

deBInfer logistic ODE example

Philipp H Boersch-Supan

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Preliminaries

First we install the deBInfer package. For this you need to install and load the devtools package first. You can do this from CRAN.

```
install.packages("devtools")  
  
#Load the devtools package.  
library(devtools)
```

Then you install deBInfer from github

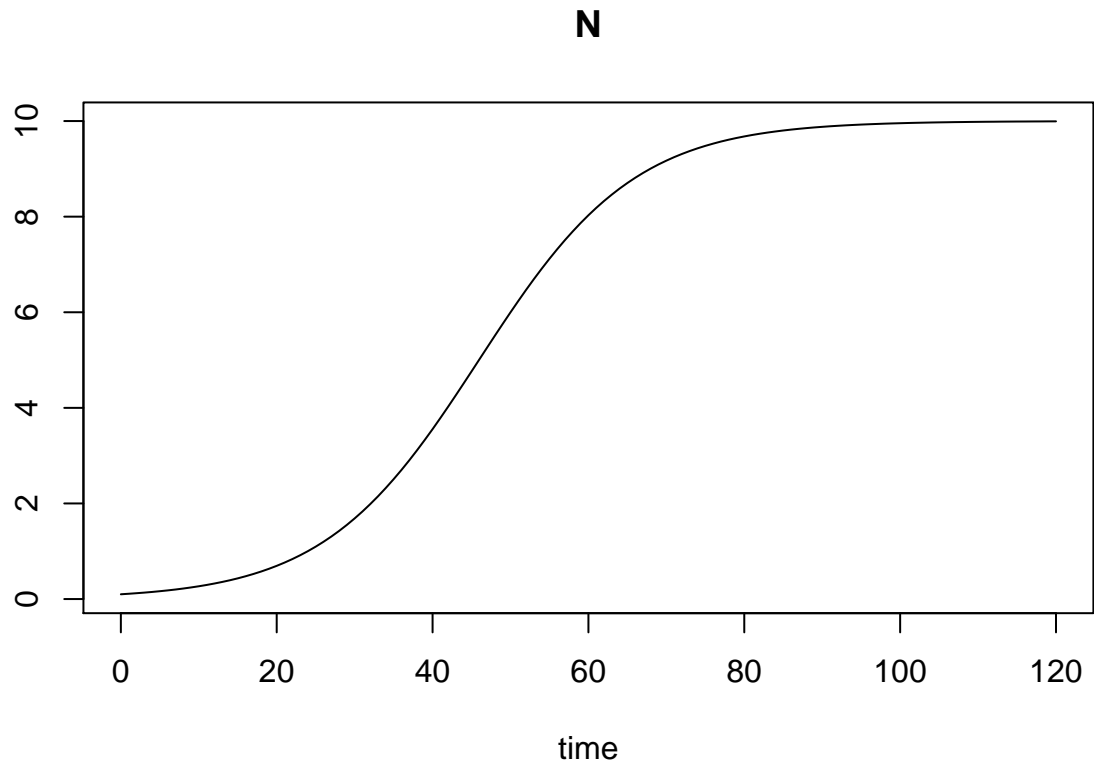
```
install_github("pboesu/debinfer")
```

Defining the DE model

We define a logistic growth ODE for deSolve.

```
library(deSolve)  
logistic_model <- function (time, y, parms) {  
  with(as.list(c(y, parms)), {  
    dN <- r * N * (1 - N / K)  
    list(dN)  
  })  
}  
y <- c(N = 0.1)  
parms <- c(r = 0.1, K = 10)  
times <- seq(0, 120, 1)  
out <- ode(y, times, logistic_model, parms, method='lsoda')
```

Which gives us the numerical solution



Simulationg observations

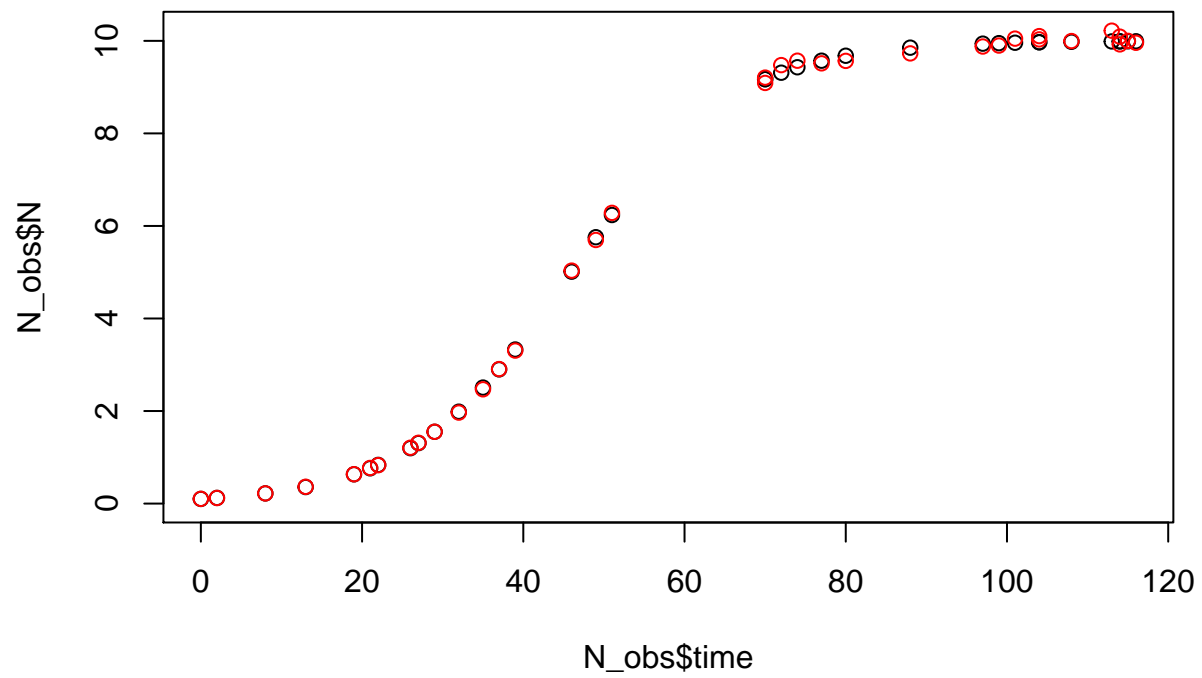
Now we simulate a noisy dataset from this equation. We sample a random subset from the integration output

```
set.seed(143)
N_obs <- as.data.frame(out[c(1,runif(35, 0, nrow(out))),]) #force include the first time-point (t=0)
```

