

# simulation & inference of transients

*Carl Boettiger, Jorge Arroyo Esquivel, Junjie Jiang, Jody Reimer, Henry Scharf, Elizabeth Wolkovich, and Kai Zhu*

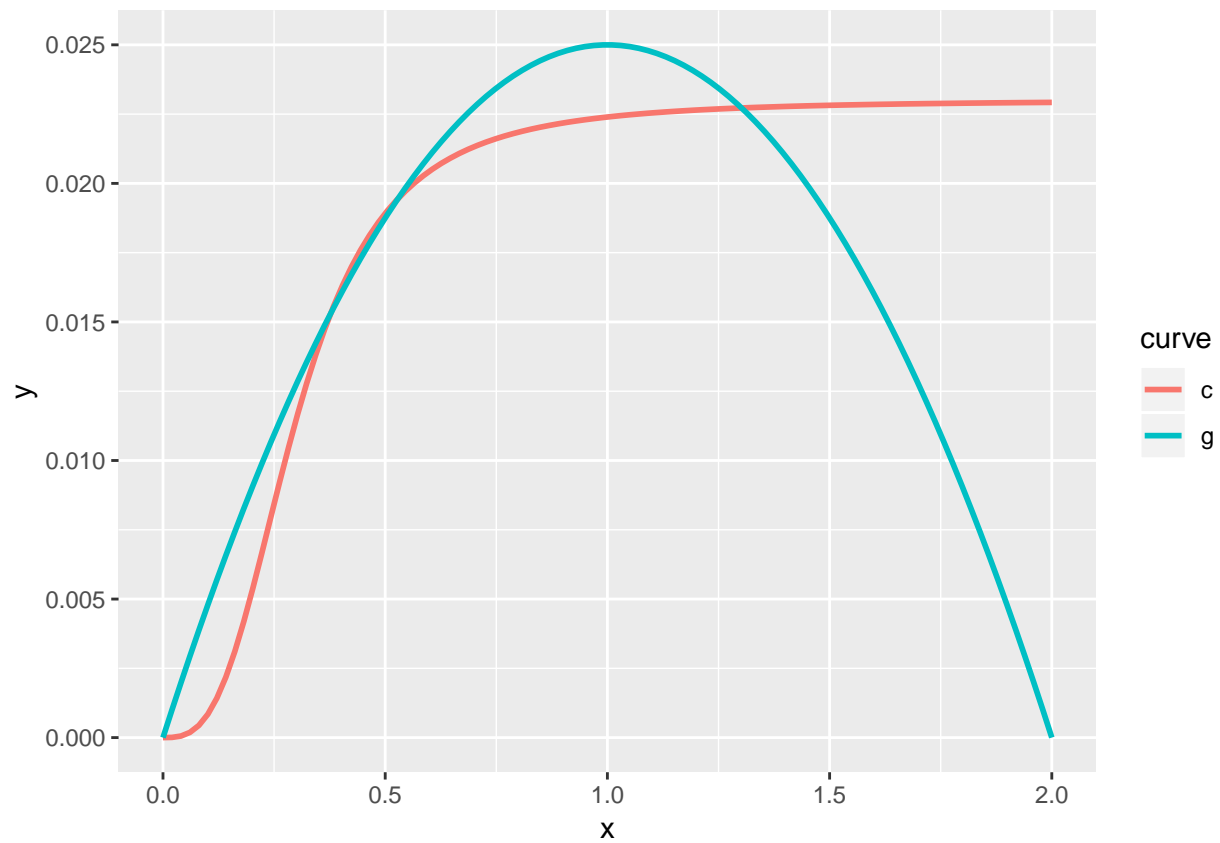
*2019-09-10*

```
library(tidyverse)
library(parallel)
library(nimble)
```

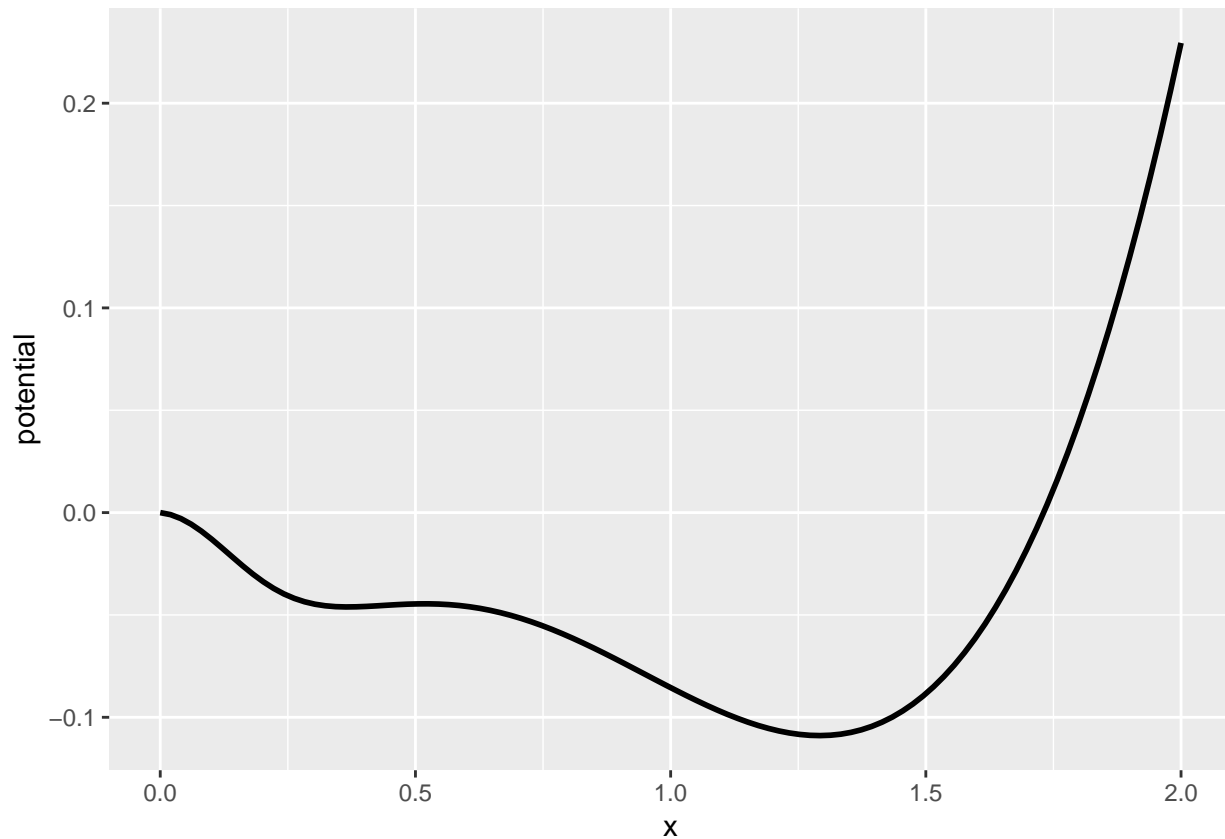
```
N <- 1e4
r <- 0.05; K <- 2
a <- 0.023; H <- 0.3; Q <- 3
x0 <- 0.2; sigma <- 0.02
growth <- function(x, r, K) x * r * (1 - x / K)
consumption <- function(x, a, H, Q) a * x^Q / (x^Q + H^Q)
```

```
theory <-
  tibble(x = seq(0,K, length.out = 100)) %>%
  mutate(g = growth(x, r, K),
         c = consumption(x, a, H, Q)) %>%
  mutate(potential = - cumsum(g - c)) %>%
  gather(curve, y, -x, -potential)
```

```
theory %>%
  ggplot(aes(x, y, col = curve)) +
  geom_line(lwd = 1)
```



```
theory %>%  
  ggplot(aes(x, potential)) +  
  geom_line(lwd = 1)
```



```
## define truncated normal distribution ----
dtruncnorm <- nimbleFunction(
  run = function(x = double(0), mean = double(0),
                 sd = double(0), log = integer(0, default = 0)) {
    returnType(double(0))
    log_prob <- dnorm(x = x, mean = mean, sd = sd, log = 1) -
      pnorm(q = 0, mean = -mean, sd = sd, log = 1)
    if(log) return(log_prob)
    else return(exp(log_prob))
  })

rtruncnorm <- nimbleFunction(
  run = function(n = integer(0, default = 1), mean = double(0),
                 sd = double(0)) {
    returnType(double(0))
    if(n != 1) print("rtruncnorm only allows n = 1; using n = 1.")
    draw <- rnorm(n = 1, mean = mean, sd = sd)
    while(draw < 0)
      draw <- rnorm(n = 1, mean = mean, sd = sd)
    return(draw)
  })

# Define stochastic model in BUGS notation ----
may <- nimble::nimbleCode({
  log(r) ~ dnorm(mu_r, sd_r)
  log(K) ~ dnorm(mu_K, sd_K)
  log(a) ~ dnorm(mu_a, sd_a)
  log(H) ~ dnorm(mu_H, sd_H)
  log(Q) ~ dnorm(mu_Q, sd_Q)
})
```

```

x0 ~ dtruncnorm(mu_x0, sd_x0)
log(sigma) ~ dnorm(mu_sigma, sd_sigma)
x[1] <- x0
for(t in 1:(N - 1)){
  mu[t] <- x[t] + x[t] * r * (1 - x[t] / K) - a * x[t]^Q / (x[t]^Q + H^Q)
  x[t + 1] ~ dtruncnorm(mean = mu[t], sd = sigma)
}
})
# constants ----
constants <- list(
  N = N,
  mu_r = log(r), sd_r = 1,
  mu_K = log(K), sd_K = 1,
  mu_a = log(a), sd_a = 1,
  mu_H = log(H), sd_H = 1,
  mu_Q = log(Q), sd_Q = 1,
  mu_x0 = x0, sd_x0 = 1,
  mu_sigma = log(sigma), sd_sigma = 1
)
## inits ----
inits <- list("log_r" = log(r), "log_K" = log(K),
             "log_a" = log(a), "log_H" = log(H), "log_Q" = log(Q),
             "log_sigma" = log(sigma), "x0" = x0)
# define and compile model ----
model <- nimbleModel(code = may, constants = constants, inits = inits)

