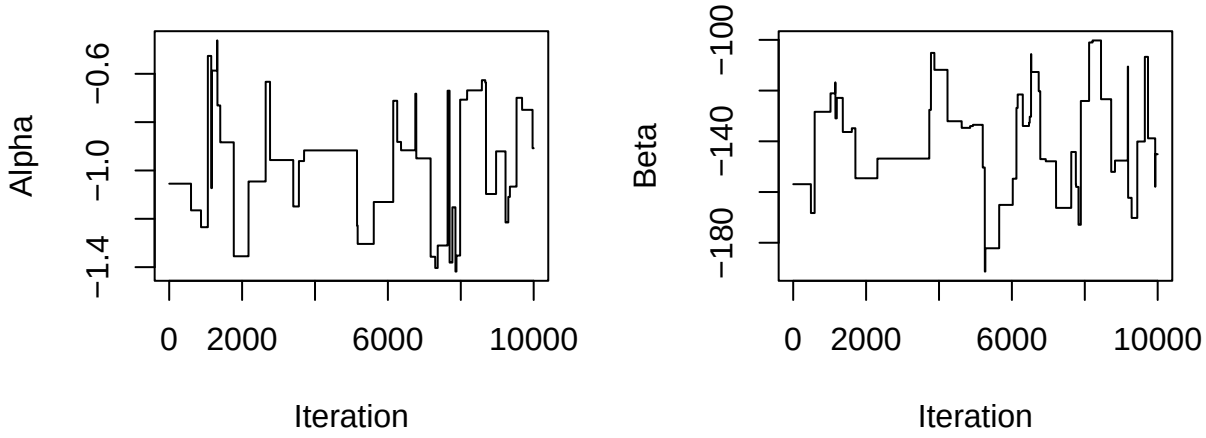

```
## Acceptance rate alpha: 0.217
## Acceptance rate beta: 0.231
```

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

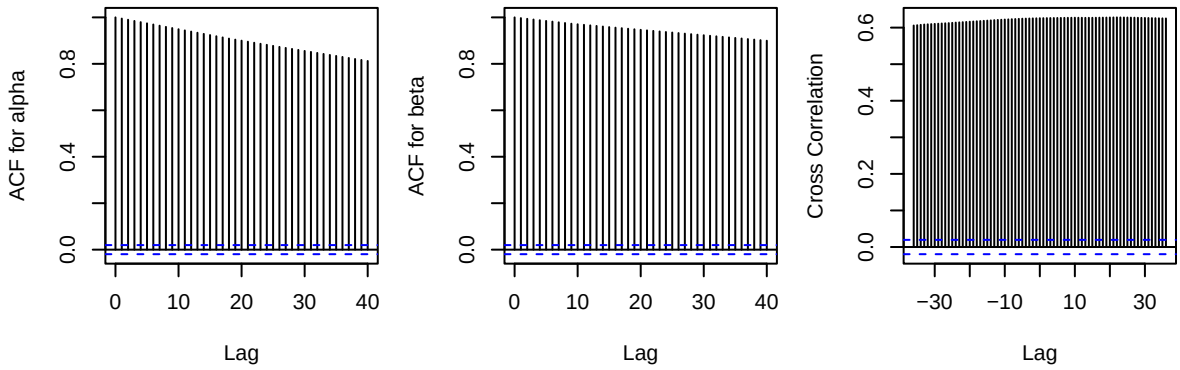
Results for high tuning parameters (50, 5000):

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

```
## Traceplots:
```




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




```
## Acceptance rate alpha: 0.00536
## Acceptance rate beta: 0.00486
```

Here the SDs of the proposal distributions are too large, so the sampler often proposes values far outside in the parameter space, leading to "adventurous" exploration and 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 sporadic jumps, and high autocorrelation over many lags. There is also high cross-correlation over many lags because if one parameter is "off", it leads to low likelihood and thus rejection of the sample, even if the other parameter would have been reasonable.

