NIMBLE User Manual

NIMBLE Development Team

Version 0.3-1

Contents

Chapter 1

Welcome to NIMBLE

NIMBLE is a system for building and sharing analysis methods for statistical models, especially for hierarchical models and computationally-intensive methods. This is an early version, 0.3-1. You can do quite a bit with it, but you can also expect it to be rough and incomplete. If you want to analyze data, we hope you will find something already useful. If you want to build algorithms, we hope you will program in NIMBLE and make an R package providing your method. We also hope you will join the mailing lists (R-nimble.org) and help improve NIMBLE by telling us what you want to do with it, what you like, and what could be better. We have a lot of ideas for how to improve it, but we want your help and ideas too.

1.1 Why something new?

There is a lot of statistical software out there. Why did we build something new? More and more, statistical models are being customized to the details of each project. That means it is often difficult to find a package whose set of available models and methods includes what you need. And more and more, statistical models are hierarchical, meaning they have some unobserved random variables between the parameters and the data. These may be random effects, shared frailties, latent states, or other such things. Or a model may be hierarchical simply due to putting Bayesian priors on parameters. Except for simple cases, hierarchical statistical models are often analyzed with computationally-intensive algorithms, the best known of which is Markov chain Monte Carlo (MCMC).

Several existing software systems have become widely used by providing a flexible way to say what the model is and then automatically providing an algorithm such as MCMC. When these work, and when MCMC is what you want, that's great. Unfortunately, there are a lot of hard models out there for which default MCMCs don't work very well. And there are also a lot of useful new and old algorithms that are not MCMC. That's why we wanted to create a system that combines a flexible system for model specification – the BUGS language – with the ability to program with those models. That's the goal of NIMBLE.

1.2 What does NIMBLE do?

NIMBLE stands for Numerical Inference of statistical Models for Bayesian and Likelihood Estimation. Although NIMBLE was motivated by algorithms for hierarchical statistical models, you could use it for simpler models too.

You can think of NIMBLE as comprising three pieces:

1. A system for writing statistical models flexibly, which is an extension of the BUGS language[1].
2. A library of algorithms such as MCMC.
3. A language, called NIMBLE, embedded within and similar in style to R, for writing algorithms that operate on BUGS models.

Both BUGS models and NIMBLE algorithms are automatically processed into C++ code, compiled, and loaded back into R with seamless interfaces.

Since NIMBLE can compile R-like functions into C++ that use the Eigen library for fast linear algebra, it can be useful for making fast numerical functions with or without BUGS models involved[2]

One of the beauties of R is that many of the high-level analysis functions are themselves written in R, so it is easy to see their code and modify them. The same is true for NIMBLE: the algorithms are themselves written in the NIMBLE language.

1.3 How to use this manual

We emphasize that you can use NIMBLE for data analysis with the algorithms provided by NIMBLE without ever using the NIMBLE language to write algorithms. So as you get started, feel free to focus on Chapters 2-8. The algorithm library in v0.3-1 is just a start, so we hope you'll let us know what you want to see and consider writing it in NIMBLE. More about NIMBLE programming comes in 9.

[1] But see Section 5.1.2 for information about limitations and extensions to how NIMBLE handles BUGS right now.

[2] The packages Rcpp and RcppEigen provide different ways of connecting C++, the Eigen library and R. In those packages you program directly in C++, while in NIMBLE you program in an R-like fashion and the NIMBLE compiler turns it into C++. Programming directly in C++ allows full access to C++, while programming in NIMBLE allows simpler code.

Chapter 2

Lightning introduction

2.1 A brief example

Here we'll give a simple example of building a model and running some algorithms on the model, as well as creating our own user-specified algorithm. The goal is to give you a sense for what one can do in the system. Later sections will provide more detail.

We'll use the *pump* model example from BUGS[1]. As you'll see later, we can read the model into NIMBLE from the files provided as the BUGS example but for now, we'll enter it directly in R.

In this "lightning introduction" we will:

1. Create the model for the pump example.
2. Compile the model.
3. Create a basic MCMC specification for the pump model.
4. Compile and run the MCMC
5. Customize the MCMC specification and compile and run that.
6. Create, compile and run a Monte Carlo Expectation Maximization (MCEM) algorithm, which illustrates some of the flexibility NIMBLE provides to combine R and NIMBLE.
7. Write a short `nimbleFunction` to generate simulations from designated nodes of any model.

2.2 Creating a model

First we define the model code, its constants, data, and initial values for MCMC.

[1] The data set describes failure times of some pumps.

```
pumpCode <- nimbleCode({
  for (i in 1:N){
      theta[i] ~ dgamma(alpha,beta);
      lambda[i] <- theta[i]*t[i];
      x[i] ~ dpois(lambda[i])
  }
  alpha ~ dexp(1.0);
  beta ~ dgamma(0.1,1.0);
})

pumpConsts <- list(N = 10,
                t = c(94.3, 15.7, 62.9, 126, 5.24,
                  31.4, 1.05, 1.05, 2.1, 10.5))

pumpData <- list(x = c(5, 1, 5, 14, 3, 19, 1, 1, 4, 22))

pumpInits <- list(alpha = 1, beta = 1,
              theta = rep(0.1, pumpConsts$N))
```

Now let's create the model and look at some of its nodes.

```
pump <- nimbleModel(code = pumpCode, name = 'pump', constants = pumpConsts,
                    data = pumpData, inits = pumpInits)

pump$getNodeNames()
```

```
##  [1] "alpha"                "beta"
##  [3] "lifted_d1_over_beta" "theta[1]"
##  [5] "theta[2]"             "theta[3]"
##  [7] "theta[4]"             "theta[5]"
##  [9] "theta[6]"             "theta[7]"
## [11] "theta[8]"             "theta[9]"
## [13] "theta[10]"            "lambda[1]"
## [15] "lambda[2]"            "lambda[3]"
## [17] "lambda[4]"            "lambda[5]"
## [19] "lambda[6]"            "lambda[7]"
## [21] "lambda[8]"            "lambda[9]"
## [23] "lambda[10]"           "x[1]"
## [25] "x[2]"                 "x[3]"
## [27] "x[4]"                 "x[5]"
## [29] "x[6]"                 "x[7]"
## [31] "x[8]"                 "x[9]"
## [33] "x[10]"
```

```
pump$x
```

```
##  [1]  5  1  5 14  3 19  1  1  4 22
```

```
pump$alpha
```

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

```
pump$theta
```

```
##  [1] 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1
```

Notice that in the list of nodes, NIMBLE has introduced a new node, `lifted_d1_over_beta`. We call this a "lifted" node. Like R, NIMBLE allows alternative parameterizations, such as the scale or rate parameterization of the gamma distribution. Choice of parameterization can generate a lifted node. It's helpful to know why they exist, but you shouldn't need to worry about them.

Thanks to the plotting capabilities of the `igraph` package that NIMBLE uses to represent the directed acyclic graph, we can plot the model (figure 2.1).

```
plot(pump$graph)
```

To simulate from the prior for `theta` (overwriting the initial values previously in the model) we first need to fully initialize the model, including any non-stochastic nodes such as lifted nodes. We do so using NIMBLE's `calculate` function and then simulate from the distribution for `theta`. First we show how to use the model's `getDependencies` method to query information about its graph.

```
pump$getDependencies(c('alpha', 'beta'))
```

```
##  [1] "alpha"               "beta"
##  [3] "lifted_d1_over_beta" "theta[1]"
##  [5] "theta[2]"            "theta[3]"
##  [7] "theta[4]"            "theta[5]"
##  [9] "theta[6]"            "theta[7]"
## [11] "theta[8]"            "theta[9]"
## [13] "theta[10]"
```

```
pump$getDependencies(c('alpha', 'beta'), determOnly = TRUE)
```

```
## [1] "lifted_d1_over_beta"
```

```
set.seed(0) ## This makes the simulations here reproducible
calculate(pump, pump$getDependencies(c('alpha', 'beta'), determOnly = TRUE))
```

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

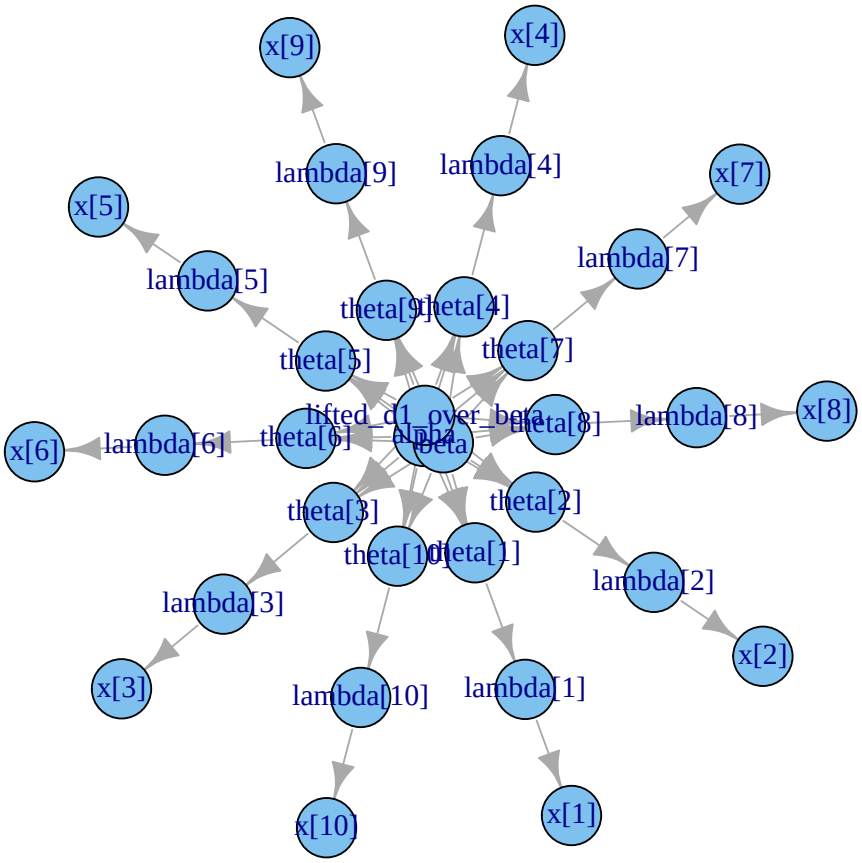


Figure 2.1: Directed Acyclic Graph plot of the pump model, thanks to the igraph package

```
simulate(pump, 'theta')
pump$theta   ## the new theta values

##  [1] 1.79181 0.29593 0.08369 0.83618 1.22254 1.15836 0.99002
##  [8] 0.30737 0.09462 0.15720

pump$lambda  ## lambda hasn't been calculated yet

##  [1] NA NA NA NA NA NA NA NA NA NA

calculate(pump, pump$getDependencies(c('theta')))

## [1] -286.7

pump$lambda  ## now it has

##  [1] 168.9674   4.6460   5.2641 105.3584   6.4061  36.3724
##  [7]   1.0395   0.3227   0.1987   1.6506
```

Notice that the first `getDependencies` call returned dependencies from `alpha` and `beta` down to the next stochastic nodes in the model. The second call requested only deterministic dependencies. We used this as the second argument to `calculate`. The call to `calculate(pump, 'theta')` expands `'theta'` to include all nodes in `theta`. After simulating into `'theta'`, we make sure to calculate its dependencies so they are kept up to date with the new `theta` values.

