Introduction to NIMBLE

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What is NIMBLE

Figure 1: Logo of the NIMBLE R package designed by Luke Larson.

NIMBLE stands for **N**umerical **I**nference for statistical **M**odels using **B**ayesian and **L**ikelihood **E**stimation. Briefly speaking, NIMBLE is an R package that implements for you MCMC algorithms to generate samples from the posterior distribution of model parameters. Freed from the burden of coding your own MCMC algorithms, you only have to specify a likelihood and priors to apply the Bayes theorem. To do so, NIMBLE uses a syntax very similar to the R syntax, which should make your life easier. This so-called BUGS language is also used by other programs like WinBUGS, OpenBUGS, and JAGS.

So why use NIMBLE you may ask? The short answer is that NIMBLE is capable of so much more than just running MCMC algorithms! First, you will work from within R, but in the background NIMBLE will translate your code in C++ for (in general) faster computation. Second, NIMBLE extends the BUGS language for writing new functions and distributions of your own, or borrow those written by others. Third, NIMBLE gives you full control of the MCMC samplers, and you may pick other algorithms than the defaults. Fourth, NIMBLE comes with a library of numerical methods other than MCMC algorithms, including sequential Monte Carlo (for particle filtering) and Monte Carlo Expectation Maximization (for maximum likelihood). Last but not least, the development team is friendly and helpful, and based on users' feedbacks, NIMBLE folks work constantly at improving the package capabilities.

Getting started

To run NIMBLE, you will need to:
1. Build a model consisting of a likelihood and priors.
2. Read in some data.
3. Specify parameters you want to make inference about.

4. Pick initial values for parameters to be estimated (for each chain).
5. Provide MCMC details namely the number of chains, the length of the burn-in period and the number of iterations following burn-in.

First things first, let's not forget to load the `nimble` package ad the other packages useful for this workshop:

```
library(nimble)
library(dplyr)
library(ggplot2)
```

Note that before you can install ***`nimble`*** *like any other R package, Windows users will need to install* ***`Rtools`****, and Mac users will need to install* ***`Xcode`****. More at https://r-nimble.org/download.*

Now let's make a example on animal survival. Say we capture, mark and release `n = 57` animals at the beginning of a winter, out of which we recapture `y = 19` animals alive. Assuming all animals are independent of each other and have the same survival probability `theta`, then `y` the number of alive animals at the end of the winter is binomial.

1. Build model

We'd like to estimate winter survival `theta`. First step is to build our model by specifying the binomial likelihood and a uniform prior on survival probability `theta`. We use the `nimbleCode()` function and wrap code within curly brackets:

```
model <- nimbleCode({
  # likelihood
  survived ~ dbinom(theta, released)
  # prior
  theta ~ dunif(0, 1)
  # derived quantity
  lifespan <- -1/log(theta)
})
```

You can check that the `model` R object contains your code:

```
model
```

```
## {
##     survived ~ dbinom(theta, released)
##     theta ~ dunif(0, 1)
##     lifespan <- -1/log(theta)
## }
```

In the code above, `survived` and `released` are known, only `theta` needs to be estimated. The line `survived ~ dbinom(theta, released)` states that the number of successes or animals that have survived over winter `survived` is distributed as (that's the `~`) as a binomial with `released` trials and probability of success or survival `theta`. Then the line `theta ~ dunif(0, 1)` assigns a uniform between 0 and 1 as a prior distribution to the survival probability. This is all you need, a likelihood and priors for model parameters, NIMBLE knows the Bayes theorem. The last line `lifespan <- - 1/log(theta)` calculates a quantity derived from `theta`, which is the expected lifespan assuming constant survival[1].

A few comments:

- The most common distributions are available in NIMBLE. Among others, there are `dbeta`, `dmultinom` and `dnorm`. If you cannot find what you need in NIMBLE, you can write your own distribution.
- It does not matter in what order you write each line of code, NIMBLE uses what is called a declarative language for building models. In brief, you write code that tells NIMBLE what you want to achieve,

[1] Cook LM, Brower LP, Croze HJ (1967) The accuracy of a population estimation from multiple recapture data. J Anim Ecol 36:57–60

and not how to get there. In contrast, an imperative language requires that you write what you want your program to do step by step.

- You can think of models in NIMBLE as graphs. A graph is made of relations (or edges) that can be of two types. A stochastic relation is signaled by a `~` sign and defines a random variable in the model, such as `survived` or `theta`. A deterministic relation is signaled by a `<-` sign, like `lifespan`. Relations define nodes on the left - the children - in terms of other nodes on the right - the parents, and relations are directed edges from parents to children. Such graphs are called directed acyclic graph or DAG (example in Figure **2**).

```
mc <- nimbleModel(model, data = list(released = 57, survived = 19))
```

```
## defining model...
## 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.
```

```
mc$plotGraph()
```

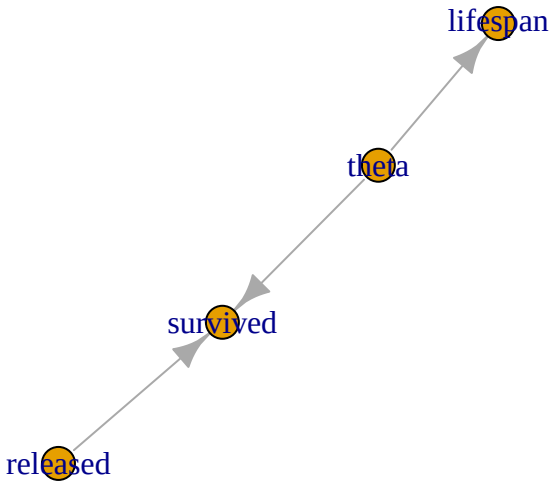


Figure 2: Graph of the animal survival model. Survived is a stochastic node defined by its parents `released` and `theta`, while `lifespan` is a deterministic node the value of which is defined exactly by the value of its parent `theta`.

2. Read in data

Second step in our workflow is to read in some data. We use a list in which each component corresponds to a known quantity in the model:

```
my.data <- list(released = 57, survived = 19)
```

You can proceed with data passed this way, but you should know a little more about how NIMBLE sees data. NIMBLE distinguishes **data** and **constants**.

- Constants are values that do not change, e.g. vectors of known index values or the indices used to define for loops.
- Data are values that you might want to change, basically anything that only appears on the left of a ~.

Declaring relevant values as constants is better for computational efficiency, but it is easy to forget, and fortunately NIMBLE will by itself distinguish data and constants.

3. Specify parameters

Third step is to tell NIMBLE which nodes in your model you would like to keep track of, in other words the quantities you'd like to do inference about. In our model we want survival `theta` and `lifespan`:

```
parameters.to.save <- c("theta", "lifespan")
```

In general you have many quantities in your model, including some of little interest that are not worth monitoring, and having full control on verbosity will prove handy.

4. Pick initial values

Fourth step is to specify initial values for all model parameters. To make sure that the MCMC algorithm explores the posterior distribution, we start different chains with different parameter values. You can specify initial values for each chain in a list and put them in yet another list:

```
init1 <- list(theta = 0.1)
init2 <- list(theta = 0.5)
init3 <- list(theta = 0.9)
initial.values <- list(init1, init2, init3)

# visualize initial values
initial.values
```

```
## [[1]]
## [[1]]$theta
## [1] 0.1
##
##
## [[2]]
## [[2]]$theta
## [1] 0.5
##
##
## [[3]]
## [[3]]$theta
## [1] 0.9
```

Alternatively, you can write a simple R function that generates random initial values:

```
initial.values <- function() list(theta = runif(1,0,1))
# visualize initial values
initial.values()
```

```
## $theta
## [1] 0.3766893
```

5. Provide MCMC details

Firth and last step, you need to tell NIMBLE the number of chains to run, say `n.chain`, how long the burn-in period should be, say `n.burnin`, and the number of iterations following the burn-in period to be used for posterior inference. In NIMBLE, you specify the total number of iterations, say `n.iter`, so that the number of posterior samples per chain is `n.iter - n.burnin`. NIMBLE also allows discarding samples after burn-in, a procedure known as thinning[2].

```
n.iter <- 5000
n.burnin <- 1000
n.chains <- 3
```

Run NIMBLE

We now have all the ingredients to run model, that is to sample in the posterior distribution of model parameters using MCMC simulations. This is accomplished using function `nimbleMCMC()`:

```
mcmc.output <- nimbleMCMC(code = model,
                          data = my.data,
                          inits = initial.values,
                          monitors = parameters.to.save,
                          niter = n.iter,
                          nburnin = n.burnin,
                          nchains = n.chains)
```

```
## defining model...
```

```
## 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...
## checking model calculations...
## model building finished.
## compiling... this may take a minute. Use 'showCompilerOutput = TRUE' to see C++ compilation details.
## compilation finished.
## running chain 1...
```

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

```
## running chain 2...
```

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

```
## running chain 3...
```

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

[2]Link, W.A. and Eaton, M.J. (2012), On thinning of chains in MCMC. Methods in Ecology and Evolution, 3: 112-115.