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: 0.217
Acceptance rate beta: 0.2316

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), 3)} ")
glue("SD alpha: {formatC(sd(alphas_2), 3)} ")
glue("Quantiles:")
quantile(alphas_2, c(0.025, 0.5, 0.975) )
```

```
## Mean alpha: -0.95
## SD alpha: 0.225
## 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), 3)} ")
glue("SD beta: {formatC(sd(betas_2), 3)} ")
glue("Quantiles:")
quantile(betas_2, c(0.025, 0.5, 0.975) )
```

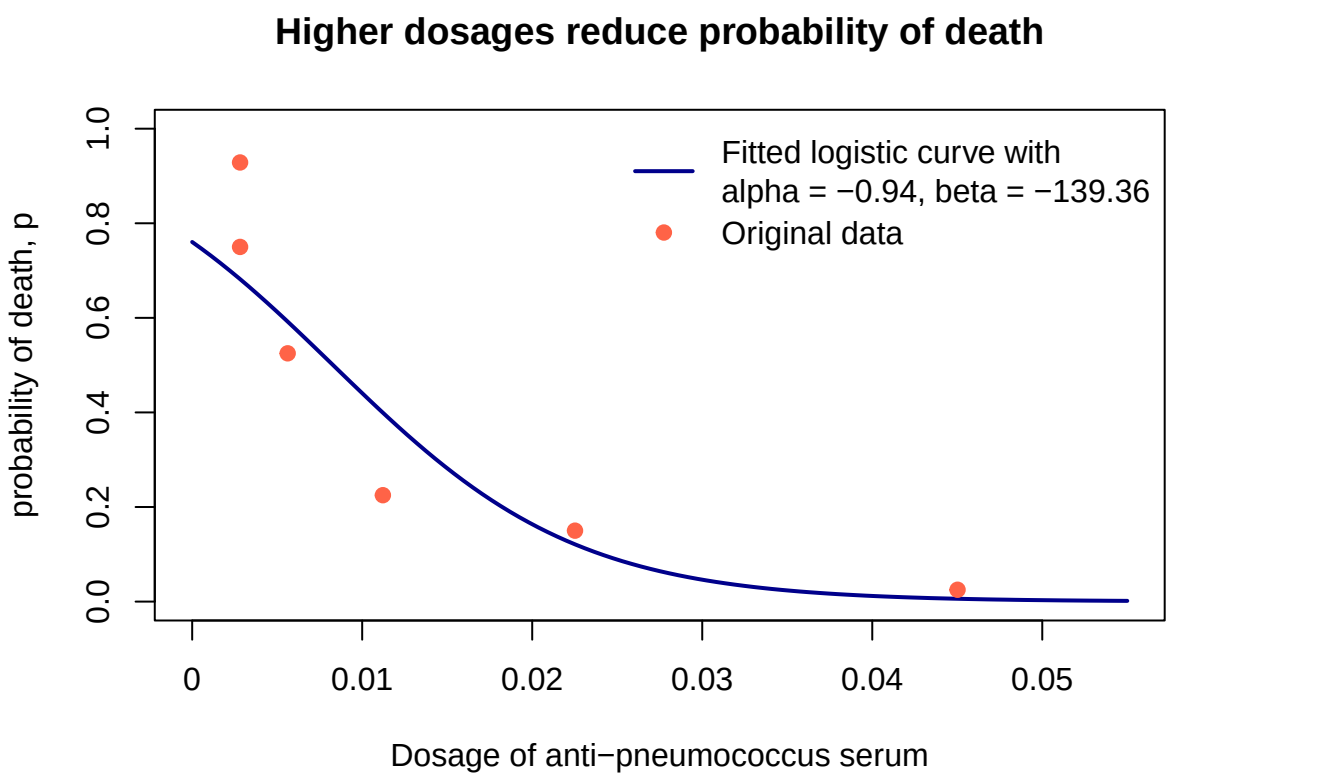
```
## Mean beta: -141
## SD beta: 24.4
## Quantiles:
##       2.5%        50%      97.5%
## -192.37525 -139.35901  -98.32787
```

5

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

```r
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( paste0("Fitted logistic curve with\nalpha = ", round(median_alpha, 2),
                          ", beta = ", round(median_beta,2) ), "Original data"),
       bty = "n", col = c("darkblue", "tomato"), lty = c(1,NA), pch = c(NA,19), lwd = c(2,NA) )
```



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 extremely high, this might again be fatal, but this was not modelled here.