2.3 Compiling the model

Next we compile the model, which means generating C++ code, compiling that code, and loading it back into R with an object that can be used just like the uncompiled model. The values in the compiled model will be initialized from those of the original model in R, but the original and compiled models are distinct objects so any subsequent changes in one will not be reflected in the other.

```
Cpump <- compileNimble(pump)
Cpump$theta

##  [1] 1.79181 0.29593 0.08369 0.83618 1.22254 1.15836 0.99002
##  [8] 0.30737 0.09462 0.15720
```

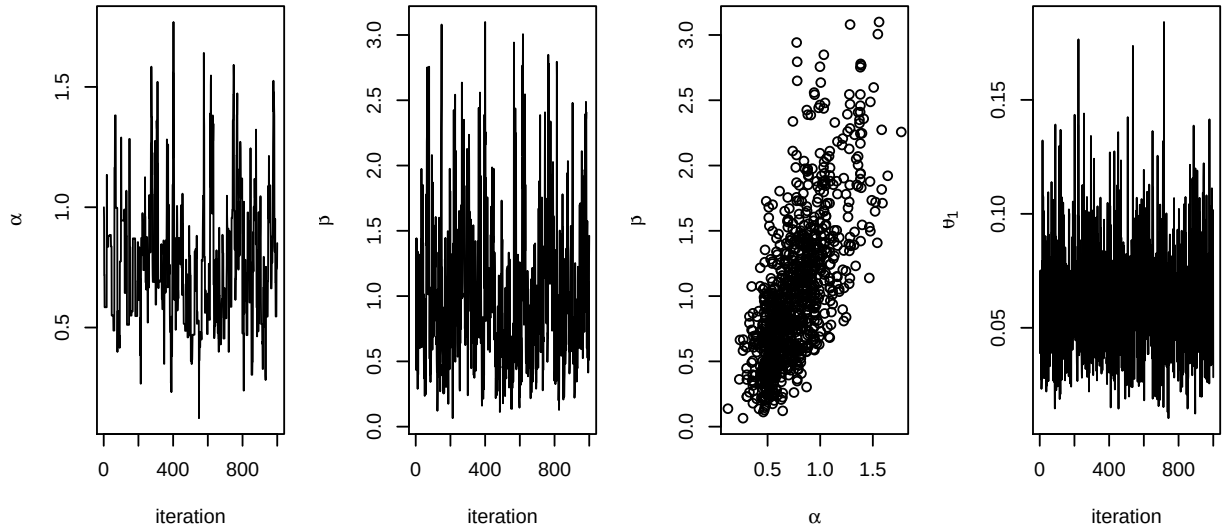
2.4 Creating, compiling and running a basic MCMC specification

At this point we have initial values for all of the nodes in the model and we have both the original and compiled versions of the model. As a first algorithm to try on our model, let's use NIMBLE's default MCMC. Note that all conjugacy is detected for all nodes except for `alpha`[2], on which the default sampler is a random walk Metropolis sampler.

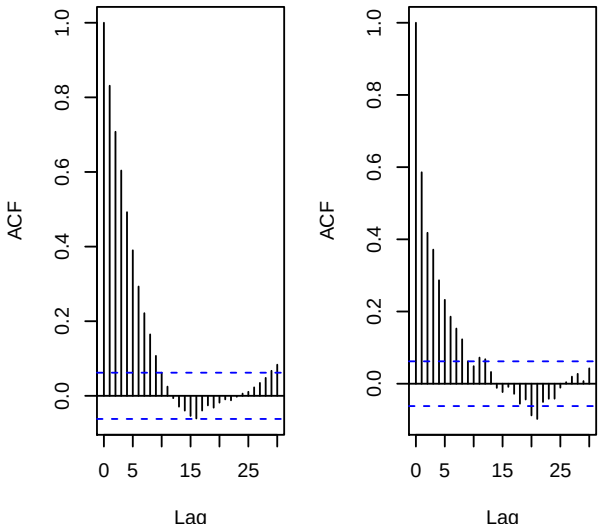
```
pumpSpec <- configureMCMC(pump, print = TRUE)

## [1] RW sampler;   targetNode: alpha,  adaptive: TRUE,  adaptInterval: 200,  scale: 1
## [2] conjugate_dgamma sampler;   targetNode: beta,  dependents_dgamma: theta[1], theta
## [3] conjugate_dgamma sampler;   targetNode: theta[1],  dependents_dpois: x[1]
## [4] conjugate_dgamma sampler;   targetNode: theta[2],  dependents_dpois: x[2]
## [5] conjugate_dgamma sampler;   targetNode: theta[3],  dependents_dpois: x[3]
## [6] conjugate_dgamma sampler;   targetNode: theta[4],  dependents_dpois: x[4]
## [7] conjugate_dgamma sampler;   targetNode: theta[5],  dependents_dpois: x[5]
## [8] conjugate_dgamma sampler;   targetNode: theta[6],  dependents_dpois: x[6]
## [9] conjugate_dgamma sampler;   targetNode: theta[7],  dependents_dpois: x[7]
## [10] conjugate_dgamma sampler;   targetNode: theta[8],  dependents_dpois: x[8]
## [11] conjugate_dgamma sampler;   targetNode: theta[9],  dependents_dpois: x[9]
## [12] conjugate_dgamma sampler;   targetNode: theta[10],  dependents_dpois: x[10]

pumpSpec$addMonitors(c('alpha', 'beta', 'theta'))

## thin = 1: alpha, beta, theta

pumpMCMC <- buildMCMC(pumpSpec)
CpumpMCMC <- compileNimble(pumpMCMC, project = pump)

niter <- 1000
set.seed(0)
CpumpMCMC$run(niter)

## NULL

samples <- as.matrix(CpumpMCMC$mvSamples)

par(mfrow = c(1, 4), mai = c(.5, .5, .1, .2))
plot(samples[ , 'alpha'], type = 'l', xlab = 'iteration',
     ylab = expression(alpha))
plot(samples[ , 'beta'], type = 'l', xlab = 'iteration',
     ylab = expression(beta))
```

[2] This is because we haven't yet set up NIMBLE to detect conjugate relationships involving an exponential distribution, but we'll add that one soon.

```
plot(samples[ , 'alpha'], samples[ , 'beta'], xlab = expression(alpha),
     ylab = expression(beta))
plot(samples[ , 'theta[1]'], type = 'l', xlab = 'iteration',
     ylab = expression(theta[1]))
```




```
acf(samples[, 'alpha']) ## plot autocorrelation of alpha sample
acf(samples[, 'beta'])  ## plot autocorrelation of beta  sample
```

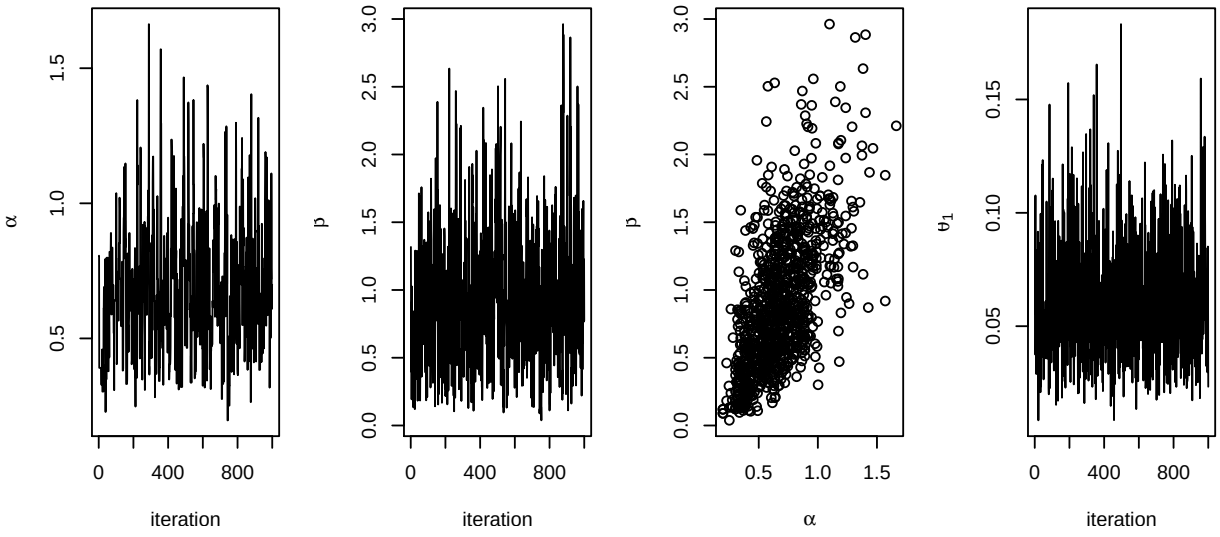


Notice the posterior correlation between `alpha` and `beta`. And a measure of the mixing for each is the autocorrelation for each, shown by the `acf` plots.