```

## defining model...

## Registering the following user-provided distributions: dtruncnorm .

## NIMBLE has registered dtruncnorm as a distribution based on its use in BUGS code. Note that if you m

## building model...

## setting data and initial values...

## running calculate on model (any error reports that follow may simply reflect missing values in model

## checking model sizes and dimensions... This model is not fully initialized. This is not an error. To

## model building finished.

```
cmodel <- compileNimble(model)
```

## compiling... this may take a minute. Use 'showCompilerOutput = TRUE' to see C++ compilation details.

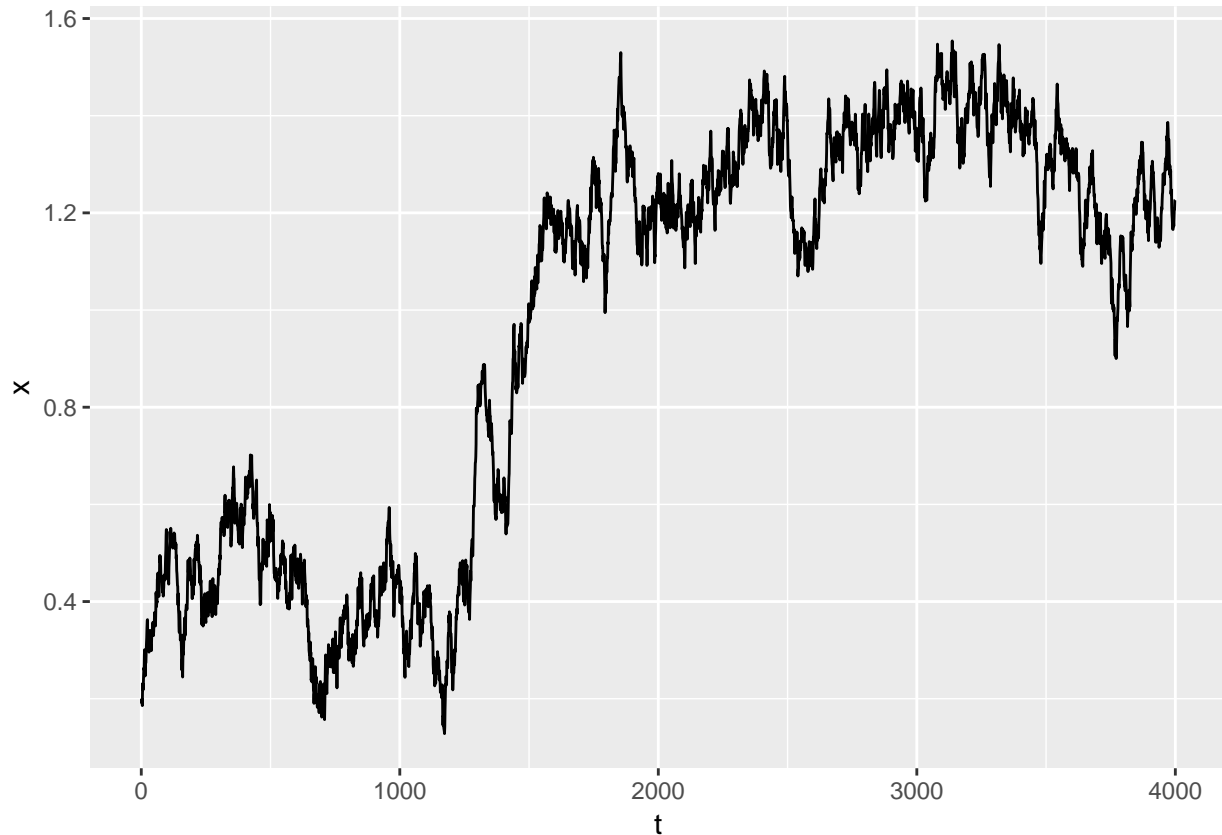
## compilation finished.

```
set.seed(1)
```

```
simulate(cmodel, nodes = c('x', 'mu'))
```

```
df <- tibble(t = seq_along(cmodel$x), x = cmodel$x)
```

```
df %>% filter(t < 4000) %>% ggplot(aes(t, x)) + geom_line()
```



```
dnorm_mod <- function(x, mean, sd, log = T){
  dnorm(x = x, mean = mean, sd = sd, log = log) -
    log(1 - pnorm(q = 0, mean = mean, sd = sd))
}

get_ll <- function(x, r, K, a, H, Q, sigma){
  TIME <- length(x)
  mu <- x + x * r * (1 - x / K) - a * x^Q / (x^Q + H^Q)
  sum(dnorm_mod(x = x[-1], mean = mu[-TIME], sd = sigma, log = T))
}

##
grid_r <- seq(1e-2, 1e-1, l=5e1)
ll_r <- sapply(grid_r, function(r) get_ll(a = cmodel$a, x = cmodel$x, r = r, K = cmodel$K,
  H = cmodel$H, Q = cmodel$Q, sigma = cmodel$sigma))

##
grid_K <- seq(1, 5, l=5e1)
ll_K <- sapply(grid_K, function(K) get_ll(a = cmodel$a, x = cmodel$x, r = cmodel$r, K = K,
  H = cmodel$H, Q = cmodel$Q, sigma = cmodel$sigma))

##
grid_a <- seq(1e-3, 1e-1, l=5e1)
ll_a <- sapply(grid_a, function(a) get_ll(a = a, x = cmodel$x, r = cmodel$r, K = cmodel$K,
  H = cmodel$H, Q = cmodel$Q, sigma = cmodel$sigma))

##
grid_H <- exp(seq(log(1e-2), log(0.7), l=5e1))
ll_H <- sapply(grid_H, function(H) get_ll(a = cmodel$a, x = cmodel$x, r = cmodel$r, K = cmodel$K,
  H = H, Q = cmodel$Q, sigma = cmodel$sigma))

##
grid_Q <- exp(seq(log(1.5), log(8), l=5e1))
```