and we “add” lognormal noise

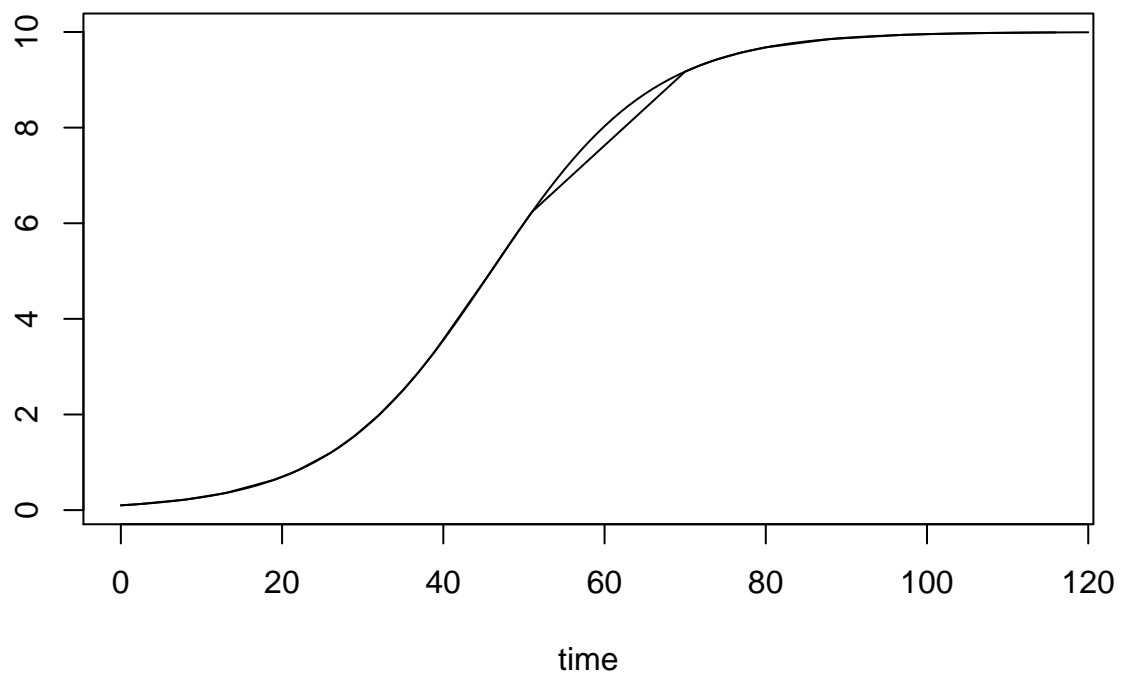
```
# add lognormal noise
parms['loglogsd.N'] <- -4.6
N_obs$N_noisy <- rlnorm(nrow(N_obs), log(N_obs$N), exp(parms['loglogsd.N']))
#observations must be ordered for solver to work
N_obs <- N_obs[order(N_obs$time),]

plot(N_obs$time, N_obs$N, ylim=c(0, max(N_obs$N, N_obs$N_noisy)))
points(N_obs$time, N_obs$N_noisy, col="red")
```



```
out_obs <- ode(y, c(0,N_obs$time), logistic_model, parms, method='lsoda')
plot(out_obs)
lines(out)
```

N



Defining an observation model and parameters for inference

We define an observation model. Note that we are sampling the log of the observation standard deviation, to ensure sampled values are strictly positive. We also use an epsilon correction for the meanlog, as the DE model can return values of 0 (or even less due to numerical precision).

```
# the observation model
logistic_obs_model<-function(data, sim.data, samp){

  llik.N<-sum(dlnorm(data$N_noisy, meanlog=log(sim.data[, "N"] + 1e-6),
                    sdlog=exp(samp[['loglogsd.N']]), log=TRUE)
            )

  llik<-llik.N

  return(llik)
}
```

We declare the parameters for inference:

```
library(deBInfer)
r <- debinfer_par(name = "r", var.type = "de", fixed = FALSE,
                  value = 0.5, prior="norm", hypers=list(mean = 0, sd = 1),
                  prop.var=0.005, samp.type="rw")

K <- debinfer_par(name = "K", var.type = "de", fixed = FALSE,
                  value = 5, prior="lnorm", hypers=list(meanlog = 1, sdlog = 1),
                  prop.var=0.1, samp.type="rw")

loglogsd.N <- debinfer_par(name = "loglogsd.N", var.type = "obs", fixed = FALSE,
                           value = -2, prior="norm", hypers=list(mean = 0, sd = 1),
                           prop.var=0.5, samp.type="rw")
```

and we also need to provide an initial condition for the differential equation:

```
N <- debinfer_par(name = "N", var.type = "init", fixed = TRUE, value = 0.1)
```

All declared parameters are collated using the `setup_debinfer` function

```
mcmc.pars <- setup_debinfer(r, K, loglogsd.N, N)
```

Conduct inference

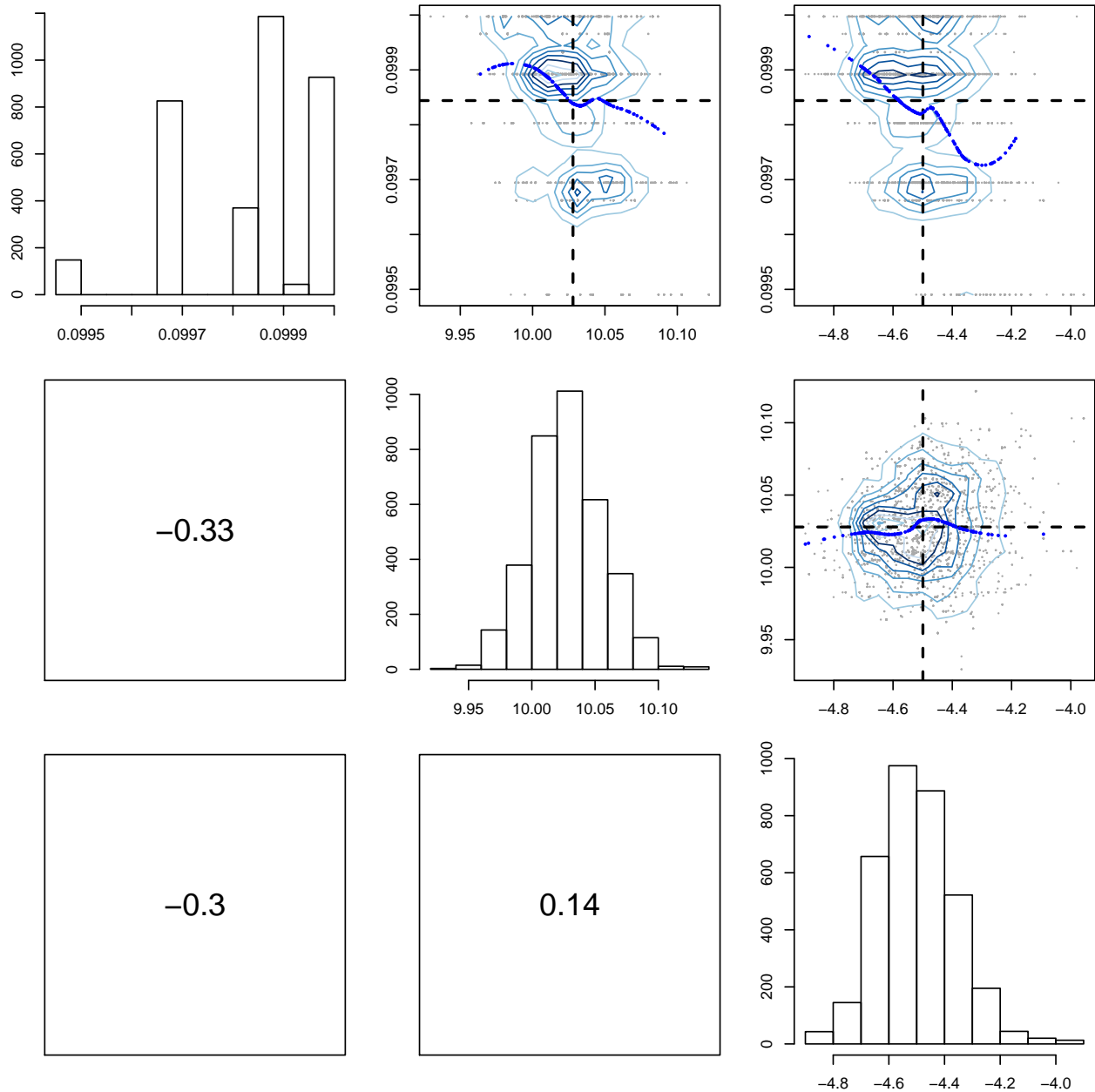
Finally we use `deBInfer` to estimate the parameters of the original model.

```
# do inference with deBInfer
# MCMC iterations
iter = 5000
# inference call
mcmc_samples <- de_mcmc(N = iter, data=N_obs, de.model=logistic_model,
```