NIMBLE goes through several steps that we will explain. Function `nimbleMCMC()` takes other arguments that you might find useful. For example, you can suppress the progress bar if you find it too depressing when running long simulations with `progressBar = FALSE`. You can also get a summary of the outputs by specifying `summary = TRUE`. Check `?nimbleMCMC` for more details.

Inspect outputs

Structure

Now let's inspect what we have in `mcmc.output`:

```
str(mcmc.output)
```

```
## List of 3
##  $ chain1: num [1:4000, 1:2] 0.876 0.876 0.876 0.876 0.876 ...
##   ..- attr(*, "dimnames")=List of 2
##   .. ..$ : NULL
##   .. ..$ : chr [1:2] "lifespan" "theta"
##  $ chain2: num [1:4000, 1:2] 1.107 0.792 0.773 1.078 1.078 ...
##   ..- attr(*, "dimnames")=List of 2
##   .. ..$ : NULL
##   .. ..$ : chr [1:2] "lifespan" "theta"
##  $ chain3: num [1:4000, 1:2] 0.864 0.864 0.864 0.864 0.864 ...
##   ..- attr(*, "dimnames")=List of 2
##   .. ..$ : NULL
##   .. ..$ : chr [1:2] "lifespan" "theta"
```

Dimensions

The R object `mcmc.output` is a list with three components, one for each MCMC chain. Let's have a look to `chain1` for example:

```
dim(mcmc.output$chain1)
```

```
## [1] 4000    2
```

```
head(mcmc.output$chain1)
```

```
##       lifespan     theta
## [1,] 0.8762681 0.3194345
## [2,] 0.8762681 0.3194345
## [3,] 0.8762681 0.3194345
## [4,] 0.8762681 0.3194345
## [5,] 0.8762681 0.3194345
## [6,] 1.0655700 0.3912280
```

Return values

```
head(mcmc.output$chain1)
```

```
##       lifespan     theta
## [1,] 0.8762681 0.3194345
## [2,] 0.8762681 0.3194345
## [3,] 0.8762681 0.3194345
## [4,] 0.8762681 0.3194345
## [5,] 0.8762681 0.3194345
## [6,] 1.0655700 0.3912280
```

Each component of the list is a matrix. In rows, you have 4000 samples from the posterior distribution of `theta`, which corresponds to `n.iter - n.burnin` iterations. In columns, you have the quantities we monitor, `theta` and `lifespan`.

Compute posterior summaries

You can compute the posterior mean of `theta`:

```
mean(mcmc.output$chain1[,'theta'])
```

```
## [1] 0.3366266
```

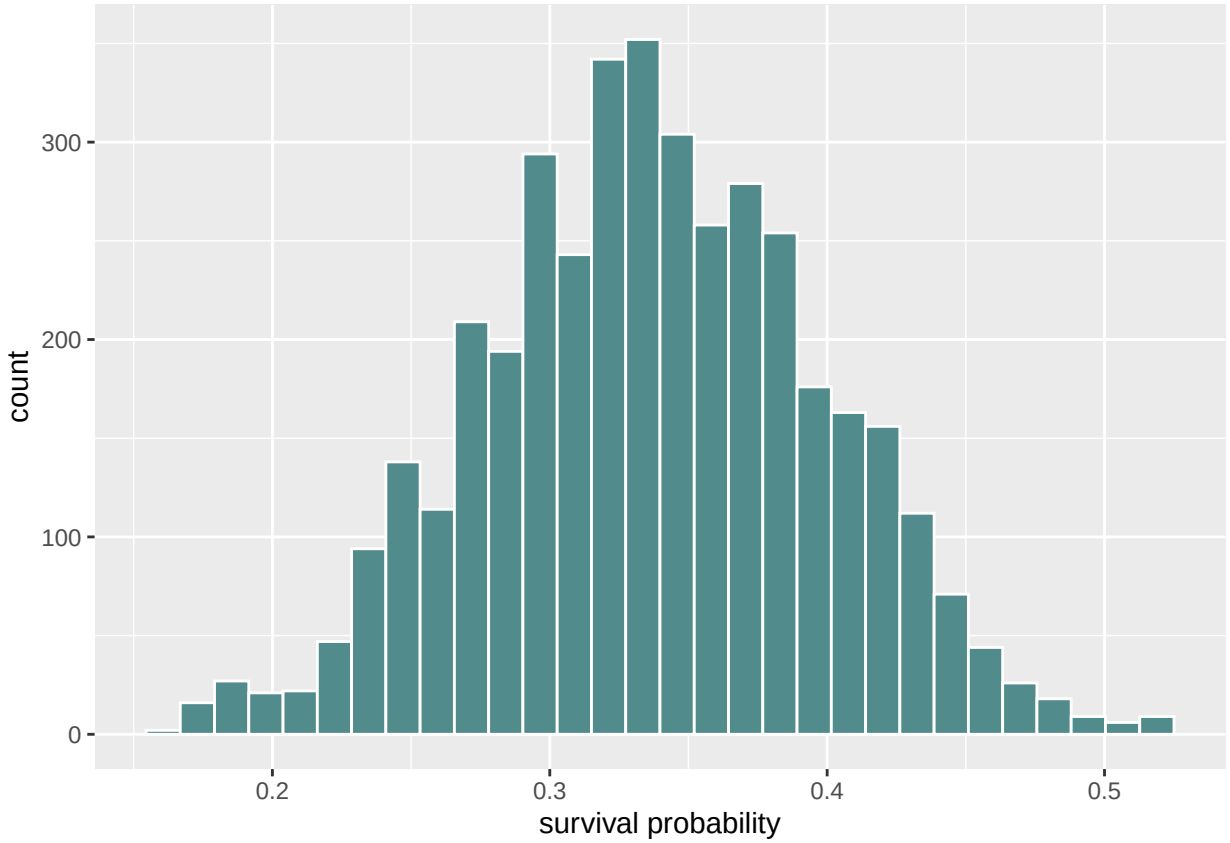
You can also obtain the 95% credible interval for `theta`:

```
quantile(mcmc.output$chain1[,'theta'], probs = c(2.5, 97.5)/100)
```

```
##      2.5%     97.5%
## 0.2239405 0.4520529
```

Let's visualise the posterior distribution of `theta` with a histogram:

```
mcmc.output %>%
  as_tibble() %>%
  ggplot() +
  geom_histogram(aes(x = chain1[,"theta"]), color = "white", fill = "darkslategray4") +
  labs(x = "survival probability")
```



There are less painful ways of doing posterior inference. The R package `MCMCvis`[3] allows to summarise

[3] https://github.com/caseyyoungflesh/MCMCvis

and visualize MCMC outputs, but there are other perfectly valid options out there like `ggmcmc`[4] and `basicMCMCplots`[5].