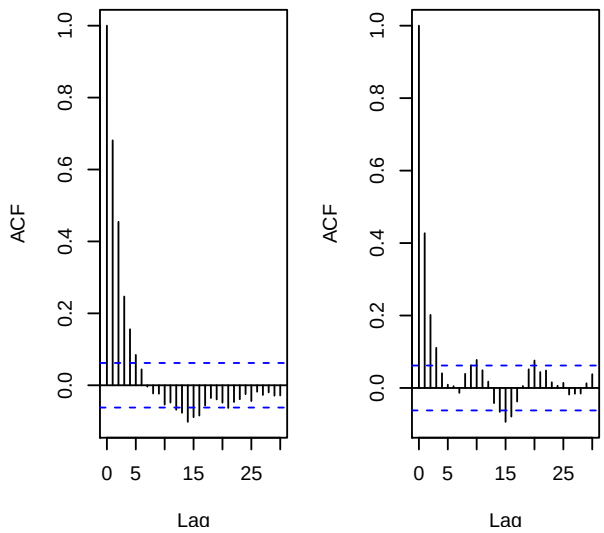
2.5 Customizing the MCMC

Let's add an adaptive block sampler on `alpha` and `beta` jointly and see if that improves the mixing.

```
pumpSpec$addSampler('RW_block', list(targetNodes = c('alpha', 'beta'),
                                     adaptInterval = 100))

## [13] RW_block sampler;   targetNodes: alpha, beta,  adaptive: TRUE,  adaptScaleOnly:

pumpMCMC2 <- buildMCMC(pumpSpec)

# need to reset the nimbleFunctions in order to add the new MCMC
CpumpNewMCMC <- compileNimble(pumpMCMC2, project  = pump, resetFunctions = TRUE)

set.seed(0);
CpumpNewMCMC$run(niter)

## NULL

samplesNew <- as.matrix(CpumpNewMCMC$mvSamples)

par(mfrow = c(1, 4), mai = c(.5, .5, .1, .2))
plot(samplesNew[ , 'alpha'], type = 'l', xlab = 'iteration',
     ylab = expression(alpha))
plot(samplesNew[ , 'beta'], type = 'l', xlab = 'iteration',
     ylab = expression(beta))
plot(samplesNew[ , 'alpha'], samplesNew[ , 'beta'], xlab = expression(alpha),
     ylab = expression(beta))
plot(samplesNew[ , 'theta[1]'], type = 'l', xlab = 'iteration',
     ylab = expression(theta[1]))
```




```
acf(samplesNew[, 'alpha']) ## plot autocorrelation of alpha sample
acf(samplesNew[, 'beta'])  ## plot autocorrelation of beta  sample
```



We can see that the block sampler has decreased the autocorrelation for both `alpha` and `beta`. Of course these are just short runs.

Once you learn the MCMC system, you can write your own samplers and include them. The entire system is written in nimbleFunctions.

2.6 Running MCEM

NIMBLE is a system for working with algorithms, not just an MCMC engine. So let's try maximizing the marginal likelihood for `alpha` and `beta` using Monte Carlo Expectation Maximization[3].

```
pump2 <- pump$newModel()

nodes <- pump2$getNodeNames(stochOnly = TRUE)

box = list( list(c('alpha','beta'), c(0, Inf)))

pumpMCEM <- buildMCEM(model = pump2, latentNodes = 'theta[1:10]',
                      boxConstraints = box)

pumpMLE <- pumpMCEM()
# Note: buildMCEM returns an R function that contains a
# nimbleFunction rather than a nimble function. That is why
# pumpMCEM() is used instead of pumpMCEM$run().

pumpMLE

##  alpha   beta
```

[3]Note that for this model, one could analytically integrate over `theta` and then numerically maximize the resulting marginal likelihood.

```
## 0.8231 1.2600
```

Both estimates are within 0.01 of the values reported by George et al. (1993)[4]

2.7 Creating your own functions

Now let's see an example of writing our own algorithm and using it on the model. We'll do something simple: simulating multiple values for a designated set of nodes and calculating every part of the model that depends on them.

Here is our `nimbleFunction`:

```
simNodesMany <- nimbleFunction(
    setup = function(model, nodes) {
        mv <- modelValues(model)
        deps <- model$getDependencies(nodes)
        allNodes <- model$getNodeNames()
    },
    run = function(n = integer()) {
        resize(mv, n)
        for(i in 1:n) {
            simulate(model, nodes)
            calculate(model, deps)
            copy(from = model, nodes = allNodes, to = mv, rowTo = i, logProb = TRUE)
        }
    })

simNodesTheta1to5 <- simNodesMany(pump, 'theta[1:5]')
```

Here are a few things to notice about the `nimbleFunction`

1. The setup code is written in R. It creates relevant information specific to our model for use in the run-time code.
2. The run-time is written in NIMBLE. It carries out the calculations using the information determined once for each set of `model` and `nodes` arguments by the setup code. The run-time code is what will be compiled.
3. A `modelValues` object is created to hold multiple sets of values for variables in the model provided.
4. The NIMBLE code requires type information about the argument `n`. In this case it is a scalar integer.
5. The for-loop looks just like R, but only sequential integer iteration is allowed.

[4] George, E.I., Makov, U.E. & Smith, A.F.M. 1993. Conjugate likelihood distributions. *Scand. J. Statist.* **20**:147-156. Their numbers were accidentally swapped in Table 2.

6. The functions `calculate` and `simulate`, which were introduced above in R, can be used in NIMBLE.

7. The special function `copy` is used here to record values from the model into the modelValues object.

8. One instance, or "specialization", `simNodesTheta1to5`, has been made by calling `simNodesMany` with the `pump` model and nodes `'theta[1:5]'` as arguments. These are used as inputs to the setup function. What is returned is an object of a uniquely generated reference class with a `run` method (member function) that will execute the `run` code.

In fact, `simNodesMany` is very similar to a standard `nimbleFunction` provided with nimble, `simNodesMV`.

Now let's execute this `nimbleFunction` in R, before compiling it.

```
set.seed(0)  ## make the calculation repeatable
pump$alpha <- pumpMLE[1]
pump$beta <- pumpMLE[2]
calculate(pump, pump$getDependencies(c('alpha','beta'), determOnly = TRUE))

## [1] 0

saveTheta <- pump$theta
simNodesTheta1to5$run(10)
simNodesTheta1to5$mv[['theta']][1:2]

## [[1]]
##  [1] 1.43718 1.53094 1.45029 0.03717 0.13310 1.15836 0.99002
##  [8] 0.30737 0.09462 0.15720
##
## [[2]]
##  [1] 0.34222 3.45823 0.82805 0.08796 0.34440 1.15836 0.99002
##  [8] 0.30737 0.09462 0.15720

simNodesTheta1to5$mv[['logProb_x']][1:2]

## [[1]]
##  [1] -115.767  -20.856  -73.444   -8.259   -3.570   -7.430
##  [7]   -1.001   -1.454   -9.841  -39.097
##
## [[2]]
##  [1] -19.688 -50.300 -37.108  -2.598  -1.825  -7.430  -1.001
##  [8]  -1.454  -9.841 -39.097
```

In this code we have initialized the values of `alpha`, `beta`, to their MLE, and recorded the `theta` values to use next. Then we have requested 10 simulations from `simNodesTheta1to5`.

Shown are the first two simulation results for `theta` and the log probabilities of `x`. Notice that `theta[6:10]` and the corresponding log probabilities for `x[6:10]` are unchanged because the nodes being simulated are only `theta[1:5]`. In R, this function runs slowly.

Finally, let's compile the function and run that version.

```
CsimNodesTheta1to5 <- compileNimble(simNodesTheta1to5,
                                    project  = pump, resetFunctions = TRUE)
Cpump$alpha <- pumpMLE[1]
Cpump$beta <- pumpMLE[2]
calculate(Cpump, Cpump$getDependencies(c('alpha','beta'), determOnly = TRUE))

## [1] 0

Cpump$theta <- saveTheta

set.seed(0)
CsimNodesTheta1to5$run(10)

## NULL

CsimNodesTheta1to5$mv[['theta']][1:2]

## [[1]]
##  [1] 1.43718 1.53094 1.45029 0.03717 0.13310 1.15836 0.99002
##  [8] 0.30737 0.09462 0.15720
##
## [[2]]
##  [1] 0.34222 3.45823 0.82805 0.08796 0.34440 1.15836 0.99002
##  [8] 0.30737 0.09462 0.15720

CsimNodesTheta1to5$mv[['logProb_x']][1:2]

## [[1]]
##  [1] -115.767  -20.856  -73.444   -8.259   -3.570   -2.593
##  [7]   -1.006   -1.180   -1.757   -2.532
##
## [[2]]
##  [1] -19.688 -50.300 -37.108  -2.598  -1.825  -2.593  -1.006
##  [8]  -1.180  -1.757  -2.532
```

Given the same initial values and the same random number generator seed, we got identical results, but it happened much faster.

Chapter 3

More Introduction

Now that we have shown a brief example, we will introduce more about the concepts and design of NIMBLE. Subsequent chapters will go into more detail about working with models and programming in NIMBLE.

One of the most important concepts behind NIMBLE is to allow a combination of high-level processing in R and low-level processing in compiled C++. For example, when we write a Metropolis-Hastings MCMC sampler in the NIMBLE language, the inspection of the model structure related to one node is done in R, and the actual sampler calculations are done in compiled C++. The theme of separating one-time high-level processing and repeated low-level processing will become clearer as we introduce more about NIMBLE's components.

3.1 NIMBLE adopts and extends the BUGS language for specifying models

We adopted the BUGS language, and we have extended it to make it more flexible. The BUGS language originally appeared in WinBUGS, then in OpenBUGS and JAGS. These systems all provide automatically-generated MCMC algorithms, but we have adopted only the language for describing models, not their systems for generating MCMCs. In fact, if you want to use those or other MCMCs in combination with NIMBLE's other algorithms, you can[1]. We adopted BUGS because it has been so successful, with over 30,000 registered users by the time they stopped counting, and with many papers and books that provide BUGS code as a way to document their statistical models. To learn the basics of BUGS, we refer you to the OpenBUGS or JAGS web sites. For the most part, if you have BUGS code, you can try NIMBLE.

NIMBLE takes BUGS code and does several things with it:

1. NIMBLE extracts all the declarations in the BUGS code to create a *model definition*. This includes a directed acyclic graph (DAG) representing the model and functions that can inspect the graph and model relationships. Usually you'll ignore the *model definition* and let NIMBLE's default options take you directly to the next step.