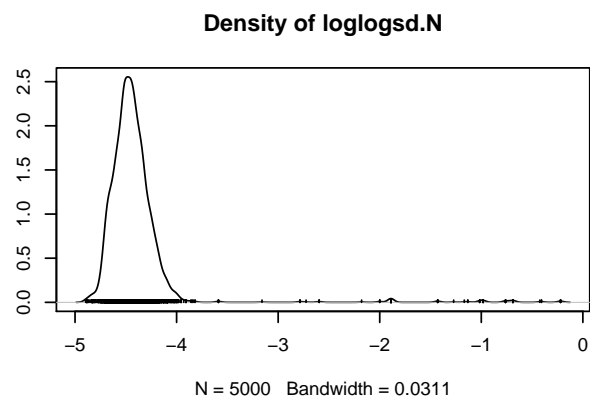
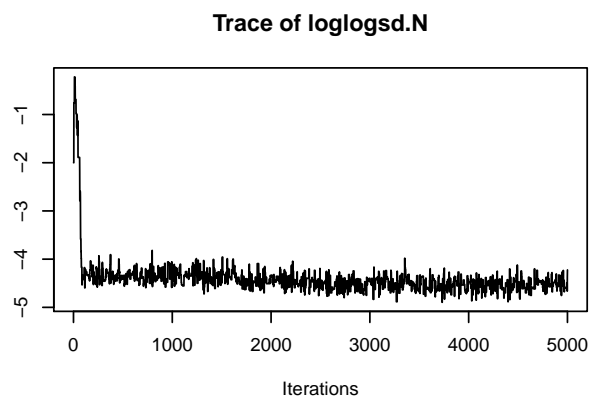
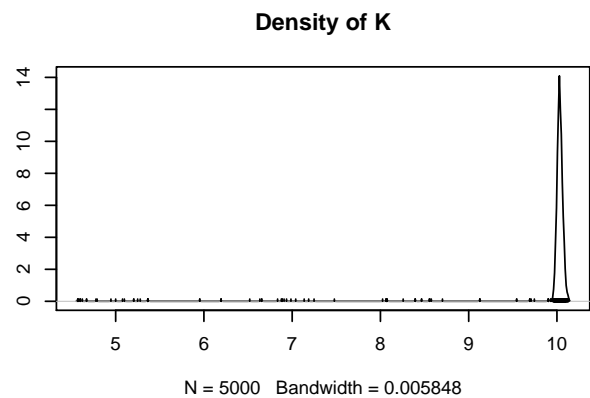
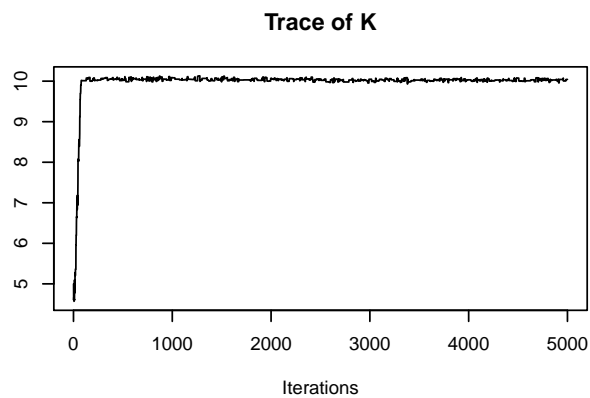
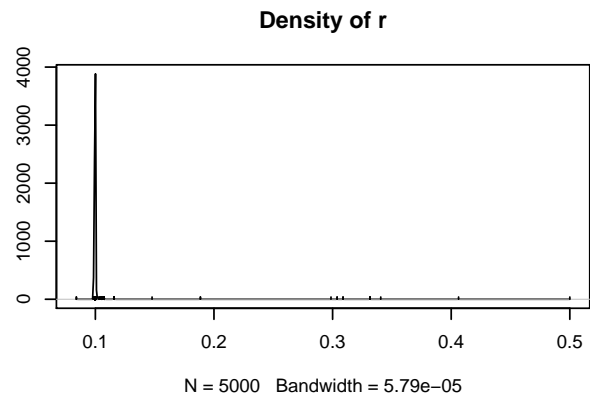
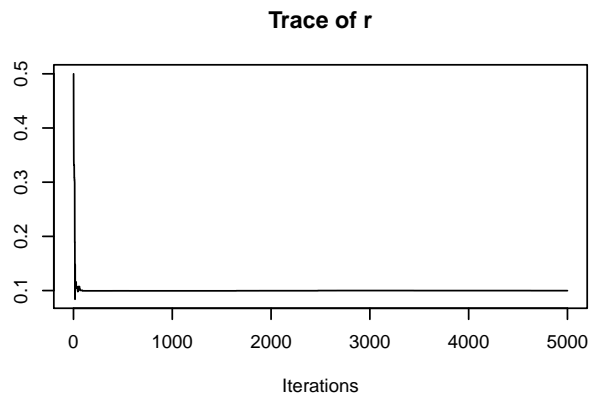
```
obs.model=logistic_obs_model, all.params=mcmc.pars,
Tmax = max(N_obs$time), data.times=N_obs$time, cnt=iter,
plot=FALSE, sizestep=0.1, which=1)
```