Let's load the package `MCMCvis`:

```
library(MCMCvis)
```

```
## Warning: package 'MCMCvis' was built under R version 4.0.5
```

Numerical summaries

To get the most common numerical summaries, the function `MCMCsummary()` does the job:

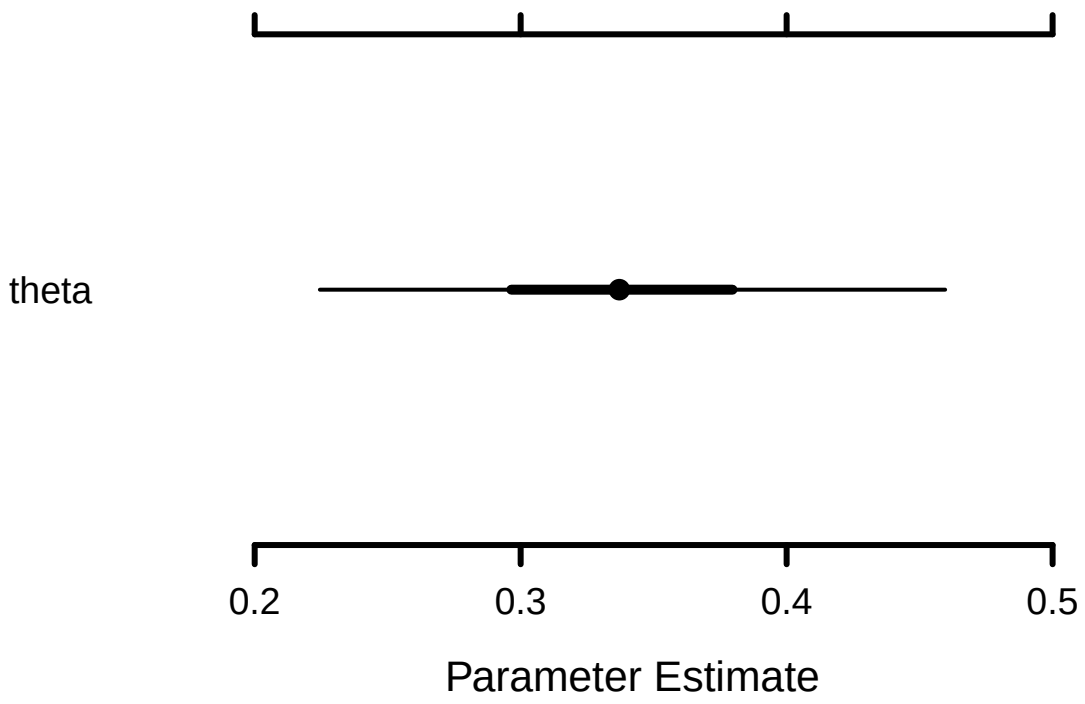
```
MCMCsummary(object = mcmc.output, round = 2)
```

```
##          mean   sd 2.5%  50% 97.5% Rhat n.eff
## lifespan 0.93 0.16 0.67 0.92  1.29    1  2715
## theta    0.34 0.06 0.22 0.34  0.46    1  2743
```

Visualize

You can use a caterpillar plot to visualise the posterior distributions of `theta` with `MCMCplot()`:

```
MCMCplot(object = mcmc.output,
         params = 'theta')
```



[4] Fernández-i-Marín, X. (2016). ggmcmc: Analysis of MCMC Samples and Bayesian Inference. Journal of Statistical Software, 70(9), 1–20

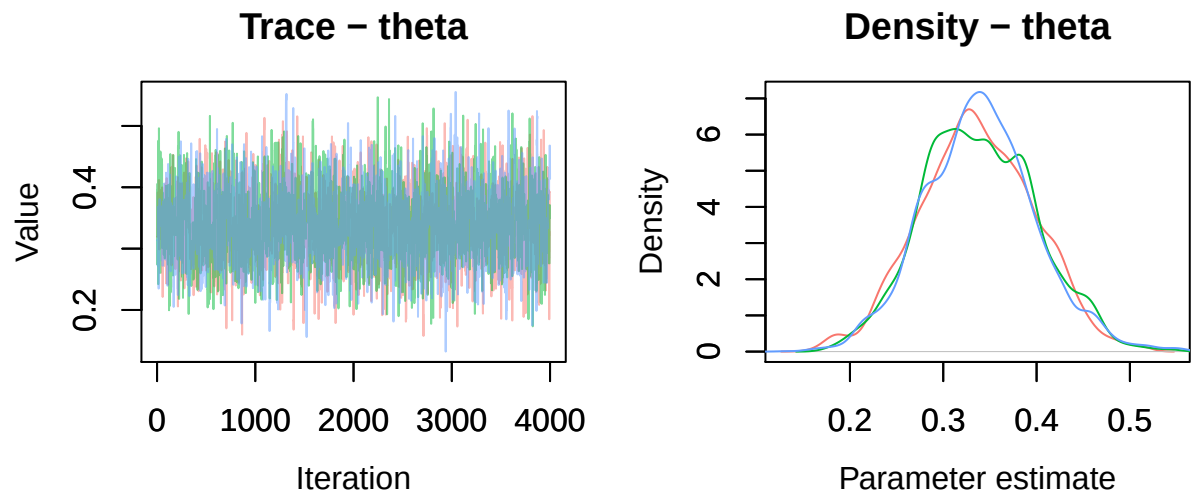
[5] https://cran.r-project.org/web/packages/basicMCMCplots/index.html

The point represents the posterior median, the thick line is the 50% credible interval and the thin line the 95% credible interval.

Trace and posterior density

The trace and posterior density of theta can be obtained with `MCMCtrace()`:

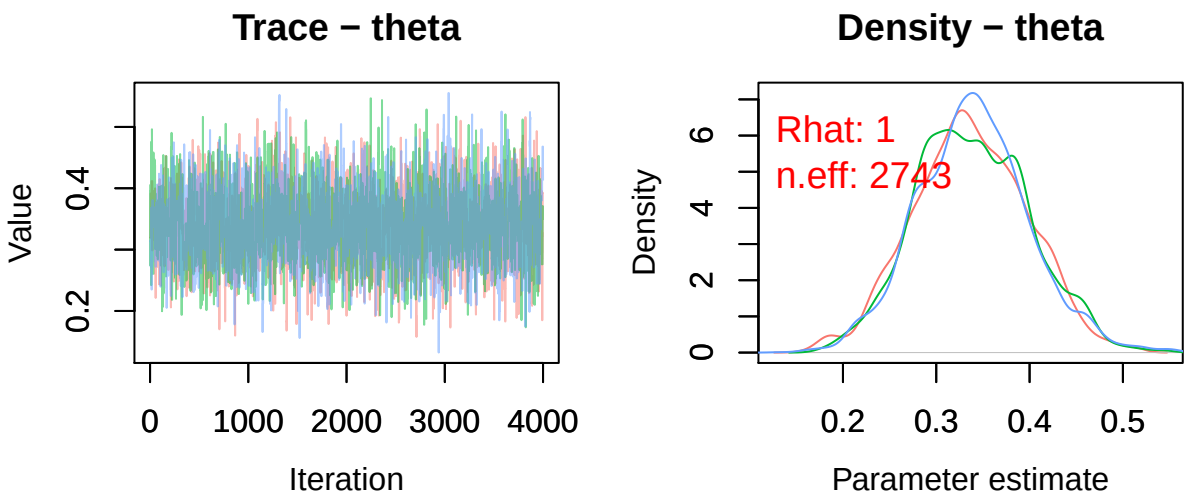
```
MCMCtrace(object = mcmc.output,
          pdf = FALSE, # no export to PDF
          ind = TRUE, # separate density lines per chain
          params = "theta")
```



Diagnostics of convergence

You can also add the diagnostics of convergence:

```
MCMCtrace(object = mcmc.output,
          pdf = FALSE,
          ind = TRUE,
          Rhat = TRUE, # add Rhat
          n.eff = TRUE, # add eff sample size
          params = "theta")
```



Derived quantities

Compute lifespan (1) We calculated lifespan directly in our model with `lifespan <- -1/log(theta)`. But you can also calculate this quantity from outside NIMBLE. This is a nice by-product of using MCMC simulations: you can obtain the posterior distribution of any quantity that is function of your model parameters by applying this function to samples from the posterior distribution of these parameters. In our example, all you need is samples from the posterior distribution of `theta`, which we pool between the three chains with:

```
theta_samples <- c(mcmc.output$chain1[,'theta'],
                   mcmc.output$chain2[,'theta'],
                   mcmc.output$chain3[,'theta'])
```

Compute lifespan (2)

To get samples from the posterior distribution of lifespan, we apply the function to calculate lifespan to the samples from the posterior distribution of survival:

```
lifespan <- -1/log(theta_samples)
```

Numerical summaries

As usual then, you can calculate the posterior mean and 95% credible interval:

```
mean(lifespan)
```

```
## [1] 0.9349671
```