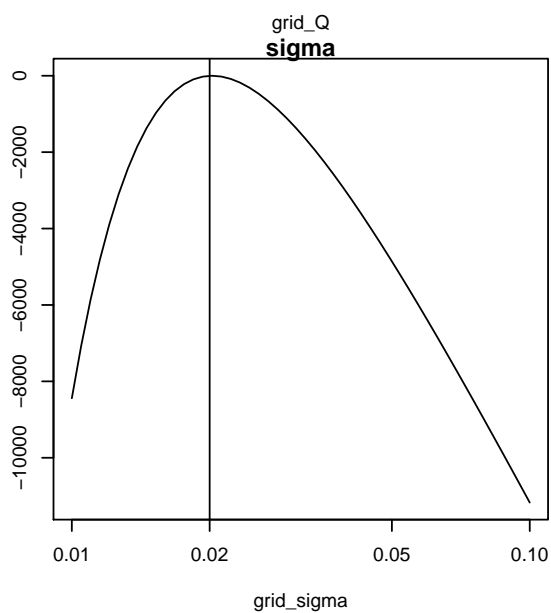
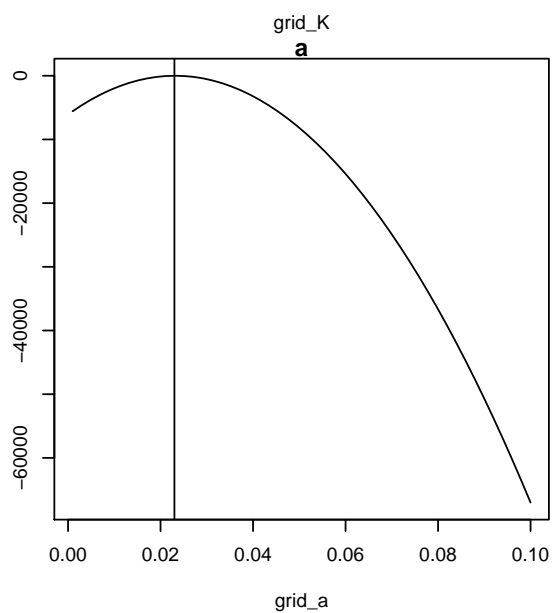
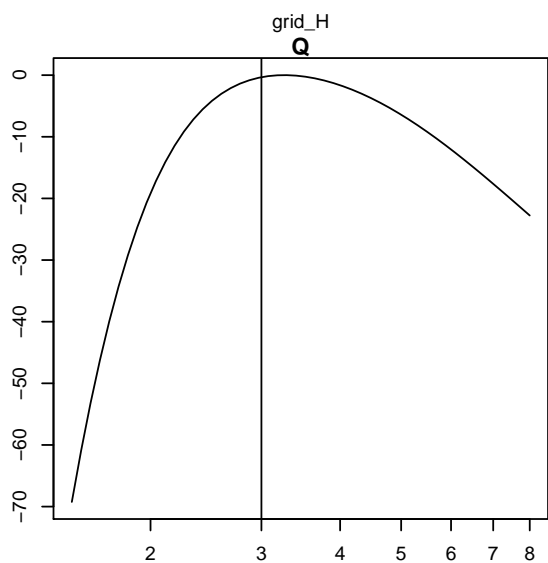
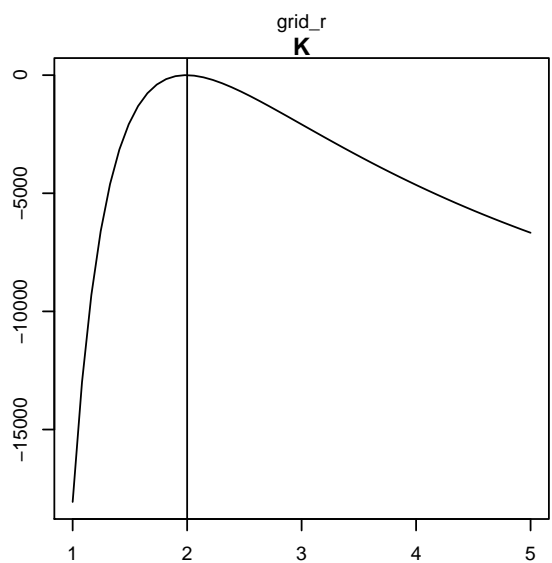
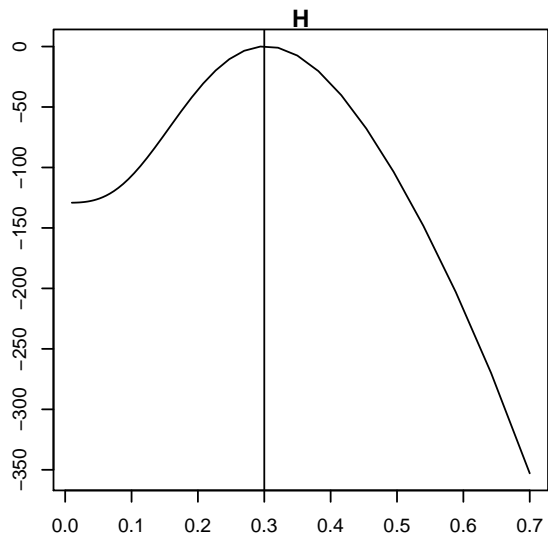
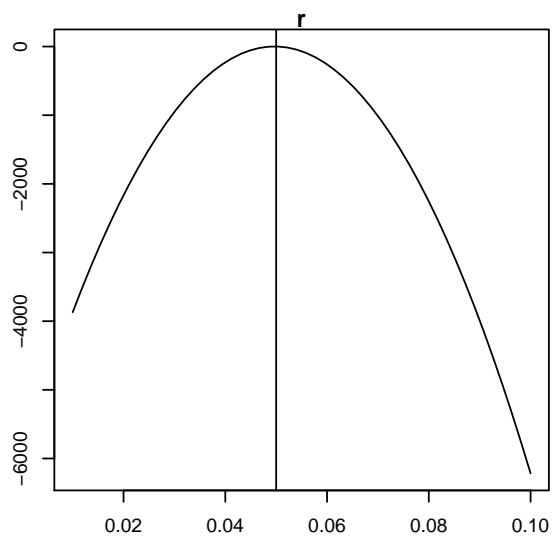
```

ll_Q <- sapply(grid_Q, function(Q) get_ll(a = cmodel$a, x = cmodel$x, r = cmodel$r, K = cmodel$K,
                                          H = cmodel$H, Q = Q, sigma = cmodel$sigma))

##
grid_sigma <- exp(seq(log(1e-2), log(1e-1), l=5e1))
ll_sigma <- sapply(grid_sigma, function(sigma)
  get_ll(a = cmodel$a, x = cmodel$x, r = cmodel$r, K = cmodel$K,
        H = cmodel$H, Q = cmodel$Q, sigma = sigma))

##
layout(matrix(1:6, 3, 2)); par(mar = c(4.1, 2, 1, 1))
plot(grid_r, (ll_r - max(ll_r)), type = "l", main = "r")
abline(v = cmodel$r)
plot(grid_K, (ll_K - max(ll_K)), type = "l", main = "K")
abline(v = cmodel$K)
plot(grid_a, (ll_a - max(ll_a)), type = "l", main = "a")
abline(v = cmodel$a)
plot(grid_H, (ll_H - max(ll_H)), type = "l", main = "H")
abline(v = cmodel$H)
plot(grid_Q, (ll_Q - max(ll_Q)), type = "l", main = "Q", log = "x")
abline(v = cmodel$Q)
plot(grid_sigma, (ll_sigma - max(ll_sigma)), log = "x", type = "l", main = "sigma")
abline(v = cmodel$sigma)