We plot the results

```
burnin = 1500
pairs(mcmc_samples, burnin = burnin, scatter=TRUE, trend=TRUE)
```



```
plot(mcmc_samples$samples)
```



```
summary(mcmc_samples$samples)
```

```
##
## Iterations = 1:5000
## Thinning interval = 1
## Number of chains = 1
## Sample size per chain = 5000
##
## 1. Empirical mean and standard deviation for each variable,
##    plus standard error of the mean:
##
##           Mean      SD Naive SE Time-series SE
```

```
## r          0.1004 0.01231 0.0001741      0.0006961
## K          9.9874 0.42553 0.0060179      0.0457233
## loglogsd.N -4.4080 0.40749 0.0057628      0.0577335
```

```
##
```

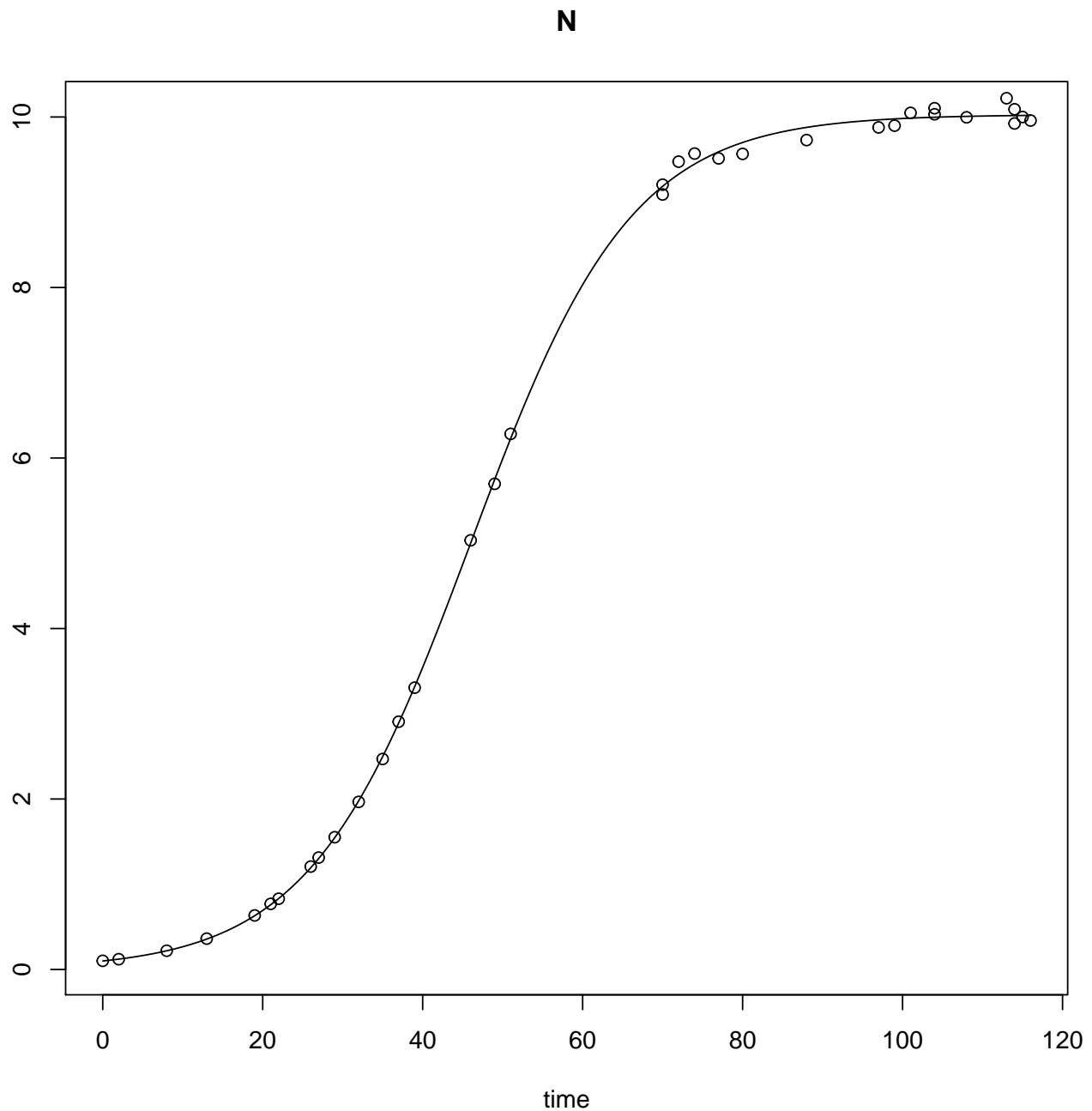
```
## 2. Quantiles for each variable:
```

```
##
```

```
##          2.5%      25%      50%      75%  97.5%
## r          0.09946 0.09949 0.0998 0.09989 0.100
## K          9.96797 10.01091 10.0312 10.05152 10.096
## loglogsd.N -4.72698 -4.56125 -4.4567 -4.34532 -4.028
```

```
#plot(N_obs$time,N_obs$N_noisy)
```

```
posterior.mean.sim <- solve_de(logistic_model, params=c(r=mean(mcmc_samples$samples[, "r"] [burnin:iter])
plot(posterior.mean.sim)
points(N_obs$time,N_obs$N_noisy)
```



Posterior credible interval (equal-tailed)

```
library(plyr)
simlist <- llply(sample(nrow(mcmc_samples$samples[burnin:iter,]), 1000),
  function(x)solve_de(logistic_model, mcmc_samples$samples[burnin:iter,][x,],
    inits=c(N = 0.1), Tmax=120, numsteps=100))

sima <- simplify2array(simlist)
dim(sima)
```

```
## [1] 100 2 1000
```