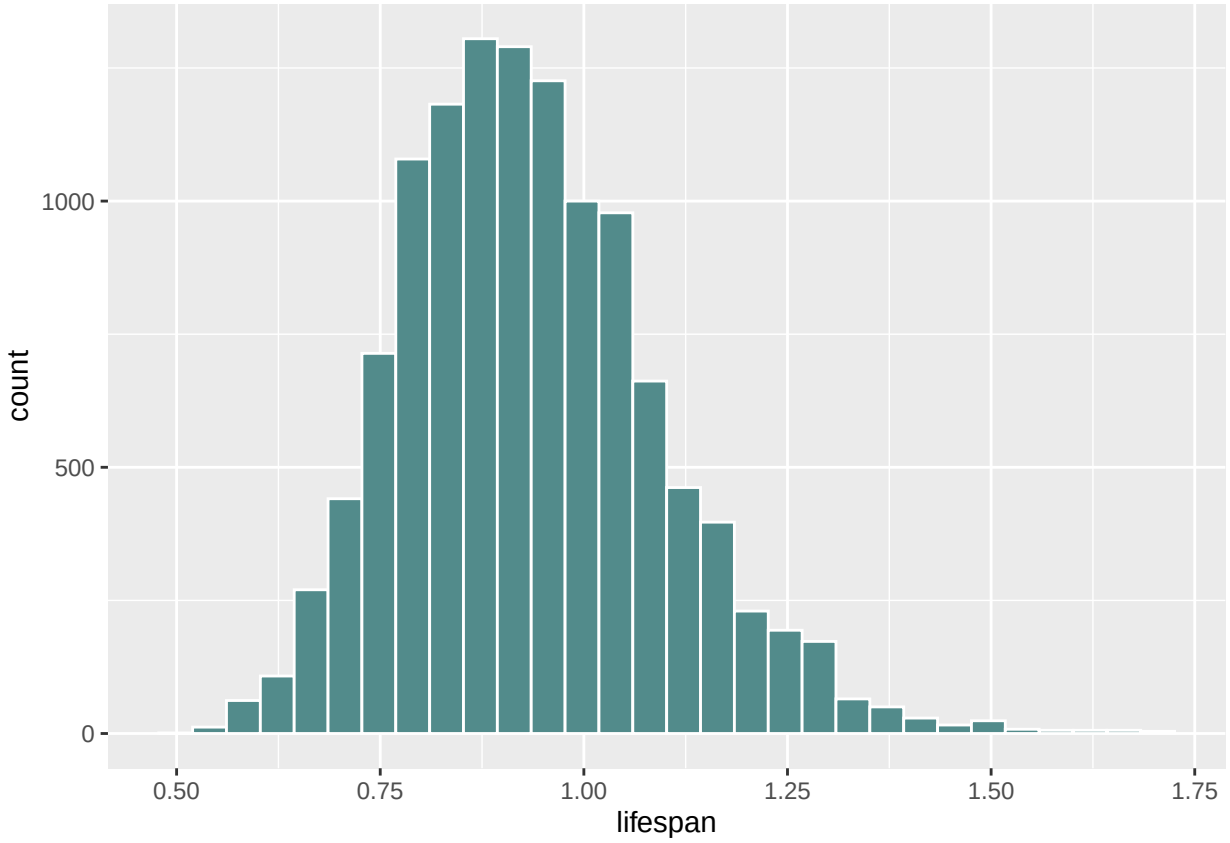
```r
quantile(lifespan, probs = c(2.5, 97.5)/100)
```

```
##      2.5%     97.5%
## 0.6694227 1.2863616
```

Visualize

You can also visualize the posterior distribution of lifespan:

```r
lifespan %>%
  as_tibble() %>%
  ggplot() +
  geom_histogram(aes(x = value), color = "white", fill = "darkslategray4") +
  labs(x = "lifespan")
```



All steps at once

Now you're good to go. For convenience the steps above are summarize in the box below. The NIMBLE workflow provided with `nimbleMCMC()` allows you to build models and make inference. This is what you can achieve with other software like WinBUGS or JAGS.

```r
# model building
model <- nimbleCode({
  # likelihood
  survived ~ dbinom(theta, released)
  # prior
  theta ~ dunif(0, 1)
  # derived quantity
```

```
  lifespan <- -1/log(theta)
})
# read in data
my.data <- list(released = 57, survived = 19)
# specify parameters to monitor
parameters.to.save <- c("theta", "lifespan")
# pick initial values
initial.values <- function() list(theta = runif(1,0,1))
# specify MCMC details
n.iter <- 5000
n.burnin <- 1000
n.chains <- 3
# run NIMBLE
mcmc.output <- nimbleMCMC(code = model,
                          data = my.data,
                          inits = initial.values,
                          monitors = parameters.to.save,
                          niter = n.iter,
                          nburnin = n.burnin,
                          nchains = n.chains)
# calculate numerical summaries
MCMCsummary(object = mcmc.output, round = 2)
# visualize parameter posterior distribution
MCMCplot(object = mcmc.output,
         params = 'theta')
# check convergence
MCMCtrace(object = mcmc.output,
          pdf = FALSE, # no export to PDF
          ind = TRUE, # separate density lines per chain
          params = "theta")
```

NIMBLE is more than just another MCMC engine. It provides a programming environment so that you have full control when building models and estimating parameters. NIMBLE allows you to write your own functions and distributions to build models, and to choose alternative MCMC samplers or code new ones. This flexibility often comes with faster convergence.

Programming

In NIMBLE you can write and use your own functions, or use existing R or C/C++ functions. This allows you to customize models the way you want.

NIMBLE functions

NIMBLE provides `nimbleFunctions` for programming. A `nimbleFunction` is like an R function, plus it can be compiled for faster computation. Going back to our animal survival example, we can write a `nimbleFunction` to compute lifespan:

```
computeLifespan <- nimbleFunction(
    run = function(theta = double(0)) { # type declarations
        ans <- -1/log(theta)
        return(ans)
        returnType(double(0))  # return type declaration
    } )
```

Within the nimbleFunction, the `run` section gives the function to be executed. It is written in the NIMBLE

language. The `theta = double(0)` and `returnType(double(0))` arguments tell NIMBLE that the input and output are single numeric values (scalars). Alternatively, `double(1)` and `double(2)` are for vectors and matrices, while `logical()`, `integer()` and `character()` are for logical, integer and character values.

You can use your `nimbleFunction` in R:

```
computeLifespan(0.8)
```

```
## [1] 4.48142
```

You can compile it and use the C++ code for faster computation:

```
CcomputeLifespan <- compileNimble(computeLifespan)
```

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

```
CcomputeLifespan(0.8)
```

```
## [1] 4.48142
```

You can also use your `nimbleFunction` in a model:

```
model <- nimbleCode({
  # likelihood
  survived ~ dbinom(theta, released)
  # prior
  theta ~ dunif(0, 1)
  # derived quantity
  lifespan <- computeLifespan(theta)
})
```

The rest of the workflow remains the same:

```
my.data <- list(survived = 19, released = 57)
parameters.to.save <- c("theta", "lifespan")
initial.values <- function() list(theta = runif(1,0,1))
n.iter <- 5000
n.burnin <- 1000
n.chains <- 3
mcmc.output <- nimbleMCMC(code = model,
                          data = my.data,
                          inits = initial.values,
                          monitors = parameters.to.save,
                          niter = n.iter,
                          nburnin = n.burnin,
                          nchains = n.chains)
```

```
## defining model...
## 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...
## checking model calculations...
## model building finished.
## compiling... this may take a minute. Use 'showCompilerOutput = TRUE' to see C++ compilation details.
## compilation finished.
```

```
## running chain 1...
## |-------------|-------------|-------------|-------------|
## |-------------------------------------------------------|
## running chain 2...
## |-------------|-------------|-------------|-------------|
## |-------------------------------------------------------|
## running chain 3...
## |-------------|-------------|-------------|-------------|
## |-------------------------------------------------------|
```

```
MCMCsummary(object = mcmc.output, round = 2)
```

```
##          mean   sd 2.5%  50% 97.5% Rhat n.eff
## lifespan 0.94 0.16 0.66 0.92  1.30    1  2538
## theta    0.34 0.06 0.22 0.34  0.46    1  2618
```

More about nimbleFunctions

With `nimbleFunctions`, you can mimic basic R syntax, do linear algebra (e.g. compute eigenvalues), operate on vectors and matrices (e.g. inverse a matrix), use logical operators (e.g. and/or) and flow control (e.g. if-else). There is also a long list of common and less common distributions that can be used with `nimbleFunctions`. To learn everything you need to know on writing `nimbleFunctions`, make sure to read chapter 11 of the NIMBLE manual at https://r-nimble.org/html_manual/cha-RCfunctions.html#cha-RCfunctions.

Calling R/C++ functions

If you're like us, and too lazy to write your own functions, you can rely on the scientific community and use existing C, C++ or R code. The trick is to write a `nimbleFunction` that wraps access to that code which can then be used by NIMBLE. As an example, imagine you'd like to use an R function `myfunction()`, either a function you wrote yourself, or a function available in your favorite R package:

```
myfunction <- function(x) {
  -1/log(x)
}
```

Now wrap this function using `nimbleRcall()` or `nimbleExternalCall()` for a C or C++ function:

```
Rmyfunction <- nimbleRcall(prototype = function(x = double(0)){},
                           Rfun = 'myfunction',
                           returnType = double(0))
```

In the call to `nimbleRcall()` above, the argument `prototype` specifies inputs (a single numeric value `double(0)`) of the R function `Rfun` that generates outputs `returnType` (a single numeric value `double(0)`).