```



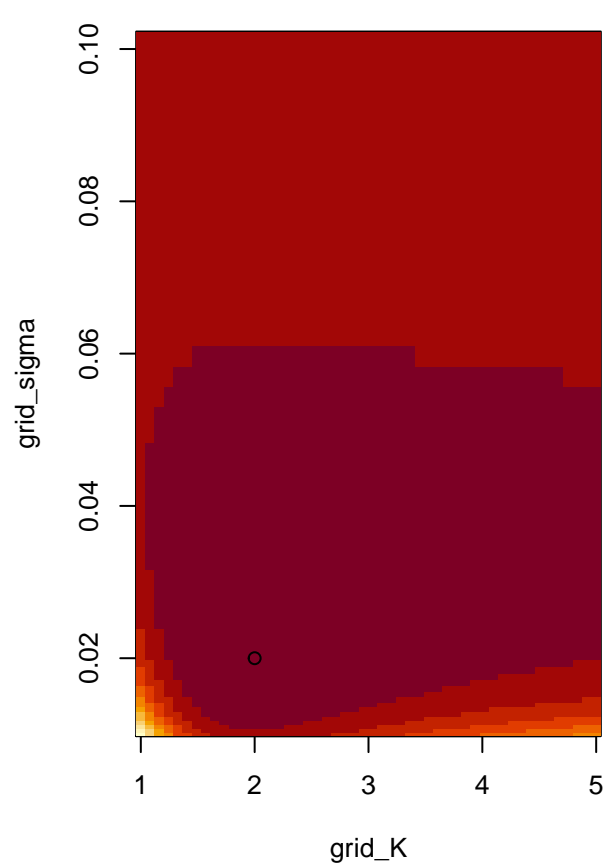
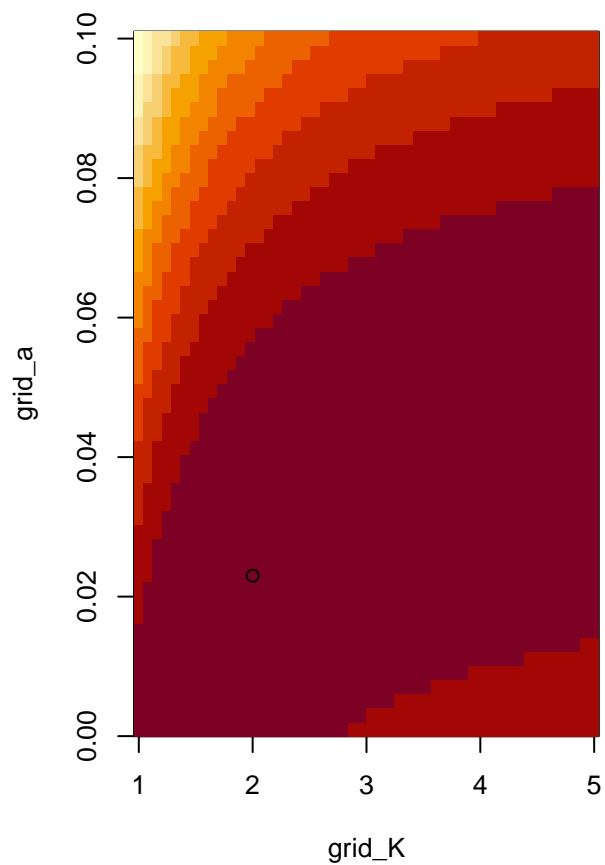
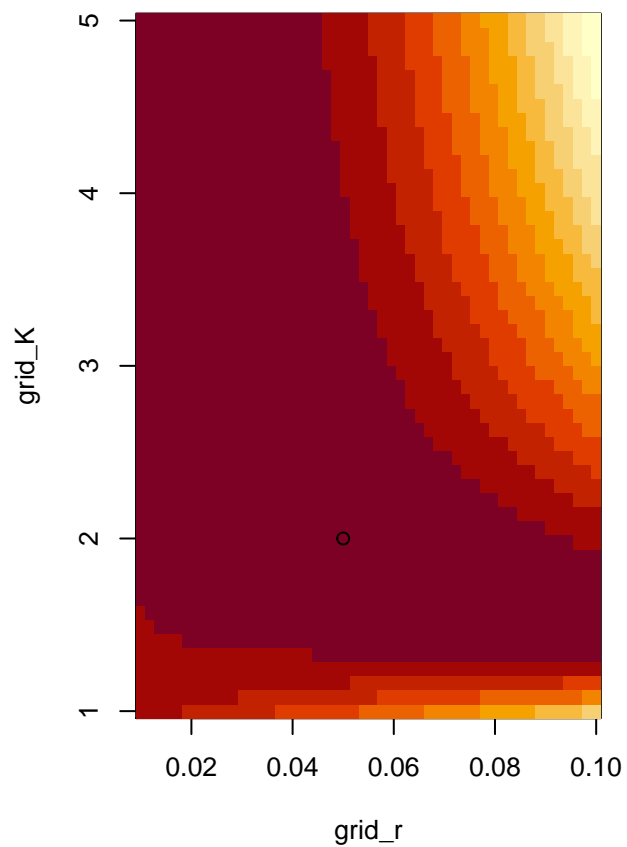
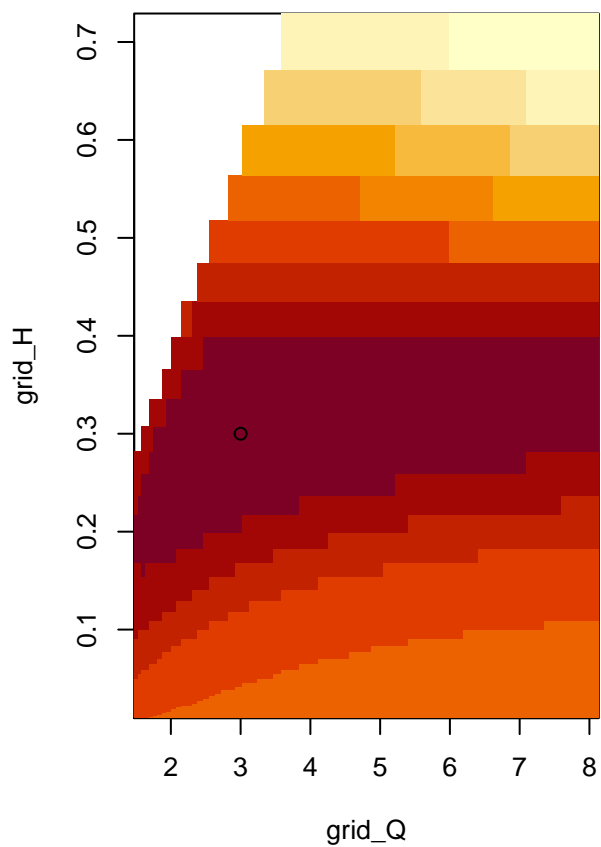
```

ll_QH <- apply(expand.grid(grid_Q, grid_H), 1, function(pair)
  if(pair[2] > (0.6 / 3) * pair[1] + 0.18 - (0.6 / 3)) NA else
  get_ll(a = cmodel$a, x = cmodel$x, r = cmodel$r, K = cmodel$K,
    H = pair[2], Q = pair[1], sigma = cmodel$sigma))
ll_Ka <- apply(expand.grid(grid_K, grid_a), 1, function(pair)
  get_ll(a = pair[2], x = cmodel$x, r = cmodel$r, K = pair[1],
    H = cmodel$H, Q = cmodel$Q, sigma = cmodel$sigma))
ll_rK <- apply(expand.grid(grid_r, grid_K), 1, function(pair)
  get_ll(x = cmodel$x, r = pair[1], K = pair[2], a = cmodel$a,
    H = cmodel$H, Q = cmodel$Q, sigma = cmodel$sigma))
ll_Ksigma <- apply(expand.grid(grid_K, grid_sigma), 1, function(pair)
  get_ll(x = cmodel$x, r = cmodel$r, K = pair[1], a = cmodel$a,
    H = cmodel$H, Q = cmodel$Q, sigma = pair[2]))

layout(matrix(1:4, 2, 2)); par(mar = c(4, 4, 1, 1))
image(grid_Q, grid_H, matrix((ll_QH - max(ll_QH, na.rm = T)), length(grid_Q), length(grid_H)))
points(cmodel$Q, cmodel$H)
##
image(grid_K, grid_a, matrix((ll_Ka - max(ll_Ka)), length(grid_K), length(grid_a)))
points(cmodel$K, cmodel$a)
##
image(grid_r, grid_K, matrix((ll_rK - max(ll_rK)), length(grid_r), length(grid_K)))
points(cmodel$r, cmodel$K)
##
image(grid_K, grid_sigma, matrix((ll_Ksigma - max(ll_Ksigma)), length(grid_a), length(grid_sigma)))
points(cmodel$K, cmodel$sigma)