[1] and will be able to do so more thoroughly in the future

2. From the *model definition*, NIMBLE builds a working model in R. This can be used to manipulate variables and operate the model from R. Operating the model includes calculating, simulating, or querying the log probability value of model nodes. These basic capabilities, along with the tools to query model structure, allow one to write programs that use the model and adapt to its structure.

3. From the working model, NIMBLE generates customized C++ code representing the model, compiles the C++, loads it back into R, and provides an R object that interfaces to it. We often call the uncompiled model the "R-model" and the compiled model the "C-model." The C-model can be used identically to the R-model, so code written to use one will work with the other. We use the word "compile" to refer to the entire process of generating C++ code, compiling it and loading it into R.

You'll learn more about specifying and manipulating models in Chapter 5-6.

3.2 The NIMBLE language for writing algorithms

NIMBLE provides a language, embedded within and similar in style to R, for writing algorithms that can operate on BUGS models. The algorithms can use NIMBLE's utilities for inspecting the structure of a model, such as determining the dependencies between variables. And the algorithms can control the model, changing values of its variables and controlling execution of its probability calculations or corresponding simulations. Finally, the algorithms can use automatically generated data structures to manage sets of model values and probabilities. In fact, the calculations of the model are themselves constructed as functions in the NIMBLE language, as are the algorithms provided in NIMBLE's algorithm library. This will make it possible in the future to extend BUGS with new distributions and new functions written in NIMBLE.

Like the models themselves, functions in the NIMBLE language are turned into C++, which is compiled, loaded, and interfaced to R.

Programming in NIMBLE involves a fundamental distinction between:

1. the steps for an algorithm that need to happen only once, at the beginning, such as inspecting the model; and

2. the steps that need to happen each time a function is called, such as MCMC iterations.

Programming in NIMBLE allows, and indeed requires, these steps to be given separately. When one writes a `nimbleFunction`, each of these parts can be provided. The former, if needed, are given in a *setup function*, and they are executed directly in R, allowing any feature of R to be used. The latter are in one or more *run-time functions*, and they are turned into C++. Run-time code is written in the NIMBLE language, which you can think of as a carefully controlled, small subset of R along with some special functions for handling models and NIMBLE's data structures.

What NIMBLE does with a `nimbleFunction` is similar to what it does with a BUGS model:

1. NIMBLE creates a working R version of the `nimbleFunction`, which you can use with an R-model or a C-model.

2. NIMBLE generates C++ code for the run-time function(s), compiles it, and loads it back into R with an interface nearly identical to the R version of the `nimbleFunction`. As for models, we refer to the uncompiled and compiled versions as R-nimbleFunctions and C-nimbleFunctions, respectively. In v0.3-1, the behavior of `nimbleFunction`s is usually very similar, but not identical, between the two versions.

You'll learn more about writing algorithms in Chapter 9.

3.3 The NIMBLE algorithm library

In v0.3-1, the NIMBLE algorithm library is fairly limited. It includes:

1. MCMC with samplers including conjugate, slice, adaptive random walk, and adaptive block. NIMBLE's MCMC system illustrates the flexibility of combining R and C++. An R function inspects the model object and creates an MCMC specification object representing choices of which kind of sampler to use for each node. This MCMC specification can be modified in R, such as adding new samplers for particular nodes, before compiling the algorithm. Since each sampler is written in NIMBLE, you can use its source code or write new samplers to insert into the MCMC. And if you want to build an entire MCMC system differently, you could do that too.

2. A `nimbleFunction` that provides a likelihood function for arbitrary sets of nodes in any model. This can be useful for simple maximum likelihood estimation of non-hierarchical models using R's optimization functions. And it can be useful for other R packages that run algorithms on any likelihood function.

3. A `nimbleFunction` that provides ability to simulate, calculate, or retrieve the summed log probability (density) of many sets of values for arbitrary sets of nodes.

4. A basic Monte Carlo Expectation Maximization (MCEM) algorithm. MCEM has its issues as an algorithm, such as potentially slow convergence to maximum likelihood (i.e. empirical Bayes in this context) estimates, but we chose it as a good illustration of how NIMBLE can be used. Each MCMC step uses NIMBLE's MCMC; the objective function for maximization is another `nimbleFunction`; and the actual maximization is done through R's `optim` function[2].

You'll learn more about the NIMBLE algorithm library in Chapter 8.

[2]In the future we plan to provide direct access to R's optimizers from within `nimbleFunction`s

Chapter 4

Getting started

4.1 Requirements to run NIMBLE

You can run NIMBLE on any of the three common operating systems: Linux, Mac, or Windows.

The following are required to run NIMBLE.

1. R, of course.
2. The igraph R package.
3. A working C++ compiler that R can use on your system. There are standard open-source C++ compilers that the R community has already made easy to install. You don't need to know anything about C++ to use NIMBLE.

NIMBLE also uses a couple of C++ libraries that you don't need to install, as they will already be on your system or are provided by NIMBLE.

1. The Eigen C++ library for linear algebra. This comes with NIMBLE, or you can use your own copy.
2. The BLAS and LAPACK numerical libraries. These come with R.

Most fairly recent versions of these requirements should work.

4.2 Installation

Since NIMBLE is an R package, you can install it in the usual way, via `install.packages()` or related mechanisms. We have not yet put in on CRAN, so you'll have to find it at R-nimble.org.

For most installations, you can ignore low-level details. However, there are some options that some users may want to utilize.

4.2.1 Using your own copy of Eigen

NIMBLE uses the Eigen C++ template library for linear algebra (http://eigen.tuxfamily.org/index.php?title=Main_Page)). Version 3.2.1 of Eigen is included in the NIMBLE package and that version will be used unless the package's configuration script finds another version on the machine. This works well, and the following is only relevant if you want to use a different (e.g., newer) version.

The configuration script looks in the standard include directories, e.g. `/usr/include` and `/usr/local/include` for the header file `Eigen/Dense`. You can specify a particular location in either of two ways:

1. Set the environment variable `EIGEN_DIR` before installing the R package, e.g., `export EIGEN_DIR=/usr/include/eigen3` in the bash shell.

2. Use `R CMD INSTALL --configure-args='--with-eigen=/path/to/eigen' nimble` or `install.packages("nimble", configure.args = "--with-eigen=/path/to/eigen")`.

In these cases, the directory should be the full path to the directory that contains the Eigen directory, e.g. `/usr/local/include`. It is not the full path to the Eigen directory itself, i.e., NOT `/usr/local/include/Eigen`.

4.2.2 Using libnimble

NIMBLE generates specialized C++ code for user-specified models and nimbleFunctions. This code uses some NIMBLE C++ library classes and functions. By default, on Linux and OS X, the library code is compiled once as a linkable library - *libnimble*. This single instance of the library is then linked with the code for each generated model. Alternatively, one can have the library code recompiled in each model's own dynamically loadable library (DLL). This does repeat the same code across models and so occupies more memory. There may be a marginal speed advantage. This is currently what happens on Windows. One can disable using *libnimble* via the configuration argument `--enable-lib`, e.g.

```
R CMD INSTALL --configure-args='--enable-lib=false' nimble
```

4.2.3 LAPACK and BLAS

NIMBLE also uses BLAS and LAPACK for some of its linear algebra (in particular calculating density values and generating random samples from multivariate distributions). NIMBLE will use the same BLAS and LAPACK installed on your system that R uses. Note that a fast (and where appropriate, threaded) BLAS can greatly increase the speed of linear algebra calculations. See Section A.3.1 of the R Installation and Administration manual for more details on providing a fast BLAS for your R installation.

4.2.4 Problems with Installation

We have tested the installation on the three commonly used platforms – OS X, Linux, Windows 7. We don't anticipate problems with installation, but we want to hear about any

and help resolve them. Please post about installation problems to the nimble-users Google group or email `nimble.stats@gmail.com`.

4.2.5 RStudio and NIMBLE

You can use NIMBLE in RStudio, but we strongly recommend that you turn off the option to display the Global Environment. Leaving it on can cause RStudio to freeze, apparently from trying to deal with some of NIMBLE's data structures.

4.3 Installing a C++ compiler for R to use

In addition to needing a C++ compiler to install the package (from source), you also need to have a C++ compiler and the utility *make* at run-time. This is needed during the R session to compile the C++ code that NIMBLE generates for a user's models and algorithms.

4.3.1 OS X

On OS X, you should install Xcode. The command-line tools, which are available as a smaller installation, should be sufficient. This is freely available from the Mac App Store. See https://developer.apple.com/xcode/downloads/ and https://itunes.apple.com/us/app/xcode/id497799835?ls=1&mt=12

For the compiler to work correctly for OS X, it is very important that the installed R be matched to the correct OS, i.e. R for snowleopard will attempt to use the incorrect compiler if the user has OS 10.9 or higher.

4.3.2 Linux

On Linux, you can install the GNU compiler suite (*gcc/g++*). You can use the package manager to install pre-built binaries. On Ubuntu, the following command will install or update *make*, *gcc* and *libc*.

```
sudo apt-get install build-essential
```

4.3.3 Windows

On Windows, you should download and install *Rtools.exe* available from http://cran.r-project.org/bin/windows/Rtools/. Select the appropriate executable corresponding to your version of R. (We strongly recommend using the most recent version of R, currently 3.1.0, and hence *Rtools31.exe*). This installer leads you through several "pages". You can accept all of the defaults. It is essential the checkbox for the "R 2.15+ toolchain" (page 4) is enabled in order to have *gcc/g++*, *make*, etc. installed. Also, we recommend that you check the PATH checkbox (page 5). This will ensure that R can locate these commands.

Advanced users may wish to change their default compilers. This can be done by editing the Makevars file, see Writing R Externsions: 1.2.1.

4.4 Customizing Compilation of the NIMBLE-generated Code

For each model or nimbleFunction, the NIMBLE package generates and compiles C++ code. This uses classes and routines available through the NIMBLE run-time library and also the Eigen library. The compilation mechanism uses R's SHLIB functionality and so the regular R configuration in `${R_HOME}/etc${R_ARCH}/Makeconf`. NIMBLE places a *Makevars* file in the directory in which the code is generated and `R CMD SHLIB` uses this file.