Now you can call your R function from a model (or any `nimbleFunctions`):

```
model <- nimbleCode({
  # likelihood
  survived ~ dbinom(theta, released)
  # prior
  theta ~ dunif(0, 1)
  lifespan <- Rmyfunction(theta)
})
```

The rest of the workflow remains the same:

```
my.data <- list(survived = 19, released = 57)
parameters.to.save <- c("theta", "lifespan")
initial.values <- function() list(theta = runif(1,0,1))
n.iter <- 5000
n.burnin <- 1000
n.chains <- 3
mcmc.output <- nimbleMCMC(code = model,
                          data = my.data,
                          inits = initial.values,
                          monitors = parameters.to.save,
                          niter = n.iter,
                          nburnin = n.burnin,
                          nchains = n.chains)
```

```
## defining model...

## 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...
## checking model calculations...
## model building finished.
## compiling... this may take a minute. Use 'showCompilerOutput = TRUE' to see C++ compilation details.
## compilation finished.
## running chain 1...

## |-------------|-------------|-------------|-------------|
## |-------------------------------------------------------|

## running chain 2...

## |-------------|-------------|-------------|-------------|
## |-------------------------------------------------------|

## running chain 3...

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

```
MCMCsummary(object = mcmc.output, round = 2)
```

```
##          mean   sd 2.5%  50% 97.5% Rhat n.eff
## lifespan 0.94 0.16 0.66 0.92  1.29    1  2865
## theta    0.34 0.06 0.22 0.34  0.46    1  2854
```

Evaluating an R function from within NIMBLE slows MCMC sampling down, but if you can live with it, the cost is easily offset by the convenience of being able to use existing R functions.

Another advantage of using `nimbleRcall()` (or `nimbleExternalCall()`) is that you can keep large objects out of your model, so that NIMBLE does not have to handle them in MCMC sampling. These objects should be constants and not change when you run NIMBLE. Letting R manipulating these objects will save you time, usually more than the time you lose by calling R from within NIMBLE.

User-defined distributions

With `nimbleFunctions` you can provide user-defined distributions to NIMBLE. You need to write functions for density (`d`) and simulation (`r`) for your distribution. As an example, we write our own binomial distribution:

```
# density
dmybinom <- nimbleFunction(
  run = function(x = double(0),
                 size = double(0),
                 prob = double(0),
                 log = integer(0, default = 1)) {
    returnType(double(0))
    # compute binomial coefficient
    lchoose <- lfactorial(size) - lfactorial(x) - lfactorial(size - x)
    # binomial density function
    logProb <- lchoose + x * log(prob) + (size - x) * log(1 - prob)
    if(log) return(logProb)
    else return(exp(logProb))
  })

# simulation using the coin flip method (p. 524 in Devroye 1986)
rmybinom <- nimbleFunction(
  run = function(n = integer(0, default = 1),
                 size = double(0),
                 prob = double(0)) {
    returnType(double(0))
    x <- 0
    y <- runif(n = size, min = 0, max = 1)
    for (j in 1:size){
      if (y[j] < prob){
        x <- x + 1
      }else{
        x <- x
      }
    }
    return(x)
  })
```

You need to define the `nimbleFunctions` in R's global environment for them to be accessed:

```
assign('dmybinom', dmybinom, .GlobalEnv)
assign('rmybinom', rmybinom, .GlobalEnv)
```

You can try out your function and simulate a random value from a binomial distribution with size 5 and probability 0.1:

```
rmybinom(n = 1, size = 5, prob = 0.1)
```

```
## [1] 0
```

```
rmybinom(n = 1, size = 5, prob = 0.8)
```

```
## [1] 5
```

All set. You can run your workflow:

```
model <- nimbleCode({
 # likelihood
 survived ~ dmybinom(prob = theta, size = released)
 # prior
 theta ~ dunif(0, 1)
})
```

```
my.data <- list(released = 57, survived = 19)
initial.values <- function() list(theta = runif(1,0,1))
n.iter <- 5000
n.burnin <- 1000
n.chains <- 3
mcmc.output <- nimbleMCMC(code = model,
 data = my.data,
 inits = initial.values,
 niter = n.iter,
 nburnin = n.burnin,
 nchains = n.chains)
```

```
## defining model...
```

```
## Registering the following user-provided distributions: dmybinom
## NIMBLE has registered dmybinom as a distribution based on its use in BUGS code. Note that if you mak
```

```
## 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...
## checking model calculations...
## model building finished.
## compiling... this may take a minute. Use 'showCompilerOutput = TRUE' to see C++ compilation details.
## compilation finished.
## running chain 1...
```

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

```
## running chain 2...
```

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

```
## running chain 3...
```

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

```
MCMCsummary(mcmc.output)
```

```
##            mean         sd      2.5%       50%     97.5% Rhat n.eff
## theta 0.3378715 0.06157776 0.2259558 0.3339566 0.4663065    1  2592
```

Having `nimbleFunctions` offers infinite possibilities to customize your models and algorithms. Besides what we covered already, you can write your own samplers. We will see an example in a minute, but first we need to tell you more about the NIMBLE workflow.

Nimble detailed workflow

So far, you have used `nimbleMCMC()` which runs the default MCMC workflow. This is perfecly fine for most applications. However, in some situations you need to customize the MCMC samplers to improve or fasten convergence. NIMBLE allows you to look under the hood by using a detailed workflow in several steps: `nimbleModel()`, `configureMCMC()`, `buildMCMC()`, `compileNimble()` and `runMCMC()`. **Note that `nimbleMCMC()` does all of this at once**.

We write the model code, read in data and pick initial values as before:

```
model <- nimbleCode({
  # likelihood
  survived ~ dbinom(theta, released)
  # prior
  theta ~ dunif(0, 1)
  # derived quantity
  lifespan <- -1/log(theta)
})
my.data <- list(survived = 19, released = 57)
initial.values <- list(theta = 0.5)
```

1. Create the model as an R object

First step is to create the model as an R object (uncompiled model) with `nimbleModel()`:

```
survival <- nimbleModel(code = model,
                        data = my.data,
                        inits = initial.values)
```

```
## defining model...
## 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...
## model building finished.
```

You can look at its nodes:

```
survival$getNodeNames()
```

```
## [1] "theta"    "lifespan" "survived"
```

You can look at the values stored at each node:

```
survival$theta
```

```
## [1] 0.5
```

```
survival$survived
```

```
## [1] 19
```

```
survival$lifespan
```

```
## [1] 1.442695
```

```
# this is -1/log(0.5)
```

We can also calculate the log-likelihood at the initial value for `theta`:

```
survival$calculate()
```

```
## [1] -5.421624
```

```
# this is dbinom(x = 19, size = 57, prob = 0.5, log = TRUE)
```

The ability in NIMBLE to access the nodes of your model and to evaluate the model likelihood can help you in identifying bugs in your code. For example, if we provide a negative initial value to `theta`, `survival$calculate()` returns `NA`.

```
survival <- nimbleModel(code = model,
                        data = my.data,
                        inits = list(theta = -0.5))
```

```
## defining model...
```

```
## 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.
```

```
survival$calculate()
```

```
## [1] NaN
```

Other example : if there are more survived than released :

```
my.data <- list(survived = 61, released = 57)
initial.values <- list(theta = 0.5)

survival <- nimbleModel(code = model,
                        data = my.data,
                        inits = initial.values)
survival$calculate()
```

```
## [1] -Inf
```

Then, to check the model is correctly initialized and without bug in the code, we can check that `model$calculate()` returns a number and not `NA` or `-Inf`.