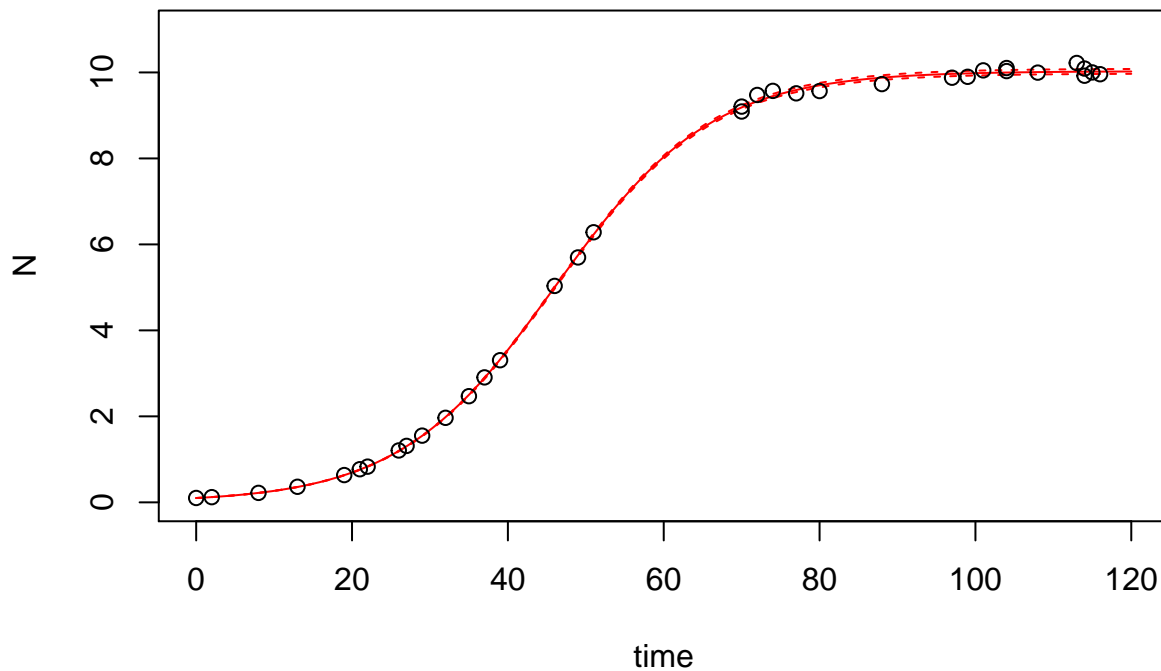


```

simCI <- aaply(sima, .margins = c(1,2), quantile, probs=c(0.025,0.5,0.975))
for (p in 2:ncol(simlist[[1]])){
  plot(simCI[,3][,c(1,p)], main="", type='n', ylim=c(0,11))

  #for (i in 1:length(simlist)){
  # lines(simlist[[i]][,c(1,p)], lty=2, col='grey')
  #}
  for (i in 1:3){
    lines(simCI[,i][,c(1,p)], lty=c(2,1,2)[i], col=c("red"))
  }
  if (dimnames(simlist[[1]])[[2]][p] == "N") points(N_obs$time, N_obs$N_noisy)
}

```



```

#str(out)
#lines(posterior.mean.sim, ylim=c(0,15))

#l_ply(simlist, function(x) lines(x[,1], x[,2]))
#lines(out[,1], out[,2], col='blue')

```

#we could also use asymmetric uniform proposals to ensure only positive values of logsd.N are sampled

```

logsd.Nunif <- debinfer_par(name = "logsd.N", var.type = "obs", fixed = FALSE,
  value = 0.01, prior="norm", hypers=list(mean = 0, sd = 1),
  prop.var=c(1,2), samp.type="rw-unif")

```

```

## Warning in if (!is.numeric(prop.var) | prop.var < 0 | length(prop.var) != :
## the condition has length > 1 and only the first element will be used

```

#in that case we need to adjust the observation model slightly

```

# the observation model
logistic_obs_model_unif<-function(data, sim.data, samp){

  llik.N<-sum(dlnorm(data$N_noisy, meanlog=log(sim.data[, "N"] + 1e-6),
                    sdlog=samp[['logsd.N']], log=TRUE)
            )

  llik<-llik.N

  return(llik)
}

mcmc.pars_unif <- setup_debinfer(r, K, logsd.Nunif, N)

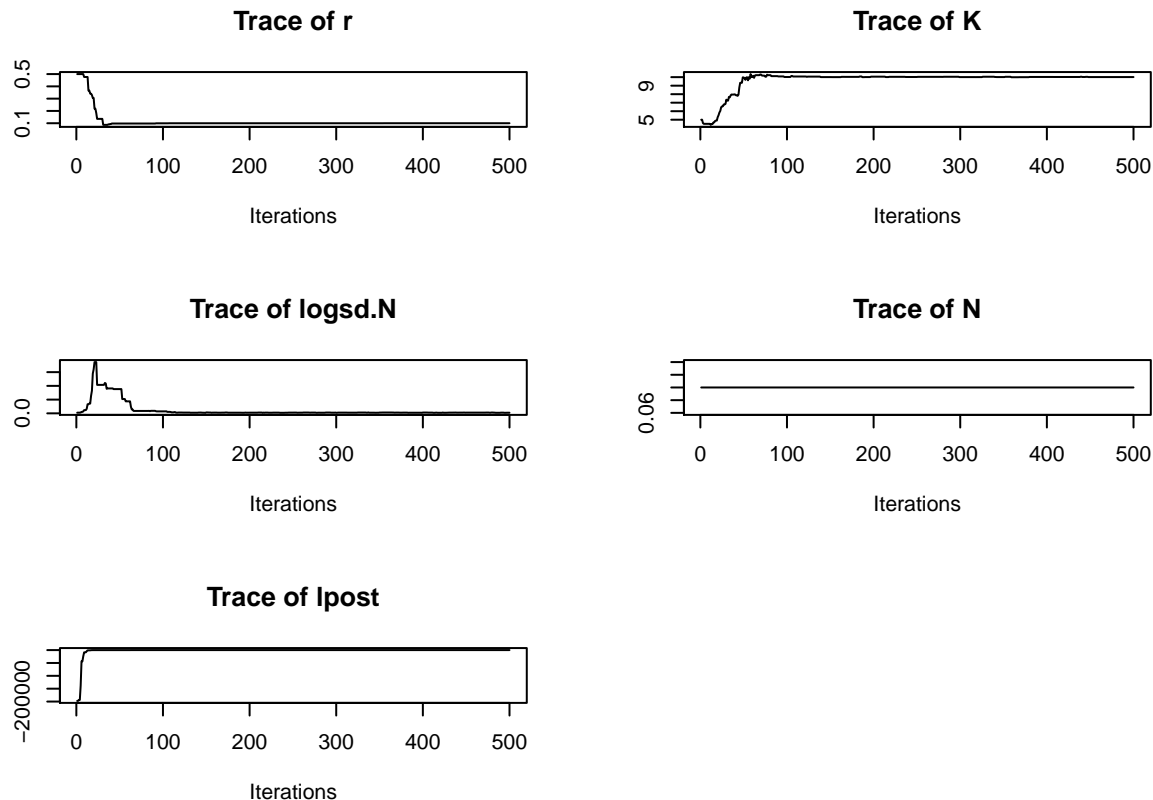
mcmc_samples_unif <- de_mcmc(N = iter, data=N_obs, de.model=logistic_model,
                             obs.model=logistic_obs_model_unif, all.params=mcmc.pars_unif,
                             Tmax = max(N_obs$time), data.times=N_obs$time, cnt=iter %/% 10,
                             plot=TRUE, sizestep=0.1, which=1)

```

```

## [1] "Order of initial conditions is N"
## [1] "initial posterior probability = -197325.858568254"
## [1] "proposing logsd.N: prob.old = 63.174; prob.new = 56.276; A = 0.0013931"
## [1] "proposing K: prob.old = 63.174; prob.new = -235.39; A = 2.1667e-130"
## [1] "proposing r: prob.old = 63.174; prob.new = -820.95; A = 0"
## [1] "sample number 500"