```





```
model$setData(x = cmodel$x)
cmodel <- compileNimble(model)
```

```
## compiling... this may take a minute. Use 'showCompilerOutput = TRUE' to see C++ compilation details.
```

```
## compilation finished.
```

```
## block sampler
system.time({
  mcmcConf <- configureMCMC(model)
  mcmcConf$getSamplers()
  mcmcConf$removeSamplers(c("x0"))
  mcmcConf$addSampler(target = c("log_r", "log_K", "log_a",
                                "log_H", "log_Q", "log_sigma"),
                      type = 'RW_block')
  mcmcConf$getSamplers()
})
```

```
## Note: Assigning an RW_block sampler to nodes with very different scales can result in low MCMC efficiency.
```

```
##   user  system elapsed
##  8.786   0.099   8.975
```

```
system.time({
  mcmc <- buildMCMC(mcmcConf)
  Cmcmc <- compileNimble(mcmc, project = model)
})
```

```
## compiling... this may take a minute. Use 'showCompilerOutput = TRUE' to see C++ compilation details.
```

```
## compilation finished.
```

```
##   user  system elapsed
## 19.747   0.782  20.874
```

```
##
n_iterations <- 1e4
system.time({
  Cmcmc$run(n_iterations, nburnin = n_iterations / 2)
})
```

```
## |-----|-----|-----|-----|
## |-----|
```

```
##   user  system elapsed
## 167.743   1.405 173.894
```

```
samples <- as.matrix(Cmcmc$mvSamples)
```

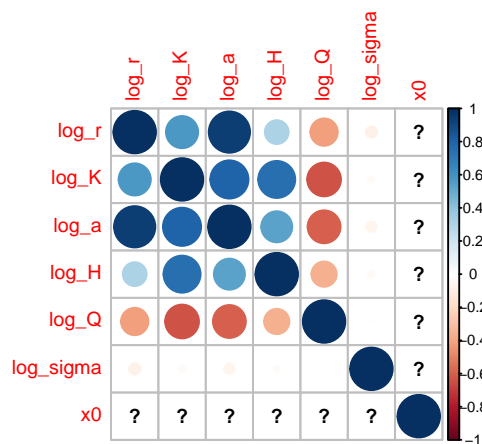
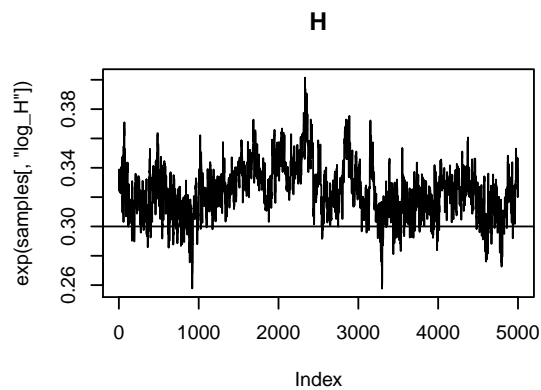
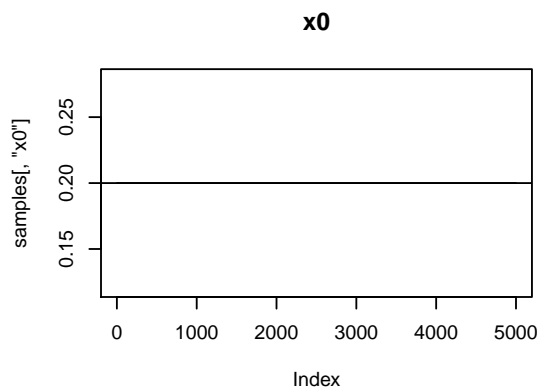
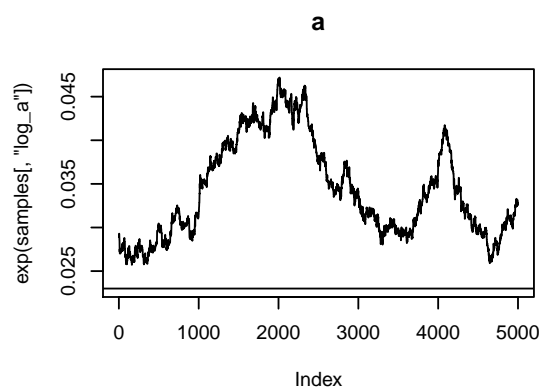
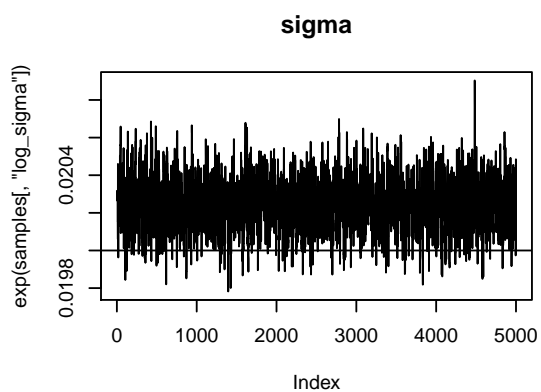
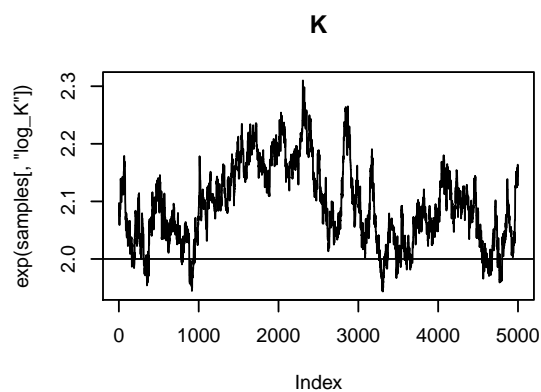
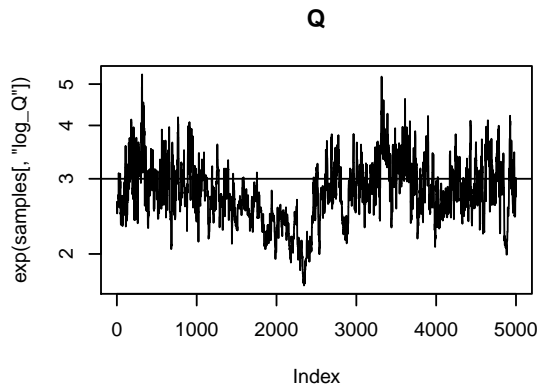
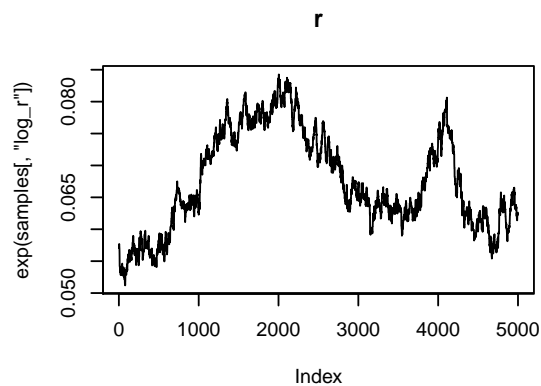
```
layout(matrix(1:8, 4, 2))
plot(exp(samples[, 'log_r']), type = "l", main = "r")
abline(h = r)
plot(exp(samples[, 'log_K']), type = "l", main = "K")
abline(h = K)
plot(exp(samples[, 'log_a']), type = "l", main = "a",
     ylim = range(exp(samples[, 'log_a']), a))
abline(h = a)
plot(exp(samples[, 'log_H']), type = "l", main = "H")
abline(h = H)
plot(exp(samples[, 'log_Q']), type = "l", main = "Q", log = "y")
```

```

abline(h = Q)
plot(exp(samples[, 'log_sigma']), type = "l", main = "sigma")
abline(h = sigma)
plot(samples[, 'x0'], type = "l", main = "x0")
abline(h = x0)
corrplot::corrplot(cor(samples[, c("log_r", "log_K", "log_a", "log_H", "log_Q", "log_sigma", "x0")]))

## Warning in cor(samples[, c("log_r", "log_K", "log_a", "log_H", "log_Q", :
## the standard deviation is zero

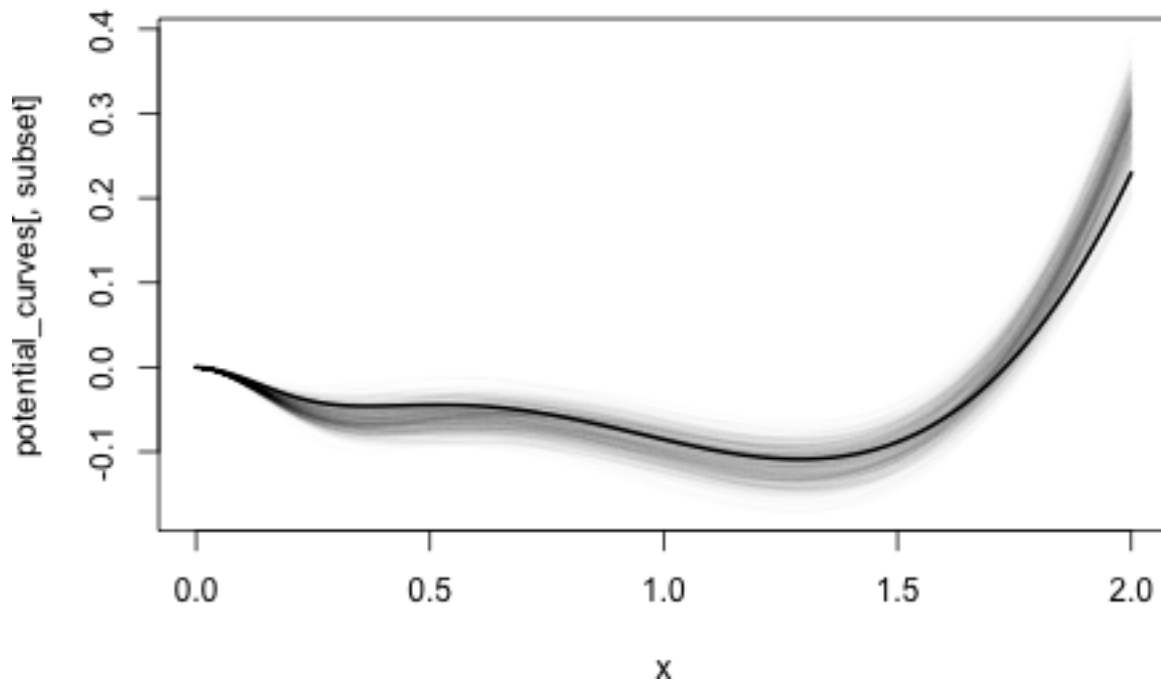
```



```

x <- seq(0, 2, l=1e2)
potential <- function(x = seq(0, 2, l = 1e2), a, r, H, Q, K){
  - cumsum(growth(x = x, r = r, K = K) -
    consumption(x = x, a = a, H = H, Q = Q))
}
potential_curves <- apply(samples, 1, function(row){
  potential(x = x, a = exp(row['log_a']), r = exp(row['log_r']),
    H = exp(row['log_H']), Q = exp(row['log_Q']), K = exp(row['log_K']))
})
subset <- sample(1:nrow(samples), min(400, nrow(samples)))
matplot(x, potential_curves[, subset], type = "l", lty = 1,
  col = scales::alpha(1, 1e-2), lwd = 2)
lines(x, potential(x = x, a = a, r = r, H = H, Q = Q, K = K), lwd = 2)