```
## defining model...
```

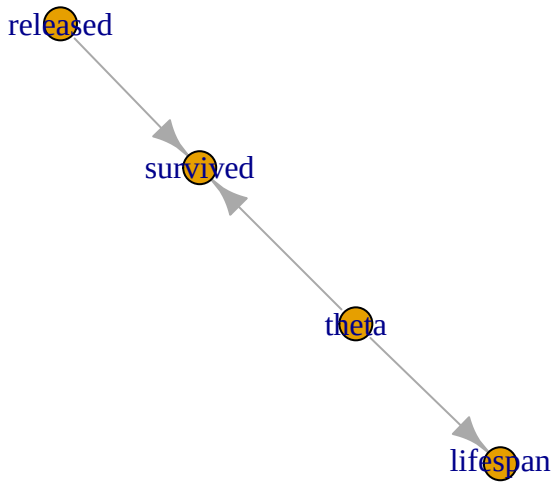
```
## building model...
```

```
## 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...
## model building finished.
```

You can obtain the graph of the model with:

```
survival$plotGraph()
```



2. Compile model

Second we compile the model with `compileNimble()`:

```
Csurvival <- compileNimble(survival)
```

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

```
## compilation finished.
```

With `compileNimble()`, the C++ code is generated, compiled and loaded back into R so that it can be used in R (compiled model):

```
Csurvival$theta
```

```
## [1] 0.5
```

Now you have two versions of the model, `survival` is in R and `Csurvival` in C++. Being able to separate the steps of model building and parameter estimation is a strength of NIMBLE. This gives you a lot of flexibility at both steps. For example, imagine you would like to fit your model with maximum likelihood, then you can do it by wrapping your model in an R function that gets the likelihood and maximise this function.

Using the C version of the model, you can write:

```
# function for negative log-likelihood to minimize
f <- function(par) {
    Csurvival[['theta']] <- par # assign par to theta
    ll <- Csurvival$calculate() # update log-likelihood with par value
    return(-ll) # return negative log-likelihood
```

```
}
# evaluate function at 0.5 and 0.9
f(0.5)
```

```
## [1] 5.421624
```

```
f(0.9)
```

```
## [1] 55.41232
```

```
# minimize function
out <- optimize(f, interval = c(0,1))
round(out$minimum, 2)
```

```
## [1] 0.33
```

By maximising the likelihood (or minimising the negative log-likelihood), you obtain the maximum likelihood estimate of animal survival, which is exactly 19 surviving animals over 57 released animals or 0.33.

3. MCMC configuration

Third we create a MCMC configuration for our model with `configureMCMC()`:

```
survivalConf <- configureMCMC(survival)
```

```
## ===== Monitors =====
## thin = 1: theta
## ===== Samplers =====
## RW sampler (1)
##   - theta
```

This steps tells you the nodes that are monitored by default, and the MCMC samplers than have been assigned to them. Here `theta` is monitored, and samples from its posterior distribution are simulated with a random walk sampler.

To monitor `lifespan` in addition to `theta`, you write:

```
survivalConf$addMonitors(c("lifespan"))
```

```
## thin = 1: theta, lifespan
```

```
survivalConf
```

```
## ===== Monitors =====
## thin = 1: theta, lifespan
## ===== Samplers =====
## RW sampler (1)
##   - theta
```

4. Create MCMC function

Fourth, we create a MCMC function with `buildMCMC()` and compile it with `compileNimble()`:

```
survivalMCMC <- buildMCMC(survivalConf)
CsurvivalMCMC <- compileNimble(survivalMCMC, project = survival)
```

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

```
## compilation finished.
```

Note that models and `nimbleFunctions` need to be compiled before they can be used to specify a project.

5. Run NIMBLE

Then, we run NIMBLE with `runMCMC()`:

```
n.iter <- 5000
n.burnin <- 1000
samples <- runMCMC(mcmc = CsurvivalMCMC,
                   niter = n.iter,
                   nburnin = n.burnin)
```

```
## running chain 1...
```

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

We run a single chain but `runMCMC()` allows you to use multiple chains as with `nimbleMCMC()`.

You can look into `samples` which contains values simulated from the posterior distribution of the parameters we monitor:

```
head(samples)
```

```
##       lifespan     theta
## [1,] 0.8271129 0.2984882
## [2,] 0.8271129 0.2984882
## [3,] 0.8271129 0.2984882
## [4,] 0.8271129 0.2984882
## [5,] 0.9143429 0.3349810
## [6,] 0.8535610 0.3098824
```

From here, you can obtain numerical summaries with `samplesSummary()`:

```
samplesSummary(samples)
```

```
##               Mean    Median    St.Dev. 95%CI_low 95%CI_upp
## lifespan 0.9374536 0.9263316 0.16156287 0.6716176 1.3033742
## theta    0.3392631 0.3397562 0.06117879 0.2256111 0.4642931
```

All steps

All steps above:

```
# model building
model <- nimbleCode({
  # likelihood
  survived ~ dbinom(theta, released)
  # prior
  theta ~ dunif(0, 1)
  # derived quantity
  lifespan <- -1/log(theta)
})
# read in data
my.data <- list(released = 57, survived = 19)
# pick initial values
initial.values <- function() list(theta = runif(1,0,1))
# create model as an R object (uncompiled model)
survival <- nimbleModel(code = model,
                        data = my.data,
                        inits = initial.values())
# compile model
```

```
Csurvival <- compileNimble(survival)
# create a MCMC configuration
survivalConf <- configureMCMC(survival)
# add lifespan to list of parameters to monitor
survivalConf$addMonitors(c("lifespan"))
# create a MCMC function and compile it
survivalMCMC <- buildMCMC(survivalConf)
CsurvivalMCMC <- compileNimble(survivalMCMC, project = survival)
# specify MCMC details
n.iter <- 5000
n.burnin <- 1000
n.chains <- 2
# run NIMBLE
samples <- runMCMC(mcmc = CsurvivalMCMC,
                   niter = n.iter,
                   nburnin = n.burnin,
                   nchain = n.chains)
# calculate numerical summaries
MCMCsummary(object = samples, round = 2)
# visualize parameter posterior distribution
MCMCplot(object = samples,
         params = 'theta')
# check convergence
MCMCtrace(object = samples,
          pdf = FALSE, # no export to PDF
          ind = TRUE, # separate density lines per chain
          params = "theta")
```

At first glance, using several steps instead of doing all these at once with `nimbleMCMC()` seems odds. Why is it useful? Mastering the whole sequence of steps allows you to play around with samplers, by changing the samplers NIMBLE picks by default, or even writing your own samplers.

MCMC samplers

Default samplers

What is the default sampler used by NIMBLE in our example? You can answer this question by inspecting the MCMC configuration obtained with `configureMCMC()`:

```
survivalConf$printSamplers()
```

```
## [1] RW sampler: theta
```

NIMBLE implements many samplers, and a list is available with `?samplers`. For example, high correlation in (regression) parameters can make independent samplers inefficient. In that situation, block sampling might help which consists in proposing candidate values from a multivariate distribution that acknowledges correlation between parameters.

Change default samplers

Now that we have control on the MCMC configuration, let's mess it up. We start by removing the default sampler:

```
survivalConf$removeSamplers(c('theta'))
survivalConf$printSamplers()
```

And we change it for a slice sampler:

```
survivalConf$addSampler(target = c('theta'),
                        type = 'slice')
survivalConf$printSamplers()
```

```
## [1] slice sampler: theta
```

Now you can resume the workflow:

```
# create a new MCMC function and compile it:
survivalMCMC2 <- buildMCMC(survivalConf)
CsurvivalMCMC2 <- compileNimble(survivalMCMC2,
                                project = survival,
                                resetFunctions = TRUE) # to compile new functions
```

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

```
## compilation finished.
```

```
                                                        # into existing project,
                                                        # need to reset nimbleFunctions
# run NIMBLE:
samples2 <- runMCMC(mcmc = CsurvivalMCMC2,
                    niter = n.iter,
                    nburnin = n.burnin)
```

```
## running chain 1...
```

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

```
# obtain numerical summaries:
samplesSummary(samples2)
```

```
##               Mean    Median    St.Dev. 95%CI_low 95%CI_upp
## lifespan 0.9354513 0.9142073 0.16459001 0.6652703 1.3060229
## theta    0.3383115 0.3349266 0.06206799 0.2224287 0.4650161
```

User-defined samplers

Allowing you to code your own sampler is another topic on which NIMBLE thrives. As an example, we focus on the Metropolis algorithm which we coded in R. We make it a `nimbleFunction` so that we can use it within our model:

```
my_metropolis <- nimbleFunction(
  name = 'my_metropolis', # fancy name for our MCMC sampler
  contains = sampler_BASE,
  setup = function(model, mvSaved, target, control) {
    # i) get dependencies for 'target' in 'model'
    calcNodes <- model$getDependencies(target)
    # ii) get sd of proposal distribution
    scale <- control$scale
  },
  run = function() {
    # (1) log-lik at current value
    initialLP <- model$getLogProb(calcNodes)
    # (2) current parameter value
    current <- model[[target]]
    # (3) logit transform
```