```

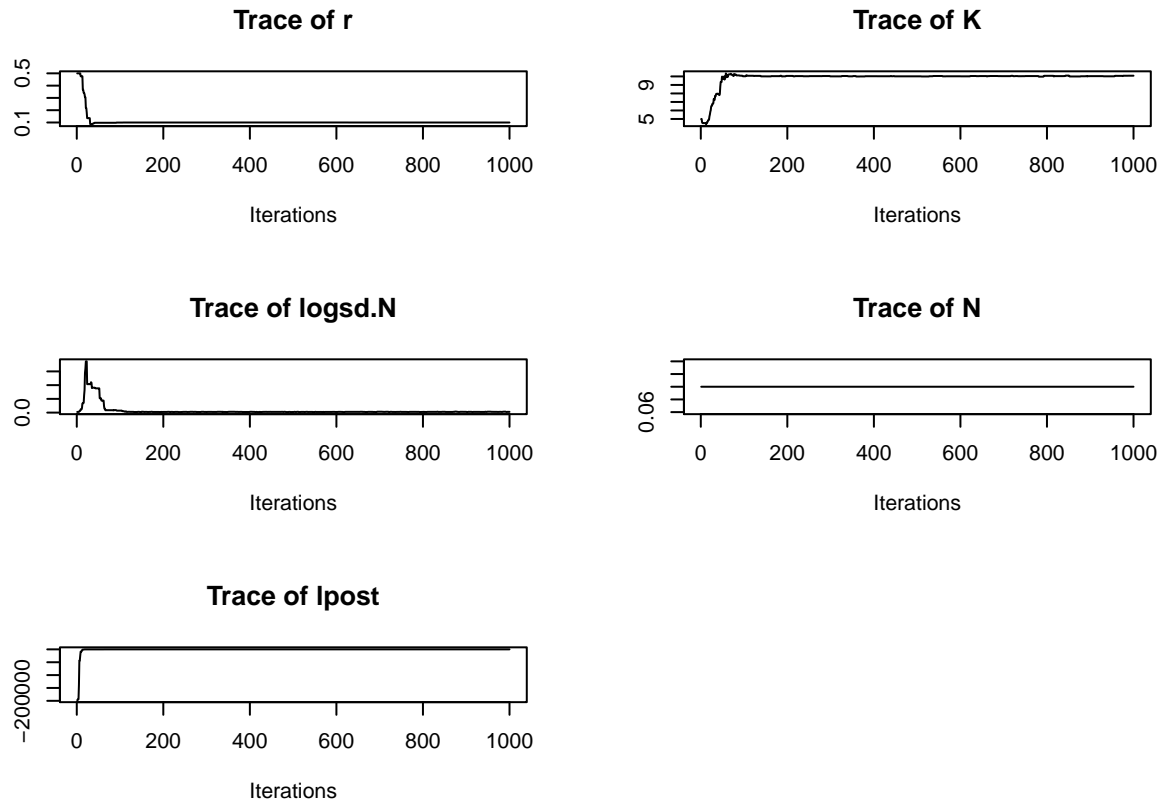


```

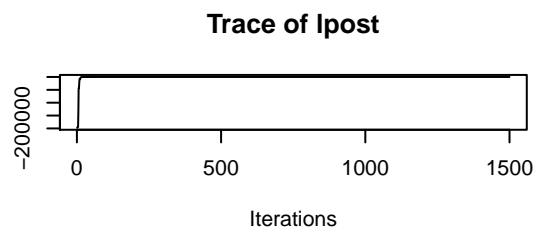
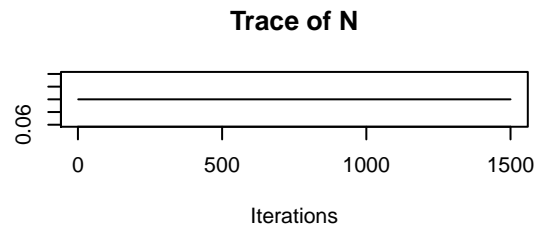
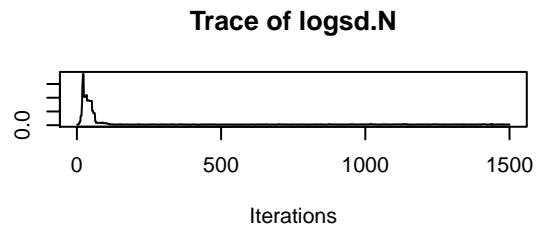
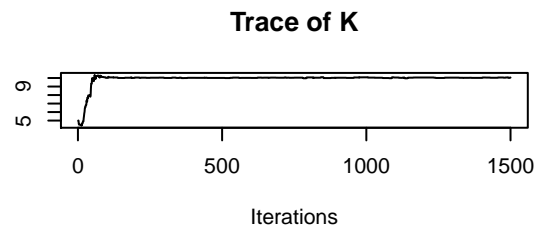
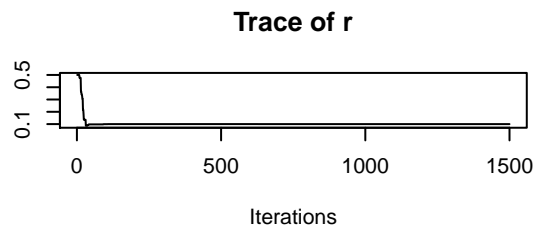
## [1] "proposing r: prob.old = 59.537; prob.new = -1131.6; A = 0"

```

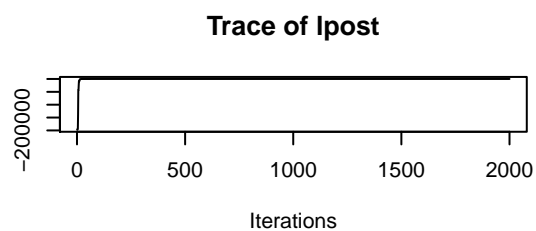
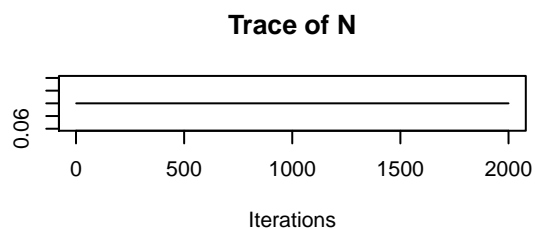
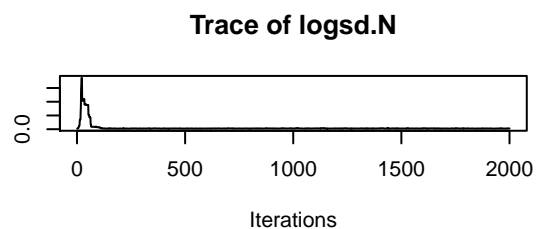
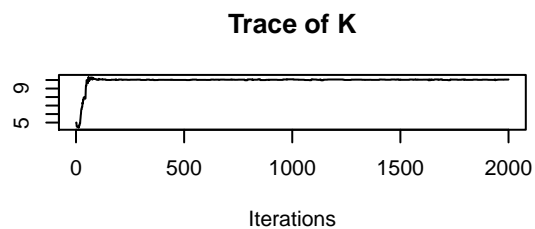
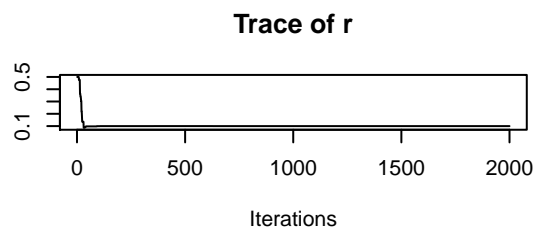
```
## [1] "proposing logsd.N: prob.old = 59.537; prob.new = 53.965; A = 0.0024396"
## [1] "proposing K: prob.old = 59.537; prob.new = 2.3222; A = 1.4189e-25"
## [1] "sample number 1000"
```