```

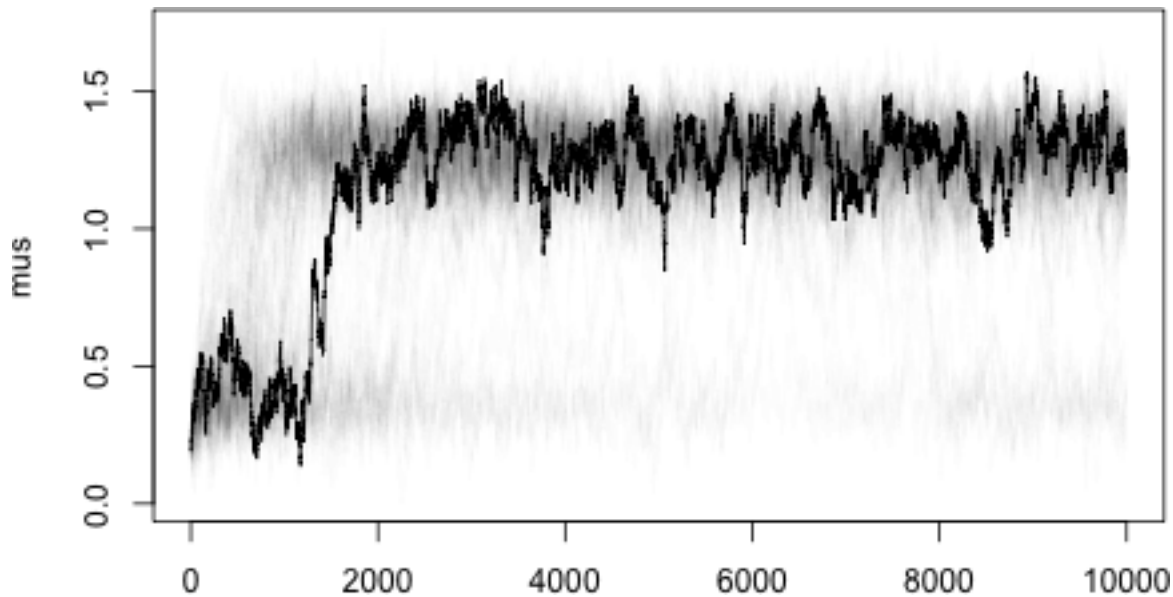


```

cl <- makeForkCluster(2)
mus <- parApply(cl, samples[sample(1:nrow(samples), 100), ], 1,
  function(row){
    x <- rep(NA, N); x[1] <- row['x0']
    mu <- rep(NA, N - 1)
    for(t in 1:(N - 1)){
      mu[t] <-
        x[t] + x[t] * exp(row['log_r']) *
          (1 - x[t] / exp(row['log_K'])) -
        exp(row['log_a']) *
          x[t]^exp(row['log_Q']) / (x[t]^exp(row['log_Q']) +
            exp(row['log_H'])^exp(row['log_Q']))
      x[t + 1] <- rtruncnorm(mean = mu[t], sd = exp(row['log_sigma']))
    }
    return(mu)
  })
stopCluster(cl)
matplot(mus, type = "l", col = scales::alpha(1, 0.01), lty = 1)

```

```
lines(cmodel$mu)
```



Notice  $a$ ,  $r$ , and  $K$  are highly correlated. Taking out two of them stabilizes somewhat, but dependence in the posterior distributions arises between other variables.

```
## block sampler
system.time({
  mcmcConf <- configureMCMC(model)
  mcmcConf$getSamplers()
  mcmcConf$removeSamplers(c("log_a", "log_K", "x0"))
  mcmcConf$addSampler(target = c("log_r", "log_H", "log_Q", "log_sigma"),
                      type = 'RW_block')
  mcmcConf$getSamplers()
})
```

## Note: Assigning an RW\_block sampler to nodes with very different scales can result in low MCMC efficiency.

```
##      user  system elapsed
##  8.839   0.091   9.036
```

```
system.time({
  mcmc <- buildMCMC(mcmcConf)
  Cmcmc <- compileNimble(mcmc, project = model, resetFunctions = T)
})
```