In all but specialized cases, the general compilation mechanism will suffice. However, one can customize this. One can specify the location of an alternative *Makevars* (or *Makevars.win*) file to use. That should define the variables `PKG_CPPFLAGS` and `PKG_LIBS`. These should contain, respectively, the pre-processor flag to locate the NIMBLE include directory, and the necessary libraries to link against (and their location as necessary), e.g., *Rlapack* and *Rblas* on Windows, and *libnimble*.

Use of this file allows users to specify additional compilation and linking flags. See the Writing R Extensions manual for more details of how this can be used and what it can contain.

Chapter 5

Building models

NIMBLE aims to be compatible with the original BUGS language and also the version used by the popular JAGS package, as well as to extend the BUGS language. However, at this point, there are some BUGS features not supported by NIMBLE, and there are some extensions that are planned but not implemented.

Here is an overview of the status of BUGS features, followed by more detailed explanations of each topic.

5.1 NIMBLE support for features of BUGS

5.1.1 Supported features of BUGS

1. Stochastic and deterministic[1] node declarations.
2. Most univariate and multivariate distributions
3. Link functions
4. Most mathematical functions
5. "for" loops for iterative declarations.
6. Arrays of nodes up to 3 dimensions.

5.1.2 Not-yet-supported features of BUGS

Eventually, we plan to make NIMBLE fully compatible with BUGS and JAGS. In this first release, the following are *not* supported.

1. Stochastic indices
2. The `I()` notation

[1] NIMBLE calls non-stochastic nodes "deterministic", whereas BUGS calls them "logical". NIMBLE uses "logical" in the way R does, to refer to boolean (TRUE/FALSE) variables.

3. Aspects of the JAGS dialect of BUGS, such as the `T()` notation and `dinterval()`.

4. The appearance of the same node on the left-hand side of both a `<-` and a ∼ declaration, allowing data assignment for the value of a stochastic node.

5. Like BUGS, NIMBLE generally determines the dimensionality and sizes of variables from the BUGS code. However, when a variable appears with blank indices, such as in `x.sum <- sum(x[])`, NIMBLE currently requires that the dimensions of x be provided.

5.1.3 Extensions to BUGS

NIMBLE also extends the BUGS language in the following ways:

1. Distribution parameters can be expressions, as in JAGS but not in WinBUGS[2]. Caveat: parameters to *multivariate* distributions (*e.g.,* `dmnorm()`) may not be expressions, but must be [appropriately indexed] model nodes.

2. Named parameters for distributions, similar to named parameters in R's distribution functions.

3. Multiple parameterizations for distributions, similar to those in R.

4. More flexible indexing of vector nodes within larger variables, such as placing a multivariate normal vector arbitrarily within a higher-dimensional object, not just in the last index.

Extension for handling "data"

In BUGS, when you define a model, you provide *the* data for the model. You can use NIMBLE that way too, but NIMBLE provides more flexibility. Consider, for example, a case where you want to use the same model for many data sets. Or, consider a case where you want to use the model to simulate many data sets from known parameters. In such cases, the model needs to know what nodes have "data"[3], but the values of the data nodes can be modified.

To accommodate such flexibility, NIMBLE separates the concept of data into two concepts:

1. "Constants", which are provided when the model is defined and can never be changed thereafter. For example, a vector of known index values, such as for block indices, helps define the model graph itself and must be provided when the model is defined. NIMBLE "constants" are like BUGS "data", because they cannot be changed.

2. "Data", which are provided when an instance of a model is created from the model definition. When data are provided, their values are used and their nodes are flagged as data so that algorithms can use that information.

[2] e.g., `y  dnorm(5 + mu, 3 * exp(tau))`

[3] because algorithms will want to query the model about its nodes

We encourage users to distinguish between data and constants when building a model via `nimbleModel()`. However, for compatibility with BUGS and JAGS, we allow users to lump together data and constants as the `constants` argument to `nimbleModel()`, in which case NIMBLE determines which are which, based on which variables appear on the left-hand side of BUGS declarations.

Future extensions to BUGS

We also plan to extend the BUGS language to support:

1. Ability to provide new functions and new distributions written NIMBLE.
2. If-then-else syntax for one-time evaluation when the model is compiled, so that the same model code can generate different models when different conditions are met.
3. Single-line declaration of common motifs such as GLMs, GLMMs, and time-series models.

5.2 Creating models

Here we describe in detail two ways to provide a BUGS model for use by NIMBLE. The first, `nimbleModel`, is the primary way to do it and was illustrated in Chapter 2 . The second, `readBUGSmodel` provides compatibility with BUGS file formats for models, variables, data, and initial values for MCMC.

5.2.1 Using `nimbleModel()` to specify a model

There are five arguments to `nimbleModel` that provide information about the model, of which `code` is the only required one. Understanding these arguments involves some basic concepts about NIMBLE and ways it differs from BUGS and JAGS, so we explain them here. The R help page (`?nimbleModel`) provides a reference for this information.

code This is R code for the BUGS model. With just a few exceptions such as `T()` and `I()` notation, BUGS code is syntactically compatible with R, so it can be held in an R object. There are three ways to make such an object, by using `nimbleCode()`, the synonym `BUGScode()`, or simply the R function `quote()`.

constants This is a named list of values that cannot be modified after creating the model definition. They may include constants such as

1. `N` in the pump example, which is required for processing the BUGS code since it appears in `for(i in 1:N)`.
2. vectors of indices, such as when the model has nodes like `y[i] ~ dnorm(mu[blockID[i]], sd)`, where `blockID` is a vector of experimental block IDs that indicate which `mu` is needed for each `y`. Since vectors of indices are used to define the model graph, they cannot be changed after model definition

3. values that appear only on the right-hand side of BUGS declarations, such as covariates/predictors in regression-style models.

However, as mentioned previously, data values can be provided via the `constants` argument for compatibility with BUGS and JAGS. NIMBLE will then determine which variables appear on the left-hand side of BUGS declarations and will treat these as data rather than constants, without any need for users to call `setData()`.

dimensions This is a named list of vectors of the sizes of variables that appear in the model with unfilled indices such as `x[,]`. For the most part, NIMBLE determines the sizes of model variables automatically, but in cases with blank index fields, dimension information is required. As described in the section below about indexing, NIMBLE currently requires square brackets with blank indices (or complete indicies such as `1:N`, of course) when the full extent of a variable is needed. The dimension argument for `x[,]` would be e.g. `list(x = c(10, 8))` if `x` is a 10-by-8 matrix. Dimension information can alternatively be taken from `constants` or `data` if these are provided. [4]

data This is a named list of values to be used as data, with `NA`s to indicate missing data.

inits This is a named list of initial values for the model. These are neither data nor constants, but rather values with which to initialize the model. For variables that are a mix of data and non-data, we recommend using NA for the data elements for clarity, but NIMBLE ignores initial values for data nodes.

5.2.2 More about specifying data nodes and values

NIMBLE distinguishes between constants and data

As described in section 5.1.3, NIMBLE considers *constants* to be values that will never change and *data* to be information about the role a node plays in the model. Nodes marked as *data* will by default be protected from any functions that would simulate over their values, but it is possible to do so or to change their values by direct assignment. *constants* are hard-coded into the model and are not variables in the model.

One can also provide variables appearing only on the right-hand side of BUGS declarations (e.g., covariates/predictors) via the `data` argument to `nimbleModel()` and these will appear as variables in the model and be flagged as data, but will not be nodes in the model. A user can change these values via direct assignment if desired.

Providing data via setData

Whereas the *constants* are a property of the *model definition* – since they may help determine the model structure itself – *data* nodes can be different in different copies of the model

[4] We have also seen cases where the dimension information inferred from the BUGS code does not match the data matrix because the model only applies to a subset of the data matrix. In a case like that, either `dimensions` must be provided to fit the entire data matrix or only the appropriate subset of the data matrix must be used in the model.

generated from the same *model definition*. For this reason, *data* is not required to be provided when the model code is processed. It can be provided later via the model member function `setData`. e.g., `pump$setData(pumpData)`, where `pumpData` is a named list of data values.

`setData` does two things: it sets the values of the data nodes, and it flags those nodes as containing data so that NIMBLE's `simulate()` functions do not overwrite data values. Values of data variables can be replaced normally, and the indication of which nodes should be treated as data can be reset by using the `resetData` method, e.g. `pump$resetData()`.

Missing data values

When a variable that functions as data in a model has missing values, one should set the nodes whose values are missing to be `NA`, either through the `data` argument when creating a model or via `setData`. The result will be that nodes with non-`NA` values will be flagged as data nodes, while nodes with `NA` values will not. Note that a node following a multivariate distribution must be either entirely observed or entirely missing.

Here's an example of running an MCMC on the *pump* model, with two of the observations taken to be missing. Our default MCMC specification will treat the missing values as unknowns to be sampled, as can be seen in the MCMC output here.

```
pumpMiss <- pump$newModel()
pumpMiss$resetData()
pumpDataNew <- pumpData
pumpDataNew$x[c(1, 3)] <- NA
pumpMiss$setData(pumpDataNew)

pumpMissSpec <- configureMCMC(pumpMiss)
pumpMissSpec$addMonitors(c('x', 'alpha', 'beta', 'theta'))

## thin = 1: alpha, beta, x, theta

pumpMissMCMC <- buildMCMC(pumpMissSpec)
Cobj <- compileNimble(pumpMiss, pumpMissMCMC)

niter <- 1000
set.seed(0)
Cobj$pumpMissMCMC$run(niter)

## NULL

samples <- as.matrix(Cobj$pumpMissMCMC$mvSamples)

samples[1:5, 13:17]

##      x[1] x[2] x[3] x[4] x[5]
## [1,]   17    1    2   14    3
## [2,]   11    1    4   14    3
```

```
## [3,]   14    1    9   14    3
## [4,]   11    1   24   14    3
## [5,]    9    1   29   14    3
```

Missing values may also occur in variables appearing on the right-hand side of BUGS declarations. Values for such variables should be passed in via the `data` argument to `nimbleModel`, with NA for the missing values. Of course in many contexts, one would want to specify (prior) distributions for the elements with missing values.

5.2.3 Using `readBUGSmodel()` to specify a model

`readBUGSmodel()` can read in the model, data/constant values and initial values in formats mostly compatible with the `bugs()` and `jags()` functions in the *R2WinBUGS* and *R2jags* packages. It can also take information directly from R objects, somewhat more flexibly than `nimbleModel()`. After processing the file inputs, it calls `nimbleModel()`.