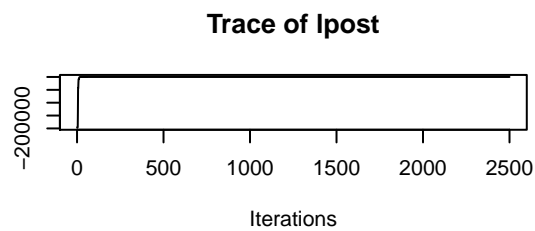
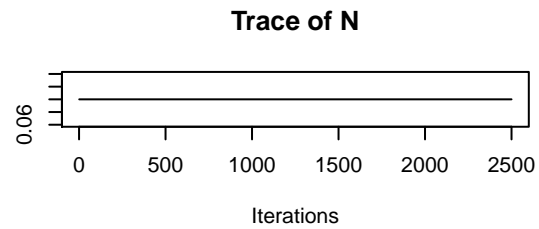
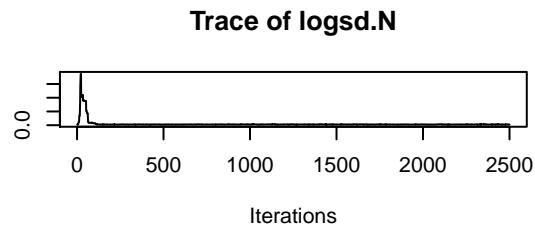
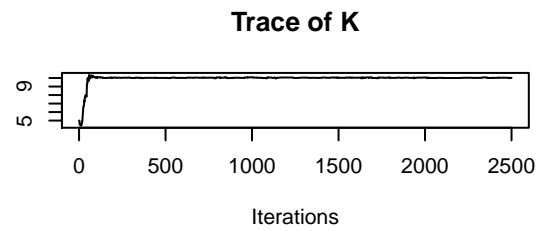
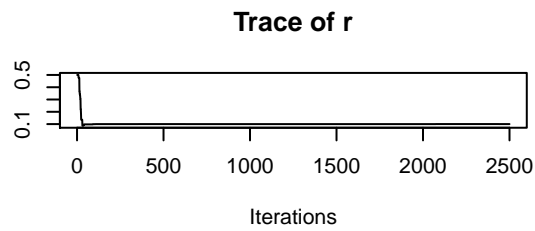
```
## [1] "proposing K: prob.old = 60.505; prob.new = 17.99; A = 3.4359e-19"
## [1] "proposing logsd.N: prob.old = 60.505; prob.new = 52.636; A = 0.00019229"
## [1] "proposing r: prob.old = 60.505; prob.new = -333820; A = 0"
## [1] "sample number 1500"
```



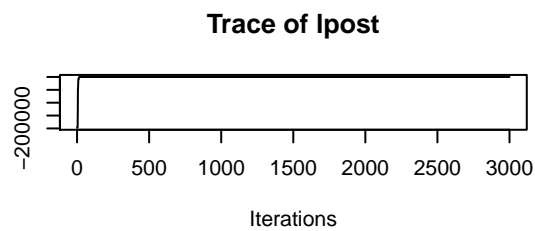
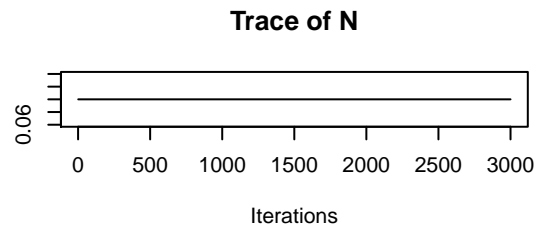
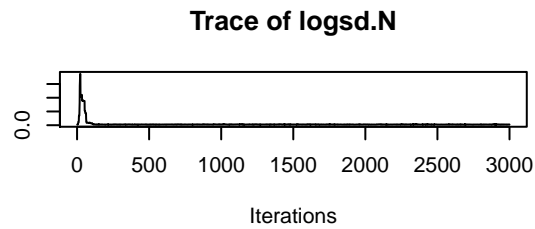
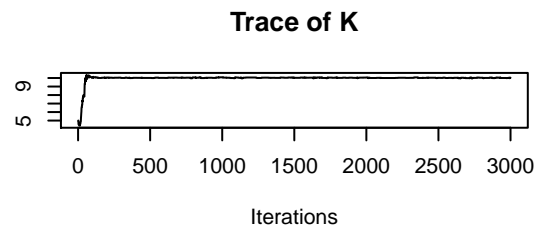
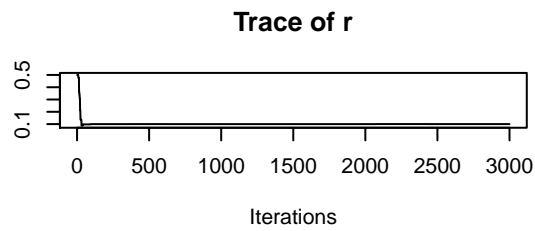
```
## [1] "proposing r: prob.old = 61.462; prob.new = -92176; A = 0"
## [1] "proposing K: prob.old = 61.462; prob.new = 60.9; A = 0.57048"
## [1] "proposing logsd.N: prob.old = 60.9; prob.new = 53.659; A = 0.00047369"
## [1] "sample number 2000"
```