## compiling... this may take a minute. Use 'showCompilerOutput = TRUE' to see C++ compilation details.

## compilation finished.

```
##      user  system elapsed
## 19.694   1.184  21.375
```

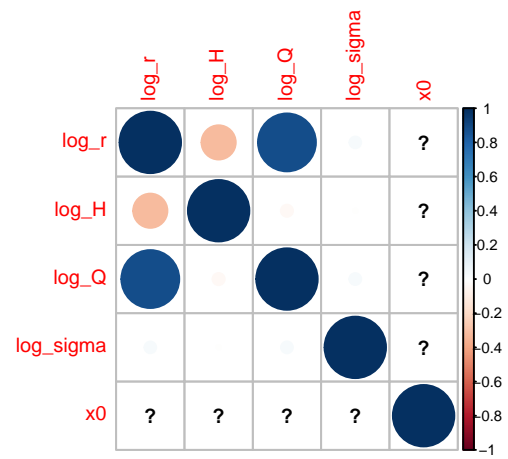
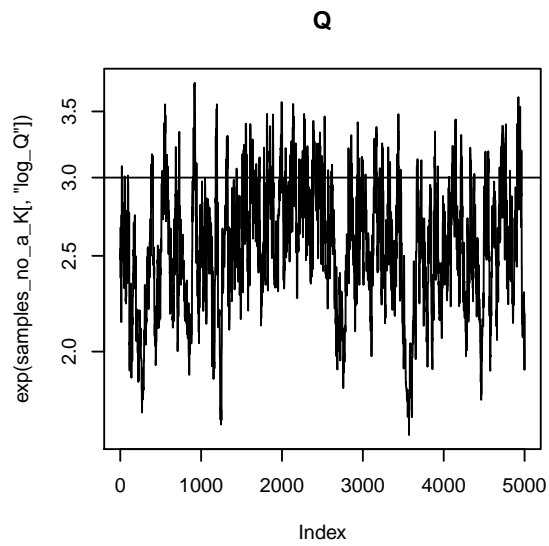
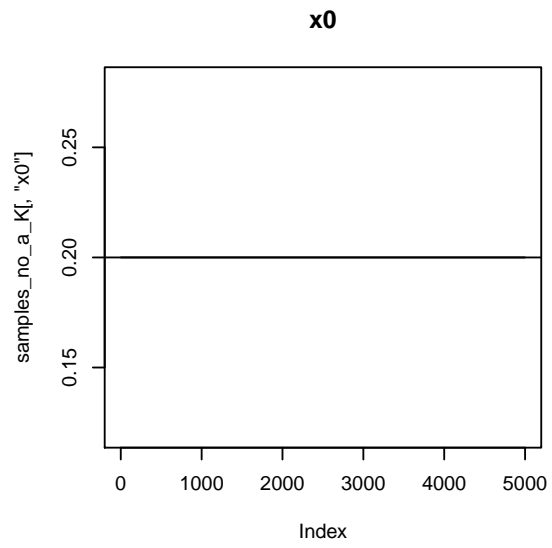
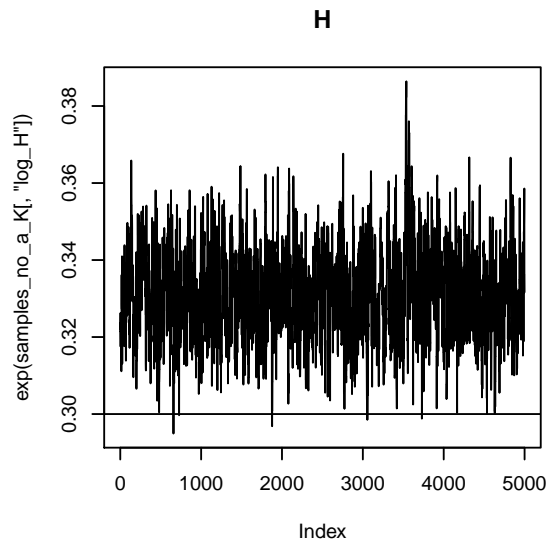
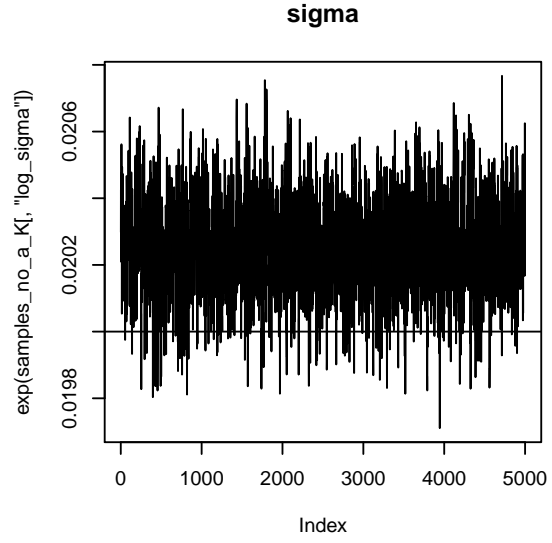
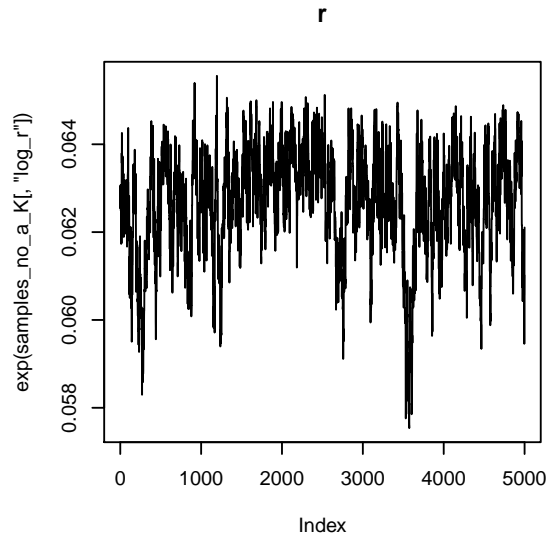
```
##
n_iterations <- 1e4
system.time({
  Cmcmc$run(n_iterations, nburnin = n_iterations / 2)
})
```

```
## |-----|-----|-----|-----|
```

```
## |-----|
##      user  system elapsed
## 114.501    0.868 116.728
samples_no_a_K <- as.matrix(Cmcmc$mvSamples)

layout(matrix(1:6, 3, 2))
plot(exp(samples_no_a_K[, 'log_r']), type = "l", main = "r")
abline(h = r)
plot(exp(samples_no_a_K[, 'log_H']), type = "l", main = "H")
abline(h = H)
plot(exp(samples_no_a_K[, 'log_Q']), type = "l", main = "Q", log = "y")
abline(h = Q)
plot(exp(samples_no_a_K[, 'log_sigma']), type = "l", main = "sigma")
abline(h = sigma)
plot(samples_no_a_K[, 'x0'], type = "l", main = "x0")
abline(h = x0)
corrplot::corrplot(cor(samples_no_a_K[, c("log_r", "log_H", "log_Q", "log_sigma", "x0")]))

## Warning in cor(samples_no_a_K[, c("log_r", "log_H", "log_Q", "log_sigma", :
## the standard deviation is zero
```