`readBUGSmodel()` can take the following arguments:

model is either a file name, an R code object such as can be passed in the `code` argument of `nimbleModel()`, or a R function whose body contains the model code.

data is either a file name or a named list specifying constants and data together, the way they would be provided for BUGS or JAGS. `readBUGSmodel()` treats values that appear on the left-hand side of BUGS declarations as data and other values as constants, so you do not need to call the `setData` method.

inits is either a file name or a named list of initial values.

For both `data` and `inits`, if a file is specified, the file should contain R code that creates objects analogous to what would populate the list if a list were provided instead. Please see the JAGS manual examples or the *classic_bugs* directory in the NIMBLE package for example syntax. NIMBLE does not handle formatting such as in some of the original BUGS examples in which data was indicated with syntax such as `data x in 'x.txt'`. Only a single set of initial values can specified in creating a model; multiple sets of initial values will (eventually) be handled in NIMBLE's MCMC implementation.

Example using `readBUGSmodel`

Let's create a model for the *pump* example from BUGS.

```
pumpDir <- system.file('classic-bugs', 'vol1', 'pump', package = 'nimble')
pumpModel <- readBUGSmodel('pump.bug', data = 'pump-data.R',
                           inits = 'pump-init.R', dir = pumpDir)
```

Note that `readBUGSmodel()` allows one to include `var` and `data` blocks in the model file as in some of the BUGS examples (such as `inhaler`). The `data` block pre-computes constant and data values. NIMBLE by and large does not need the information given in a `var` block

but occasionally this is used to determine dimensionality, such as in the case of syntax like `xbar <- mean(x[])` where `x` is a variable that appears only on the right-hand side of BUGS expressions.

5.2.4 A note on introduced nodes

In some cases, NIMBLE introduces new nodes into the model that were not specified in the BUGS code for the model, such as the `lifted_d1_over_beta` node in the introductory example. For this reason, it is important that programs written to adapt to different model structures use NIMBLE's systems for querying the model graph. For example, a call to `pump$getDependencies("beta")` will correctly include `lifted_d1_over_beta` in the results. If one skips this step and assumes the nodes are only those that appear in the BUGS code, one may not get correct results.

It can be helpful to know the situations in which lifted nodes are generated. These include:

- When distribution parameters are expressions, NIMBLE creates a new deterministic node that contains the expression for a given parameter. The node is then a direct descendant of the new deterministic node. This is an optional feature, but it is currently enabled in all cases.
- As discussed in 5.3.4 the use of link functions causes new nodes to be introduced.
- Use of alternative parameterizations of distributions. For example when a user provides the precision of a normal distribution as `tau`, NIMBLE creates a new node `sd <- 1/sqrt(tau)` and uses `sd` as a parameter in the normal distribution. If many nodes use the same `tau`, only one new `sd` node will be created, so the computation `1/sqrt(tau)` will not be repeated redundantly. More about NIMBLE's parameterizations is described below.

5.3 More details on NIMBLE support of BUGS features

5.3.1 Distributions

NIMBLE supports most of the distributions allowed in BUGS and JAGS. Table 5.1 lists the distributions currently supported.

To understand how NIMBLE handles alternative parameterizations, it is useful to distinguish three cases, using the `gamma` distribution as an example:

1. A *canonical* parameterization is used directly for computations. Usually this is the parameterization in the `Rmath` header of R's C implementation of distributions. For `gamma`, this is (shape, scale).
2. The *BUGS* parameterization is the one defined in the original BUGS language. For `gamma`, this is (shape, rate).

3. An *alternative* parameterization is one that must be converted into the *canonical* parameterization. For example, NIMBLE provides a (mean, sd) parameterization and creates nodes to calculate (shape, scale) from (mean, sd). In the case of `gamma`, the *BUGS* parameterization is also an *alternative* parameterization.

Since NIMBLE aims to provide compatibility with existing BUGS and JAGS code, the order of parameters places the *BUGS* parameterization first. For example, the NIMBLE definition of a `gamma`, in R format, is `dgamma( shape, rate, scale, mean, sd)`. Like R, if parameter names are not given, they are taken in order, so that (shape, rate) is the default. This happens to match R's order of parameters, but it need not. If names are given, they can be given in any order. NIMBLE knows that rate is an alternative to scale and that (mean, sd) are an alternative to (shape, scale or rate).

The file *distsDefs_table.R* in the R directory of the source package is the definitive source for the NIMBLE's distributions and parameterizations.

We plan to, but do not currently, handle the following distributions: double exponential (Laplace), beta-binomial, Dirichlet-multinomial, F, Pareto, inverse Wishart, and various forms of multivariate t.

We will shortly add the distribution aliases allowed in JAGS: `dbinom`, `dnbinom`, `dweibull`, `ddirich`.

Name	Usage	Density	Lower	Upper
Bernoulli	`dbern(prob = p)` $0 < p < 1$	$p^x(1-p)^{1-x}$	0	1
Beta	`dbeta(shape1 = a, shape2 = b)` $a > 0$, $b > 0$	$\frac{x^{a-1}(1-x)^{b-1}}{\beta(a,b)}$	0	1
Binomial	`dbin(prob = p, size = n)` $0 < p < 1$, $n \in \mathbb{N}^*$	$\binom{n}{x} p^x (1-p)^{n-x}$	0	n
Categorical	`dcat(prob = p)` $p \in (\mathbb{R}^+)^N$	$\frac{p_x}{\sum_i p_i}$	1	N
Chi-square	`dchisq(df = k)` $k > 0$	$\frac{x^{\frac{k}{2}-1}\exp(-x/2)}{2^{\frac{k}{2}}\Gamma(\frac{k}{2})}$	0	
Dirichlet	`ddirch(alpha)` $\alpha_j \geq 0$	$\Gamma(\sum_i \alpha_i)\prod_j \frac{x_j^{\alpha_j - 1}}{\Gamma(\alpha_j)}$	0	
Exponential	`dexp(rate = lambda)` $\lambda > 0$	$\lambda \exp(-\lambda x)$	0	
Gamma	`dgamma(shape = r, rate = λ)` $\lambda > 0$, $r > 0$	$\frac{\lambda^r x^{r-1}\exp(-\lambda x)}{\Gamma(r)}$	0	
Logistic	`dlogis(location = μ, rate = τ)` $\tau > 0$	$\frac{\tau \exp\{(x-\mu)\tau\}}{[1+\exp\{(x-\mu)\tau\}]^2}$		
Log-normal	`dlnorm(mu, tau)` $\tau > 0$	$\left(\frac{\tau}{2\pi}\right)^{\frac{1}{2}} x^{-1} \exp\left\{-\tau(\log(x)-\mu)^2/2\right\}$	0	
Multinomial	`dmulti(prob = b,size = n)` $\sum_j x_j = n$	$n! \prod_j \frac{p_j^{x_j}}{x_j!}$		
Multivariate normal	`dmnorm(mu, prec = Λ)` Λ positive definite	$(2\pi)^{-\frac{d}{2}}\lvert\Lambda\rvert^{\frac{1}{2}} \exp\{-(x-\mu)^T\Lambda(x-\mu)/2\}$		
Negative binomial	`dnegbin(prob = p, size = r)` $0 < p \leq 1$, $r \geq 0$	$\binom{x+r-1}{x} p^r (1-p)^x$	0	
Normal	`dnorm(mu, tau)` $\tau > 0$	$\left(\frac{\tau}{2\pi}\right)^{\frac{1}{2}} \exp\{-\tau(x-\mu)^2/2\}$		
Poisson	`dpois(lambda)` $\lambda > 0$	$\frac{\exp(-\lambda)\lambda^x}{x!}$	0	
Student t	`dt(mu, tau, df = k)` $\tau > 0$, $k > 0$	$\frac{\Gamma(\frac{k+1}{2})}{\Gamma(\frac{k}{2})}\left(\frac{\tau}{k\pi}\right)^{\frac{1}{2}}\left\{1+\frac{\tau(x-\mu)^2}{k}\right\}^{-\frac{(k+1)}{2}}$		
Uniform	`dunif(min = a,max = b)` $a < b$	$\frac{1}{b-a}$	a	b
Weibull	`dweib(shape = v, lambda)` $v > 0$, $\lambda > 0$	$v\lambda x^{v-1}\exp(-\lambda x^v)$	0	
Wishart	`dwish(R, df = k)` R $p \times p$ pos. def., $k \geq p$	$\frac{\lvert x\rvert^{(k-p-1)/2}\lvert R\rvert^{k/2}\exp\{-\mathrm{tr}(Rx/2)\}}{2^{pk/2}\Gamma_p(k/2)}$		

Table 5.1: Distributions with their default order of parameters. The value of the random variable is denoted by x.

5.3.2 List of parameterizations

NIMBLE extends BUGS by allowing different standard parameterizations of distributions. These are listed in Table 5.2.

Alternative Parameterization	NIMBLE re-parameterization
`dbeta(mean, sd)`	`dbeta(shape1 = mean^2 * (1 - mean) / sd^2 - mean, shape2 = mean * (1 - mean)^2 / sd^2 + mean - 1)`
`dexp(scale)`	`dexp(rate = 1/scale)`
`dgamma(shape, scale)`	*none*
`dgamma(mean, sd)`	`dgamma(shape = mean^2 / sd^2, scale = sd^2 / mean)`
`dweib(shape, scale)`	*none*
`dweib(shape, rate)`	`dweib(shape, scale = 1/rate)`
`dlnorm(mu, sd)`	*none*
`dlogis(location, scale)`	*none*
`dnorm(mu, sd)`	*none*
`dnorm(mu, var)`	`dnorm(mu, sd = sqrt(var))`
`dt(mu, sigma, df)`	*none*
`dmnorm(mu, cov)`	`dnorm(mu, chol = chol(cov), prec_param = FALSE)`
`dmnorm(mu, chol)`	`dnorm(mu, chol, prec_param = FALSE)`
`dwish(S, df)`	`dwish(chol = chol(S), df, scale_param = TRUE)`

Table 5.2: Alternative distribution parameterizations. The first column indicates the supported parameterizations for distributions given in Table 5.1 with their *BUGS* parameterization. The second column indicates the relationship to the *canonical* parameterization used in NIMBLE. In cases where the the *BUGS* parameterization is not the *canonical* one, the latter is listed in this table with *none* in the second column.