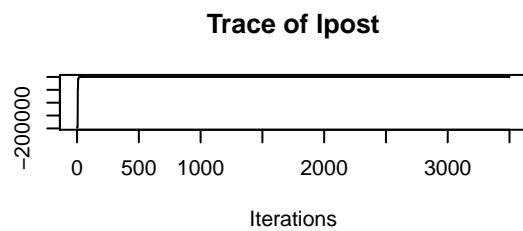
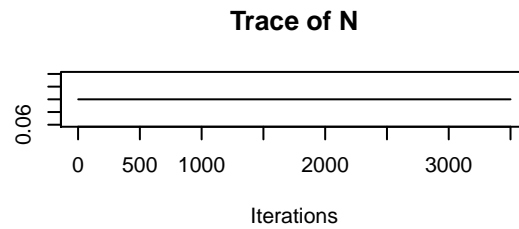
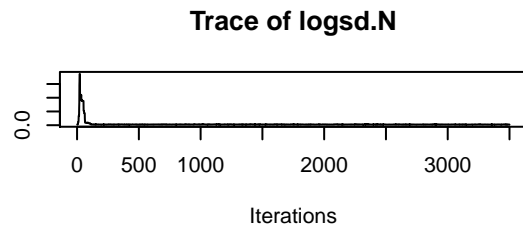
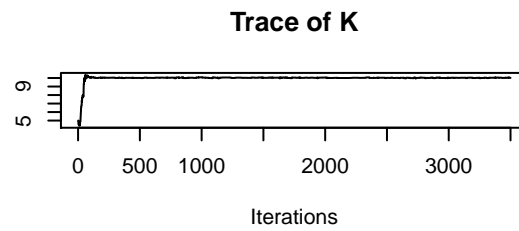
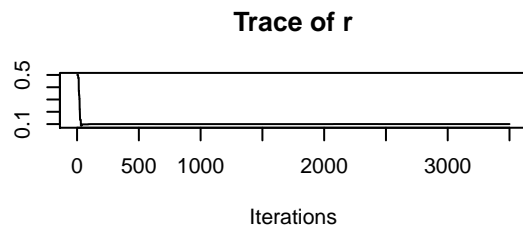
```
## [1] "proposing r: prob.old = 63.489; prob.new = -103.31; A = 3.6221e-73"
## [1] "proposing K: prob.old = 63.489; prob.new = -81.159; A = 1.5138e-63"
## [1] "proposing logsd.N: prob.old = 63.489; prob.new = 63.478; A = 0.99257"
## [1] "sample number 2500"
```



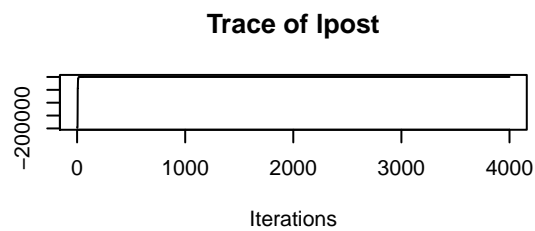
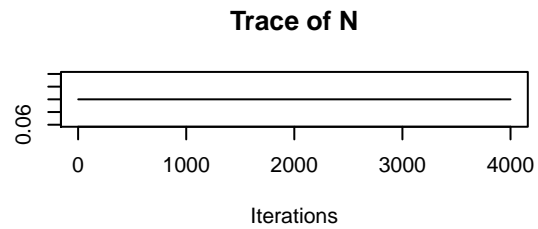
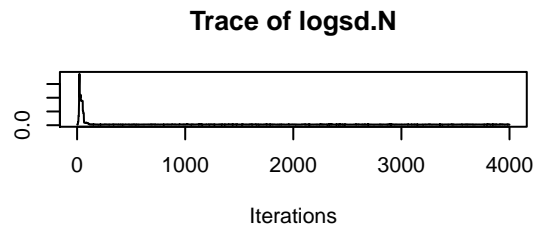
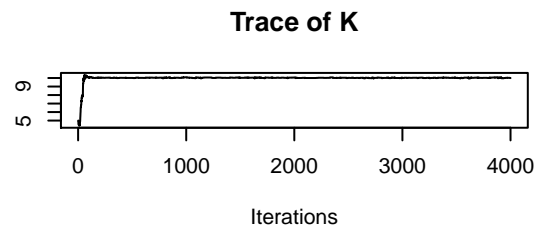
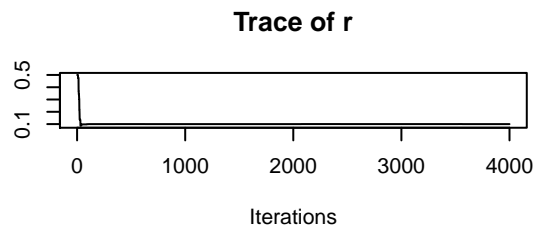
```
## [1] "proposing logsd.N: prob.old = 63.079; prob.new = 50.212; A = 1.3109e-06"
## [1] "proposing K: prob.old = 63.079; prob.new = 62.472; A = 0.54506"
## [1] "proposing r: prob.old = 63.079; prob.new = -32227; A = 0"
## [1] "sample number 3000"
```



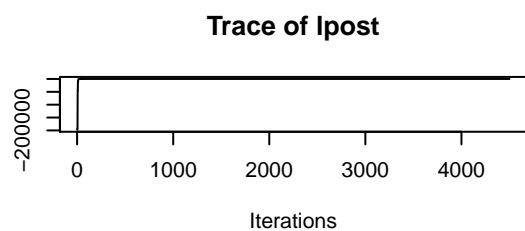
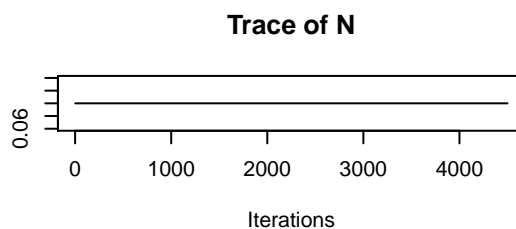
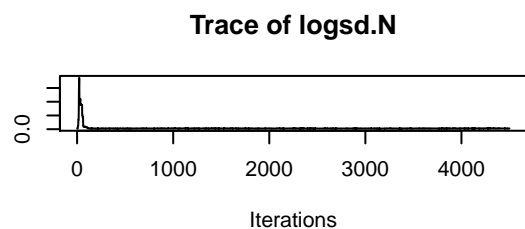
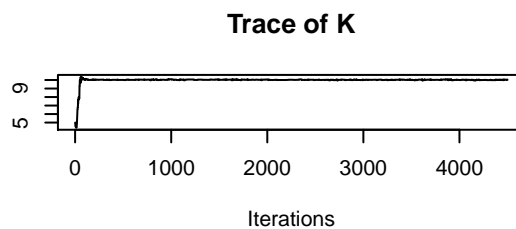
```
## [1] "proposing K: prob.old = 63.446; prob.new = 50.537; A = 2.4756e-06"
## [1] "proposing logsd.N: prob.old = 63.446; prob.new = 39.198; A = 5.5353e-11"
## [1] "proposing r: prob.old = 63.446; prob.new = -80342; A = 0"
## [1] "sample number 3500"
```



```
## [1] "proposing r: prob.old = 60.726; prob.new = -223110; A = 0"
## [1] "proposing logsd.N: prob.old = 60.726; prob.new = 58.709; A = 0.15692"
## [1] "proposing K: prob.old = 58.709; prob.new = -18.732; A = 2.3327e-34"
## [1] "sample number 4000"
```

```
## [1] "proposing r: prob.old = 62.404; prob.new = -49424; A = 0"
## [1] "proposing logsd.N: prob.old = 62.404; prob.new = 62.416; A = 1.0673"
## [1] "proposing K: prob.old = 62.416; prob.new = 61.392; A = 0.35938"
## [1] "sample number 4500"
```



```
## [1] "proposing logsd.N: prob.old = 61.597; prob.new = 56.528; A = 0.0038677"
## [1] "proposing r: prob.old = 61.597; prob.new = -66996; A = 0"
## [1] "proposing K: prob.old = 61.597; prob.new = 22.872; A = 1.5202e-17"
## [1] "sample number 5000"
```