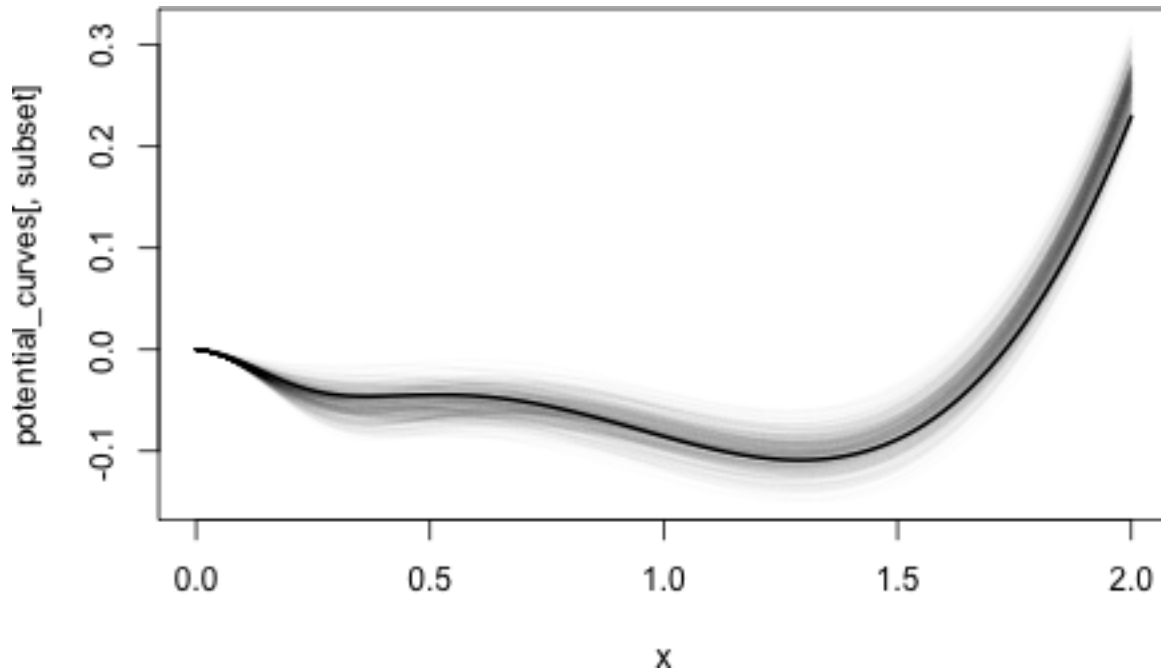




```

x <- seq(0, 2, l=1e2)
potential_curves <- apply(samples_no_a_K, 1, function(row){
  potential(x = x, a = exp(row['log_a']), r = exp(row['log_r']),
    H = exp(row['log_H']), Q = exp(row['log_Q']), K = exp(row['log_K']))
})
matplot(x, potential_curves[, subset], type = "l", lty = 1,
  col = scales::alpha(1, 1e-2), lwd = 2)
lines(x, potential(x = x, a = a, r = r, H = H, Q = Q, K = K), lwd = 2)

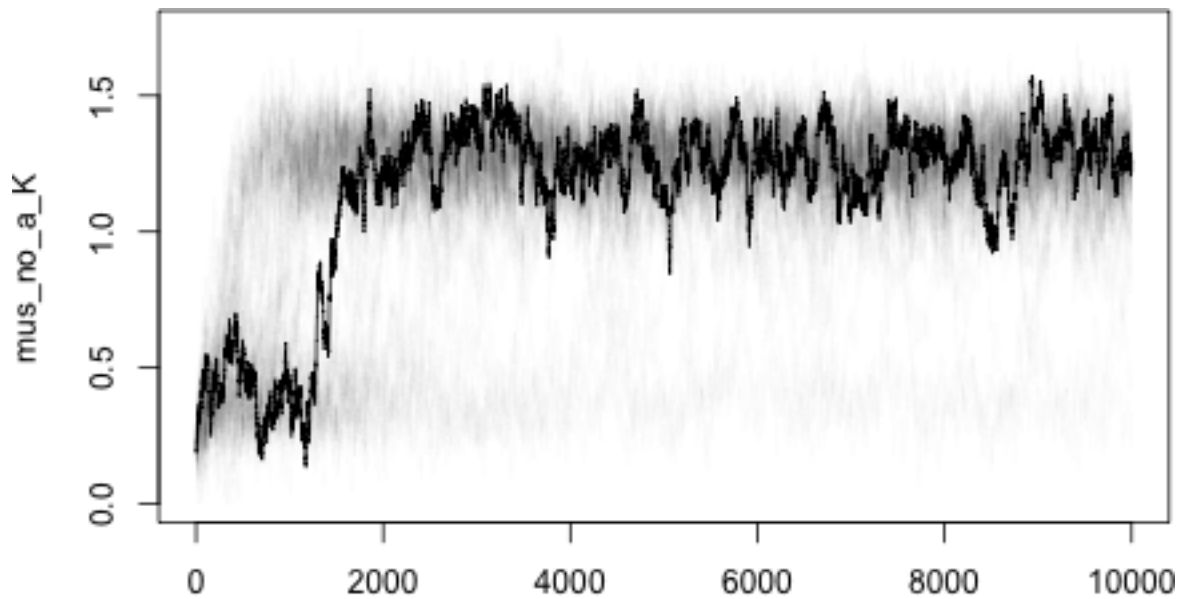
```



```

cl <- makeForkCluster(2)
mus_no_a_K <- parApply(cl, samples_no_a_K[sample(1:nrow(samples_no_a_K), 100), ], 1,
  function(row){
    x <- rep(NA, N); x[1] <- row['x0']
    mu <- rep(NA, N - 1)
    for(t in 1:(N - 1)){
      mu[t] <-
        x[t] + x[t] * exp(row['log_r']) *
          (1 - x[t] / exp(row['log_K'])) -
        exp(row['log_a']) *
          x[t]^exp(row['log_Q']) / (x[t]^exp(row['log_Q']) +
            exp(row['log_H'])^exp(row['log_Q']))
      x[t + 1] <- rtruncnorm(mean = mu[t], sd = exp(row['log_sigma']))
    }
    return(mu)
  })
stopCluster(cl)
matplot(mus_no_a_K, type = "l", col = scales::alpha(1, 0.01), lty = 1)
lines(cmodel$mu)

```



```

N_intro <- 700
constants$N <- N_intro
model <- nimbleModel(code = may, constants = constants, inits = inits)
model$setData(x = cmodel$x[1:N_intro])
cmodel <- compileNimble(model)
## block sampler
system.time({
  mcmcConf <- configureMCMC(model)
  mcmcConf$getSamplers()
  mcmcConf$removeSamplers(c("x0"))
  mcmcConf$addSampler(target = c("log_r", "log_K", "log_a",
                                "log_H", "log_Q", "log_sigma"),
                      type = 'RW_block')
  mcmcConf$getSamplers()
})
system.time({
  mcmc <- buildMCMC(mcmcConf)
  Cmcmc <- compileNimble(mcmc, project = model)
})
##
n_iterations <- 1e4
system.time({
  Cmcmc$run(n_iterations, nburnin = n_iterations / 2)
})
samples <- as.matrix(Cmcmc$mvSamples)

```

```

layout(matrix(1:8, 4, 2))
plot(exp(samples[, 'log_r']), type = "l", main = "r")
abline(h = r)
plot(exp(samples[, 'log_K']), type = "l", main = "K")
abline(h = K)
plot(exp(samples[, 'log_a']), type = "l", main = "a",
      ylim = range(exp(samples[, 'log_a']), a))
abline(h = a)
plot(exp(samples[, 'log_H']), type = "l", main = "H")

```

```

abline(h = H)
plot(exp(samples[, 'log_Q']), type = "l", main = "Q", log = "y")
abline(h = Q)
plot(exp(samples[, 'log_sigma']), type = "l", main = "sigma")
abline(h = sigma)
plot(samples[, 'x0'], type = "l", main = "x0")
abline(h = x0)
corrplot::corrplot(cor(samples[, c("log_r", "log_K", "log_a", "log_H", "log_Q", "log_sigma", "x0")]))

x <- seq(0, 2, l=1e2)
potential <- function(x = seq(0, 2, l = 1e2), a, r, H, Q, K){
  - cumsum(growth(x = x, r = r, K = K) -
            consumption(x = x, a = a, H = H, Q = Q))
}
potential_curves <- apply(samples, 1, function(row){
  potential(x = x, a = exp(row['log_a']), r = exp(row['log_r']),
            H = exp(row['log_H']), Q = exp(row['log_Q']), K = exp(row['log_K']))
})
subset <- sample(1:nrow(samples), min(400, nrow(samples)))
matplot(x, potential_curves[, subset], type = "l", lty = 1,
        col = scales::alpha(1, 1e-2), lwd = 2)
lines(x, potential(x = x, a = a, r = r, H = H, Q = Q, K = K), lwd = 2)

cl <- makeForkCluster(2)
mus <- parApply(cl, samples[sample(1:nrow(samples), 100), ], 1,
               function(row){
  x <- rep(NA, N); x[1] <- row['x0']
  mu <- rep(NA, N - 1)
  for(t in 1:(N - 1)){
    mu[t] <-
      x[t] + x[t] * exp(row['log_r']) *
        (1 - x[t] / exp(row['log_K'])) -
      exp(row['log_a']) *
        x[t]^exp(row['log_Q']) / (x[t]^(row['log_Q']) +
      exp(row['log_H'])^(row['log_Q']))
    x[t + 1] <- rtruncnorm(mean = mu[t], sd = exp(row['log_sigma']))
  }
  return(mu)
})
stopCluster(cl)
matplot(mus, type = "l", col = scales::alpha(1, 0.01), lty = 1)
lines(cmodel$mu)

```