5.3.3 List of BUGS language functions

NIMBLE provides a wide variety of operators and functions for use in defining models (Tables 5.3-5.4). Note that by virtue of how we set up models using the NIMBLE language, these are the same operators and functions that one can use in a NIMBLE function, as discussed further in Chapter 9.

For the most part NIMBLE supports the functions used in BUGS and JAGS, with exceptions indicated in the table. Additional functions provided by NIMBLE are also listed. For distribution functions, currently "r" and "d" functions are provided for each distribution, and when called from `nimbleFunctions` only the BUGS parameterization is available in v0.3-1, and in fact sometimes that is provided differently. See 9.5.17. Currently "r" functions only return one random draw at a time, and the first argument must always be 1. For multivariate distribution functions the `prec_param` or `scale_param` argument must be provided, indicating when a covariance or precision matrix has been given. In a future release we will provide a variety of distribution functions, including density, cumulative distribution

and quantile functions, using the same syntax as `dnorm`, `pnorm`, `qnorm`. We will also extend the alternative parameterizations with named parameters to `nimbleFunctions`.

5.3.4 List of link functions

NIMBLE allows the link functions listed in Table 5.5.

Link functions are specified as functions applied to a variable on the left hand side of a BUGS expression. To handle link functions, NIMBLE does some processing that inserts an additional node into the model. For example, the declaration `logit(p[i]) ~ dnorm(mu[i],1)`, is equivalent to the follow two declarations:

- `logit_p[i] ~ dnorm(mu[i], 1)`,
- `p[i] <- expit(logit_p[i])`

where `expit` is the inverse of `logit`. When the BUGS expression defines a deterministic node, such as `logit(p) <- b0 + b1*x`, the same operations are performed except that `logit_p` is a deterministic node.

5.3.5 Indexing

NIMBLE allows flexible indexing that is compatible with BUGS and JAGS.

In particular NIMBLE allows

- `x[i]`
- `x[i:j]`
- `x[i:j,k:l]` and indexing of higher dimensional arrays
- `x[i:j, ]`
- `x[3*i+7]`
- `x[(3*i):(5*i+1)]`

When calling functions such as `mean` and `sum` on a vector variable, the square brackets are required but can have blank indices, e.g. `xbar <- mean(x[])` if `x` is a vector and `xbar <- mean(x[,])` if `x` is a matrix [5].

NIMBLE does not allow multivariate nodes to be indicated without square brackets, which is an incompatibility with JAGS. Therefore a statement like `xbar <- mean(x)` in JAGS must be converted to `xbar <- mean(x[])` for NIMBLE.

Here's an example of indexing in the context of multivariate nodes, showing two ways to do the indexing. The first provides indices, so no `dimensions` argument is needed, while the second omits the indices and provides a `dimensions` argument instead.

[5] This is a case where the dimension of x must be provided when defining the model.

Usage	Description	Comments	Status	Accepts vector input
`x | y`, `x & y`	logical OR (|) and AND(&)		✓	
`!x`	logical not		✓	
`x > y`, `x >= y`	greater than (and or equal to)		✓	
`x < y`, `x <= y`	less than (and or equal to)		✓	
`x != y`, `x == y`	(not) equals		✓	
`x + y`, `x - y`, `x * y`	component-wise operators	mix of scalar and vector ok	✓	✓
`x / y`,	component-wise division	vector x and scalar y ok	✓	✓
`x^y`, `pow(x, y)`	power	x^y	✓	
`x %% y`	modulo (remainder)		✓	
`min(x1, x2)`, `max(x1, x2)`	min. (max.) of two scalars		✓	
`exp(x)`	exponential		✓	✓
`log(x)`	natural logarithm		✓	✓
`sqrt(x)`	square root		✓	✓
`abs(x)`	absolute value		✓	✓
`step(x)`	step function at 0	0 if $x < 0$, 1 if $x > 0$	✓	✓
`equals(x, y)`	equality of two scalars	1 if $x == y$, 0 if $x! = y$	✓	
`cube(x)`	third power	x^3	✓	✓
`sin(x)`, `cos(x)`, `tan(x)`	trigonometric functions		✓	✓
`asin(x)`, `acos(x)`, `atan(x)`	inverse trigonometric functions		✓	✓
`asinh(x)`, `acosh(x)`, `atanh(x)`	inv. hyperbolic trig. functions		✓	✓
`logit(x)`	logit	$\log(x/(1-x))$	✓	✓
`ilogit(x)`, `expit(x)`	inverse logit	$\exp(x)/(1+\exp(x))$	✓	✓
`probit(x)`	probit (Gaussian quantile)	$\Phi^{-1}(x)$	✓	✓
`iprobit(x)`, `phi(x)`	inverse probit (Gaussian CDF)	$\Phi(x)$	✓	✓
`cloglog(x)`	complementary log log	$\log(-\log(1-x))$	✓	✓
`icloglog(x)`	inverse complementary log log	$1-\exp(-\exp(x))$	✓	✓
`ceiling(x)`	ceiling function	$\lceil(x)\rceil$	✓	✓
`floor(x)`	floor function	$\lfloor(x)\rfloor$	✓	✓
`round(x)`	round to integer		✓	✓
`trunc(x)`	truncation to integer		✓	✓
`lgamma(x)`, `loggam(x)`	log gamma function	$\log\Gamma(x)$	✓	✓
`log1p(x)`	log of 1 + x	$\log(1+x)$	✓	✓
`lfactorial(x)`, `logfact(x)`	log factorial	$\log x!$	✓	✓
`log1p(x)`	log one-plus	$log(x+1)$	✓	✓
`dDIST(x, PARAMS)`	"d" distribution functions	canonical parameterization	✓	
`rDIST(1, PARAMS)`	"r" distribution functions	canonical parameterization	✓	
`sort(x)`				
`rank(x, s)`				
`ranked(x, s)`				
`order(x)`				

Table 5.3: Functions operating on scalars, many of which can operate on each element (component-wise) of vectors and matrices. Status column indicates if the function is currently provided in NIMBLE.

Usage	Description	Comments	Status
`inverse(x)`	matrix inverse	`x` symmetric, positive definite	✓
`chol(x)`	matrix Cholesky factorization	`x` symmetric, positive definite	✓
`eigen(x)`	matrix eigendecomposition		
`svd(x)`	matrix singular value decomposition		
`t(x)`	matrix transpose	$x^\top$	✓
`x%*%y`	matrix multiply	xy; x, y conformant	✓
`inprod(x, y)`	dot product	$x^\top y$	✓
`logdet(x)`	log matrix determinant	$\log \lvert x \rvert$	✓
`asRow(x)`	convert vector `x` to 1-row matrix	sometimes automatic	✓
`asCol(x)`	convert vector `x` to 1-column matrix	sometimes automatic	✓
`sum(x)`	sum of elements of `x`		✓
`mean(x)`	mean of elements of `x`		✓
`sd(x)`	standard deviation of elements of `x`		✓
`prod(x)`	product of elements of `x`		✓
`min(x)`, `max(x)`	min. (max.) of elements of `x`		✓
`pmin(x, y)`, `pmax(x, y)`	vector of mins (maxs) of elements of `x` and `y`		✓
`interp.lin(x, v1, v2)`	linear interpolation		

Table 5.4: Functions operating on vectors and matrices. Status column indicates if the function is currently provided in NIMBLE.

Link function	Description	Range	Inverse
`cloglog(y) <- x`	Complementary log log	$0 < y < 1$	`y <- icloglog(x)`
`log(y) <- x`	Log	$0 < y$	`y <- exp(x)`
`logit(y) <- x`	Logit	$0 < y < 1$	`y <- expit(x)`
`probit(y) <- x`	Probit	$0 < y < 1$	`y <- iprobit(x)`

Table 5.5: Link functions

```
code <- nimbleCode({
  y[1:K] ~ dmulti(p[1:K], n)
  p[1:K] ~ ddirch(alpha[1:K])
  log(alpha[1:K]) ~ dmnorm(alpha0[1:K], R[1:K, 1:K])
})

K <- 5
model <- nimbleModel(code, constants = list(n = 3, K = K,
                           alpha0 = rep(0, K), R = diag(K)))

codeAlt <- nimbleCode({
  y[] ~ dmulti(p[], n)
  p[] ~ ddirch(alpha[])
  log(alpha[]) ~ dmnorm(alpha0[], R[ , ])
```

```
})

model <- nimbleModel(codeAlt, constants = list(n = 3, K = K,
                              alpha0 = rep(0, K), R = diag(K)),
                    dimensions = list(y = K, p = K, alpha = K))
```

A limitation to NIMBLE at present is that it allows only contiguous indexed blocks. In particular, it does not allow:

- Non-contiguous sub-indexing such as `c(1, 3, 4, 8)` or `seq(2, 10, by = 2)`
- Logical sub-indexing such as `c(TRUE, FALSE, TRUE)`

5.3.6 Censoring and truncation

`T()` and `dinterval()` provide for truncation and censoring, respectively, in the JAGS dialect of BUGS. These will be enabled in a release of NIMBLE in the near term. JAGS provides `I()` for backwards compatibility with BUGS, only for the case that the node to which `I()` is applied has fixed parameters and we will enable this usage in NIMBLE as well. For more discussion of truncation vs. censoring, please see the JAGS manual.

5.4 Compiling models

A compiled model inherits all the information from the uncompiled model and is initialized from its values. However, once the C++ version of the model is created, these are two distinct models and changing values in one model does not affect the other model. However, they are considered to have a one-to-one relationship: You can make a second copy of the uncompiled model and from that a second compiled model, but you cannot make two compiled models from the same uncompiled model.

Continuing the example from above, compilation is done as follows.

```
CpumpModel <- compileNimble(pumpModel)
```

The `compileNimble` function will be described in more detail later. Additional arguments can specific what directory to use for C++ code and what other NIMBLE objects are part of the same project.

Once one has the C-model in hand one can manipulate it in exactly the same way one manipulates the R-model. Both versions of the model are represented in R as Reference Class objects inheriting from the same base class.

Chapter 6

Using NIMBLE models from R

6.1 Some basic concepts and terminology

Before going further, we need some basic concepts and terminology to be able to speak about NIMBLE clearly.