```
    lcurrent <- log(current / (1 - current))
    # (4) propose candidate value
    lproposal <- lcurrent  + rnorm(1, mean = 0, scale)
    # (5) back-transform
    proposal <- plogis(lproposal)
    # (6) plug candidate value in model
    model[[target]] <<- proposal
    # (7) log-lik at candidate value
    proposalLP <- model$calculate(calcNodes)
    # (8) compute lik ratio on log scale
    lMHR <- proposalLP - initialLP
    # (9) spin continuous spinner and compare to ratio
    if(runif(1,0,1) < exp(lMHR)) {
      # (10) if candidate value is accepted, update current value
      copy(from = model, to = mvSaved, nodes = calcNodes, logProb = TRUE, row = 1)
    } else {
      ## (11) if candidate value is accepted, keep current value
      copy(from = mvSaved, to = model, nodes = calcNodes, logProb = TRUE, row = 1)
    }
  },
  methods = list(
    reset = function() {}
  )
)
```

Compared to `nimbleFunctions` we wrote earlier, `my_metropolis()` contains a `setup` function which - i) gets the dependencies of the parameter to update in the `run` function with Metropolis, the target node, that would be `theta` in our example and - ii) extracts control parameters, that would be `scale` the standard deviation of the proposal distribution in our example. Then the `run` function implements the steps of the Metropolis algorithm: (1) get the log-likelihood function evaluated at the current value, (2) get the current value, (3) apply the logit transform to it, (4) propose a candidate value by perturbing the current value with some normal noise controled by the standard deviation `scale`, (5) back-transform the candidate value and (6) plug it in the model, (7) calculate the log-likelihood function at the candidate value, (8) compute the Metropolis ratio on the log scale, (9) compare output of a spinner and the Metropolis ratio to decide whether to (10) accept the candidate value and copy from the model to `mvSaved` or (11) reject it and keep the current value by copying from `mvSaved` to the model. Because this `nimbleFunction` is to be used as a MCMC sampler, several constraints need to be respected like having a `contains = sampler_BASE` statement or using the four arguments `model`, `mvSaved`, `target` and `control` in the `setup` function. Of course, NIMBLE implements a more advanced and efficient version of the Metropolis algorithm, you can look into it at https://github.com/cran/nimble/blob/master/R/MCMC_samplers.R#L184.

Now that we have our user-defined MCMC algorithm, we can change the default sampler for our new sampler. We start from scratch:

```
model <- nimbleCode({
  # likelihood
  survived ~ dbinom(theta, released)
  # prior
  theta ~ dunif(0, 1)
})
my.data <- list(survived = 19, released = 57)
initial.values <- function() list(theta = runif(1,0,1))
survival <- nimbleModel(code = model,
                        data = my.data,
                        inits = initial.values())
```

```
## defining model...
## 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...
## model building finished.
```

```
Csurvival <- compileNimble(survival)
```

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

```
survivalConf <- configureMCMC(survival)
```

```
## ===== Monitors =====
## thin = 1: theta
## ===== Samplers =====
## RW sampler (1)
##   - theta
```

We print the samplers used by default, remove the default sampler for `theta`, replace it with our `my_metropolis()` sampler with the standard deviation of the proposal distribution set to 0.1, and print again to make sure NIMBLE now uses our new sampler:

```
survivalConf$printSamplers()
```

```
## [1] RW sampler: theta
```

```
survivalConf$removeSamplers(c('theta'))
survivalConf$addSampler(target = 'theta',
                        type = 'my_metropolis',
                        control = list(scale = 0.1)) # standard deviation
                                                     # of proposal distribution
survivalConf$printSamplers()
```

```
## [1] my_metropolis sampler: theta,  scale: 0.1
```

The rest of the workflow is unchanged:

```
survivalMCMC <- buildMCMC(survivalConf)
CsurvivalMCMC <- compileNimble(survivalMCMC,
                               project = survival)
```

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

```
samples <- runMCMC(mcmc = CsurvivalMCMC,
                   niter = 5000,
                   nburnin = 1000)
```

```
## running chain 1...
## |-------------|-------------|-------------|-------------|
## |-------------------------------------------------------|
```

```
samplesSummary(samples)
```

```
##            Mean    Median    St.Dev. 95%CI_low 95%CI_upp
## theta 0.3344994 0.3334362 0.06121351 0.2192959 0.4669104
```

Tips and tricks

Precision vs standard deviation

In other sotware like JAGS, the normal distribution is parameterized with mean `mu` and a parameter called precision, often denoted `tau`, the inverse of the variance you are used to. Say we use a normal prior on some parameter `epsilon` with `epsilon ~ dnorm(mu, tau)`. We'd like this prior to be vague, therefore `tau` should be small, say 0.01 so that the variance of the normal distribution is large, $1/0.01 = 100$ here. This subtlety is the source of problems (and frustration) when you forget that the second parameter is precision and use `epsilon ~ dnorm(mu, 100)`, because then the variance is actually $1/100 = 0.01$ and the prior is very informative, and peaked on `mu`. In NIMBLE you can use this parameterisation as well as the more natural parameterisation `epsilon ~ dnorm(mu, sd = 100)` which avoids confusion.

Indexing

NIMBLE does not guess the dimensions of objects. In other software like JAGS you can write `sum.x <- sum(x[])` to calculate the sum over all components of `x`. In NIMBLE you need to write `sum.x <- sum(x[1:n])` to sum the components of `x` from 1 up to n. Specifying dimensions can be annoying, but it useful as it forces us to think of what we are doing and to keep the code self-explaining.

Faster compilation

You might have noticed that compilation in NIMBLE takes time. When you have large models (with lots of nodes), compilation can take forever. You can set `calculate = FALSE` in `nimbleModel()` to disable the calculation of all deterministic nodes and log-likelihood. You can also use `useConjugacy = FALSE` in `configureMCMC()` to disable the search for conjugate samplers. With the animal survival example, you would do:

```
model <- nimbleCode({
  # likelihood
  survived ~ dbinom(theta, released)
  # prior
  theta ~ dunif(0, 1)
})
my.data <- list(survived = 19, released = 57)
initial.values <- function() list(theta = runif(1,0,1))
survival <- nimbleModel(code = model,
                        data = my.data,
                        inits = initial.values(),
                        calculate = FALSE) # first tip
```

```
## defining model...
```

```
## building model...
```

```
## setting data and initial values...
```

```
## checking model sizes and dimensions...
## model building finished.
```

```
Csurvival <- compileNimble(survival)
```

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

```
survivalConf <- configureMCMC(survival)
```

```
## ===== Monitors =====
## thin = 1: theta
```

```
## ===== Samplers =====
## RW sampler (1)
##   - theta
```

```
survivalMCMC <- buildMCMC(survivalConf, useConjugacy = FALSE) # second tip
CsurvivalMCMC <- compileNimble(survivalMCMC,
                               project = survival)
```

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

```
samples <- runMCMC(mcmc = CsurvivalMCMC,
                   niter = 5000,
                   nburnin = 1000)
```

```
## running chain 1...
```

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

```
samplesSummary(samples)
```

```
##            Mean    Median    St.Dev. 95%CI_low 95%CI_upp
## theta 0.3412494 0.3397304 0.06139642  0.230306 0.4611938
```

Updating MCMC chains

Sometimes it is useful to run your MCMC chains a little bit longer to improve convergence. Re-starting from the run in previous section, you can use:

```
niter_ad <- 6000
CsurvivalMCMC$run(niter_ad, reset = FALSE)
```

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

```
## NULL
```

Then you can extract the matrix of previous MCMC samples augmented with new ones and obtain numerical summaries:

```
more_samples <- as.matrix(CsurvivalMCMC$mvSamples)
dim(more_samples)
```

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

You can check that `more_samples` contains 10000 samples, 4000 from the call to `runMCMC()` plus 6000 additional samples.

Reproducibility

If you want your results to be reproducible, you can control the state of R the random number generator with the `setSeed` argument in functions `nimbleMCMC()` and `runMCMC()`. Going back to the animal survival example, you can check that two calls to `nimbleMCMC()` give the same results when `setSeed` is set to the same value:

```
## defining model...
```

```
## 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...
## checking model calculations...
## model building finished.
## compiling... this may take a minute. Use 'showCompilerOutput = TRUE' to see C++ compilation details.
## compilation finished.
## running chain 1...
## |-------------|-------------|-------------|-------------|
## |-------------------------------------------------------|
## running chain 2...
## |-------------|-------------|-------------|-------------|
## |-------------------------------------------------------|
## running chain 3...
## |-------------|-------------|-------------|-------------|
## |-------------------------------------------------------|
## defining model...
## 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...
## checking model calculations...
## model building finished.
## compiling... this may take a minute. Use 'showCompilerOutput = TRUE' to see C++ compilation details.
## compilation finished.
## running chain 1...
## |-------------|-------------|-------------|-------------|
## |-------------------------------------------------------|
## running chain 2...
## |-------------|-------------|-------------|-------------|
## |-------------------------------------------------------|
## running chain 3...
## |-------------|-------------|-------------|-------------|
## |-------------------------------------------------------|
##            Mean    Median    St.Dev. 95%CI_low 95%CI_upp
## theta 0.3386766 0.3360208 0.05968472 0.2282263 0.4608244
##            Mean    Median    St.Dev. 95%CI_low 95%CI_upp
## theta 0.3386766 0.3360208 0.05968472 0.2282263 0.4608244
```

Parallelization

To speed up your analyses, you can run MCMC chains in parallel. This is what the package `jagsUI`[6] accomplishes for JAGS users. Here, we use the `parallel` package for parallel computation:

```
library(parallel)
```

First you create a cluster using the total amount of cores you have but one to make sure your computer can go on working:

[6] https://github.com/kenkellner/jagsUI

```
nbcores <- detectCores() - 1
my_cluster <- makeCluster(nbcores)
```

Then you wrap your workflow in a function to be run in parallel:

```
workflow <- function(seed, data) {

  library(nimble)

  model <- nimbleCode({
    # likelihood
    survived ~ dbinom(theta, released)
    # prior
    theta ~ dunif(0, 1)
  })

  set.seed(123) # for reproducibility
  initial.values <- function() list(theta = runif(1,0,1))

  survival <- nimbleModel(code = model,
                          data = data,
                          inits = initial.values())
  Csurvival <- compileNimble(survival)
  survivalMCMC <- buildMCMC(Csurvival)
  CsurvivalMCMC <- compileNimble(survivalMCMC)

  samples <- runMCMC(mcmc = CsurvivalMCMC,
                     niter = 5000,
                     nburnin = 1000,
                     setSeed = seed)

  return(samples)
}
```

Now we run the code using `parLapply()`, which uses cluster nodes to execute our workflow:

```
output <- parLapply(cl = my_cluster,
                    X = c(2022, 666),
                    fun = workflow,
                    data = list(survived = 19, released = 57))
```

In the call to `parLapply`, we specify `X = c(2022, 666)` to ensure reproducibility. We use two values 2022 and 666 to set the seed in `workflow()`, which means we run two instances of our workflow, or two MCMC chains. Note that we also have a line `set.seed(123)` in the `workflow()` function to ensure reproducibility while drawing randomly initial values.

It's good practice to close the cluster with `stopCluster()` so that processes do not continue to run in the background and slow down other processes:

```
stopCluster(my_cluster)
```

By inspecting the results, you can see that the object `output` is a list with two components, one for each MCMC chain:

```
str(output)
```

```
## List of 2
```

```
##  $ : num [1:4000, 1] 0.393 0.369 0.346 0.346 0.346 ...
##   ..- attr(*, "dimnames")=List of 2
##   .. ..$ : NULL
##   .. ..$ : chr "theta"
##  $ : num [1:4000, 1] 0.435 0.435 0.435 0.435 0.243 ...
##   ..- attr(*, "dimnames")=List of 2
##   .. ..$ : NULL
##   .. ..$ : chr "theta"
```

Eventually, you can obtain numerical summaries:

```
MCMCsummary(output)
```

```
##            mean         sd      2.5%       50%     97.5% Rhat n.eff
## theta 0.3361363 0.06147798 0.2215332 0.3334801 0.4594087    1  1779
```

NIMBLE tutorial: https://r-nimble.org/nimbleExamples/parallelizing_NIMBLE.html.

Incomplete initialization

When you run `nimbleMCMC()` or `nimbleModel()`, you may get warnings thrown at you by NIMBLE like *'This model is not fully initialized'* or the value is NA or NaN even after trying to calculate **(see here)**. This is not necessarily an error, but it reflects missing values in model variables (incomplete initialization). In this situation, NIMBLE will initialize nodes with NAs by drawing from priors, and it will work or not. When possible, try to initialize all nodes (full initialization). The process can be a bit of a headache, but it helps understanding the model structure better. Going back to our animal survival example, let's purposedly forget to provide an initial value for `theta`:

```
model <- nimbleCode({
  # likelihood
  survived ~ dbinom(theta, released)
  # prior
  theta ~ dunif(0, 1)
})
#initial.values <- list(theta = runif(1,0,1))
survival <- nimbleModel(code = model,
                        data = list(survived = 19, released = 57))
```

```
## defining model...
```

```
## 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.
```

To see which variables are not initialized, we use `initializeInfo()`:

```
# survival$calculate() # gives NA
survival$initializeInfo()
```

```
## Missing values (NAs) or non-finite values were found in model variables: theta. This is not an error
```

Now that we know `theta` was not initialized, we can fix the issue and resume our workflow:

```
survival$theta <- 0.5 # assign initial value to theta
survival$calculate() # now ok
```

```
## [1] -5.421624
```

```
Csurvival <- compileNimble(survival)
```

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

```
survivalMCMC <- buildMCMC(Csurvival)
```

```
## ===== Monitors =====
## thin = 1: theta
## ===== Samplers =====
## RW sampler (1)
##   - theta
```

```
CsurvivalMCMC <- compileNimble(survivalMCMC)
```

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

```
samples <- runMCMC(mcmc = CsurvivalMCMC,
                   niter = 5000,
                   nburnin = 1000)
```

```
## running chain 1...
```

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

```
samplesSummary(samples)
```

```
##            Mean  Median    St.Dev. 95%CI_low 95%CI_upp
## theta 0.3358678 0.33346 0.06087566 0.2190501 0.4602376
```

Vectorization

Vectorization is the process of replacing a loop by a vector so that instead of processing a single value at a time, you process a set of values at once. As an example, instead of writing:

```
for(i in 1:n){
  x[i] <- mu + epsilon[i]
}
```

you would write:

```
x[1:n] <- mu + epsilon[1:n]
```

Vectorization can make your code more efficient by manipulating one vector node `x[1:n]` instead of `n` nodes `x[1]`, ..., `x[n]`.

Take-home messages

- NIMBLE is an R package that implements for you MCMC algorithms to generate samples from the posterior distribution of model parameters. You only have to specify a likelihood and priors using the BUGS language to apply the Bayes theorem.
- NIMBLE is more than just another MCMC engine. It provides a programming environment so that you have full control when building models and estimating parameters.
- At the core of NIMBLE are `nimbleFunctions` which you can write and compile for faster computation. With `nimbleFunctions` you can mimic basic R syntax, work with vectors and matrices, use logical operators and flow control, and specify many distributions.

- There are two workflows to run NIMBLE. In most situations, `nimbleMCMC()` will serve you well. When you need more control, you can adopt a detailed workflow with `nimbleModel()`, `configureMCMC()`, `buildMCMC()`, `compileNimble()` and `runMCMC()`.
- By having full control of the workflow, you can change default MCMC samplers and even write your own samplers.

Useful resources

- The NIMBLE folks make a lot of useful resources available through the official website https://r-nimble.org.
- The NIMBLE manual https://r-nimble.org/html_manual/cha-welcome-nimble.html reads like a book with clear explanations and relevant examples.
- You can learn a lot by going through examples at https://r-nimble.org/examples and training material from NIMBLE workshops at https://github.com/nimble-training.
- You can keep the NIMBLE cheatsheet https://r-nimble.org/cheatsheets/NimbleCheatSheet.pdf near you to remind yourself of the workflow, how to write and use models, or which functions and distributions are available.
- If you have questions, feel free to get in touch with the community of NIMBLE users by emailing the discussion group https://groups.google.com/forum/#!forum/nimble-users. This is a great place to learn, and folks who take the time to answer questions are kind and provide constructive answers. When possible, make sure to provide a reproducible example illustrating your problem.

Citation

- Last, you can cite the following reference when using NIMBLE in a publication:

  de Valpine, P., D. Turek, C. J. Paciorek, C. Anderson-Bergman, D. Temple Lang, and R. Bodik (2017). Programming With Models: Writing Statistical Algorithms for General Model Structures With NIMBLE. *Journal of Computational and Graphical Statistics* **26** (2): 403–13.