Say we have the following BUGS code

```
mc <- nimbleCode({
    a ~ dnorm(0, 0.001)
    for(i in 1:5) {
        y[i] ~ dnorm(a, 0.1)
        for(j in 1:3)
            z[i,j] ~ dnorm(y[i], sd = 0.1)
    }
})

model <- nimbleModel(mc, data = list(z = matrix(rnorm(15), nrow = 5)))
```

In NIMBLE terminology:

- The *variables* of this model are a and y.
- The *nodes* of this model are `a`, `y[1]`, ..., `y[5]`, and `z[1,1]`, ..., `z[5, 3]`.
- the *node functions* of this model are `a ~ dnorm(0, 0.001)`, `y[i] ~ dnorm(a, 0.1)` and `z[i,j] ~ dnorm(y[i], sd = 0.1)`. Sometimes the distinction between nodes and node functions is important, but when it is not important we may refer to both simply as *nodes*.

6.2 Accessing variables

Model variables can be accessed and set just as in R using `$` and `[[ ]]`. For example

```
model$a <- 5
model$a

## [1] 5

model[['a']]

## [1] 5

model$y[2:4] <- rnorm(3)
model$y

## [1]      NA -1.2518 -0.6632  0.1652      NA

model[['y']][c(1, 5)] <- rnorm(2)
model$y

## [1]  2.1748 -1.2518 -0.6632  0.1652  0.2907

model$z[1,]

## [1] -0.0216 -1.6069  0.2034
```

6.2.1 Accessing log probabilities via logProb variables

For each variable that contains at least one stochastic scalar node, NIMBLE generates a model variable with the prefix "logProb_" that usually matches the variable's size. For example

```
model$logProb_y

## [1] NA NA NA NA NA

calculate(model, 'y')

## [1] -16.59

model$logProb_y

## [1] -2.469 -4.024 -3.674 -3.239 -3.179
```

Creation of `logProb` variables for stochastic multivariate nodes is trickier, because they can represent an arbitrary block of a larger variable. In general NIMBLE records the logProb values using the lowest possible indices. For example, if `x[5:10, 15:20]` follows a Wishart distribution, its log probability (density) value will be stored in `logProb_x[5, 15]`. When

possible, NIMBLE will reduce the dimensions of the corresponding logProb variable. For example, in

```
for(i in 1:10) x[i,] ~ dmnorm(mu[], prec[,])
```

`x` may be 10×20 (dimensions must be provided), but `logProb_x` will be 10×1. For the most part you do not need to worry about how NIMBLE is storing the log probability values, because you can always get them using `getLogProb`.

6.3 Accessing nodes

While nodes that are part of a variable can be accessed as above, each node also has its own name that be used to access it directly. For example, `y[2]` has the name "y[2]" and can be accessed by that name as follows:

```
model[['y[2]']]

## [1] -1.252

model[['y[2]']] <- -5
model$y

## [1]  2.1748 -5.0000 -0.6632  0.1652  0.2907

model[['z[2, 3]']]

## [1] -2.154

model[['z[2:4, 1:2]']][1, 2]

## [1] -1.098

model$z[2, 2]

## [1] -1.098
```

Notice that node names can include index blocks, such as `model[['z[2:4, 1:2]']]`, and these are not strictly required to correspond to actual nodes. Such blocks can be subsequently sub-indexed in the regular R manner.

6.3.1 How nodes are named

Every node has a name that is a character string including its indices, with a space after every comma. For example, `X[1, 2, 3]` has the name "X[1, 2, 3]". Nodes following multivariate distributions have names that include their index blocks. For example, a BUGS declaration creating a multivariate node for `X[6:10, 3]` has the name "X[6:10, 3]".

The definitive source for node names in a model is `getNodeNames()`, described below. For example

```
multiVarCode <- nimbleCode({
    X[1, 1:5] ~ dmnorm(mu[], cov[,])
    X[6:10, 3] ~ dmnorm(mu[], cov[,])
})

multiVarModel <- nimbleModel(multiVarCode, dimensions = list(mu = 5, cov = c(5,5)))

multiVarModel$getNodeNames()

## [1] "lifted_chol_cov_1to5_1to5[1:5, 1:5]"
## [2] "X[1, 1:5]"
## [3] "X[6:10, 3]"
```

You can see one lifted node for the Cholesky decomposition of `cov`, and the two multivariate normal nodes.

In the event you need to ensure that a name is formatted correctly, you can use R's `parse()` and `deparse()` functions. For example, to get the spaces correctly inserted into "X[1,1:5]":

```
deparse(parse(text = "X[1,1:5]", keep.source = FALSE)[[1]])

## [1] "X[1, 1:5]"
```

The `keep.source = FALSE` makes `parse()` more efficient.

6.3.2 Why use node names?

Syntax like `pump[["x[2, 3]"]]` may seem strange at first. To see its utility, consider the example of writing the nimbleFunction given in 2.7. By giving every scalar node a name, even if it is part of a multivariate variable, one can write functions in R or NIMBLE that access any single node by a name. This is particularly useful for NIMBLE, which resolves how to access a particular node during the compilation process.

6.4 `calculate()`, `simulate()`, and `getLogProb()`

The three basic ways to operate a model are to calculate nodes, simulate into nodes, or get the log probabilities (or probability densities) that have already been calculated. In more detail:

calculate For a stochastic node, `calculate` determines the log probability value, stores it, and returns it. For a deterministic node, `calculate` executes the deterministic calculation and returns 0.

simulate For a stochastic node, `simulate` generates a random draw. For deterministic nodes, `simulate` is equivalent to `calculate` without returning 0. `simulate` always returns `NULL` (or `void` in C++).

getLogProb `getLogProb` simply returns the most recently calculated log probability value, or 0 for a deterministic node.

There are two ways to access `calculate`, `simulate`, and `getLogProb`. The primary way is via the functions with those names, which can use arbitrary collections of nodes. In that case, `calculate` and `getLogProb` return the sum of the log probabilities from each node. The other way is to directly access the corresponding function for each node in a model. Normally you'll use the first way, but we'll show you both.

6.4.1 For arbitrary collections of nodes

```
model$y

## [1]  2.1748 -5.0000 -0.6632  0.1652  0.2907

simulate(model, 'y[1:3]')
model$y

## [1] 6.2679 8.5769 3.1255 0.1652 0.2907

simulate(model, 'y')
model$y

## [1] 10.3638 -0.7319  1.7390 11.2717  4.1535

model$z

##         [,1]    [,2]    [,3]
## [1,] -0.0216 -1.6069  0.2034
## [2,]  2.0866 -1.0978 -2.1542
## [3,]  0.5998  1.6349  0.3827
## [4,]  0.2366 -0.2201 -0.4214
## [5,] -0.6389 -1.2344 -2.2250

simulate(model, c('y[1:3]', 'z[1:5, 1:3]'))
model$y

## [1]  7.1787  3.6497  0.6323 11.2717  4.1535

model$z
```

```
##          [,1]    [,2]    [,3]
## [1,] -0.0216 -1.6069  0.2034
## [2,]  2.0866 -1.0978 -2.1542
## [3,]  0.5998  1.6349  0.3827
## [4,]  0.2366 -0.2201 -0.4214
## [5,] -0.6389 -1.2344 -2.2250

simulate(model, c('z[1:5, 1:3]'), includeData = TRUE)
model$z

##         [,1]    [,2]    [,3]
## [1,]  7.088  7.0959  7.3236
## [2,]  3.794  3.7199  3.7240
## [3,]  0.613  0.7931  0.6332
## [4,] 11.312 11.3335 11.1923
## [5,]  4.266  4.1383  4.3164
```

Notice that

1. inputs like `'y[1:3]'` are automatically expanded into `c('y[1]', 'y[2]', 'y[3]')`. In fact, simply `'y'` will be expanded into all nodes within `y`.
2. an abitrary number of nodes can be provided as a character vector
3. simulations will be done in the order provided, so in practice the nodes will often be obtained by functions like `getDependencies` described below. These return nodes in topologically sorted order, which means no node comes before something it depends on.
4. The data nodes `z` were not simulated over until `includeData = TRUE` was used.
5. In v0.3-1 it is not allowed to leave an index blank. For example `simulate(model, 'z[1,]')` is an error.

Use of `calculate` and `getLogProb` is simliar to `simulate`, except that they return the sum of the log probabilities (densities) of the nodes requested, and they have not `includeData` argument.

6.4.2 Direct access to each node's functions

Access to the underlying `calculate`, `simulate`, and `getLogProb` functions built by NIMBLE can be had as follows:

```
y2lp <- model$nodes[['y[2]']]$calculate()
y2lp

## [1] -2.161
```

```
model$nodes[['y[2]']]$getLogProb()

## [1] -2.161
```

6.5 Querying model parameters

Models also have a system for querying the value of any distribution parameter, including parameters from alternative parameterizations. In v0.3-1, this is an advanced topic to be described later.

6.6 Querying model structure

NIMBLE provides functionality by which one can determine the structure of a model. This can be used directly from R or in the setup code of an algorithm as discussed in Chapter 9. These functions also work with the compiled version of a model.

Here we demonstrate this functionality using the *pump* example because it has a few more interesting components than the example above.

6.6.1 `getNodeNames()` and `getVarNames()`

First we'll see how to determine the nodes and variables in a model.

```
pump$getNodeNames()

##  [1] "alpha"               "beta"
##  [3] "lifted_d1_over_beta" "theta[1]"
##  [5] "theta[2]"            "theta[3]"
##  [7] "theta[4]"            "theta[5]"
##  [9] "theta[6]"            "theta[7]"
## [11] "theta[8]"            "theta[9]"
## [13] "theta[10]"           "lambda[1]"
## [15] "lambda[2]"           "lambda[3]"
## [17] "lambda[4]"           "lambda[5]"
## [19] "lambda[6]"           "lambda[7]"
## [21] "lambda[8]"           "lambda[9]"
## [23] "lambda[10]"          "x[1]"
## [25] "x[2]"                "x[3]"
## [27] "x[4]"                "x[5]"
## [29] "x[6]"                "x[7]"
## [31] "x[8]"                "x[9]"
## [33] "x[10]"

pump$getNodeNames(determOnly = TRUE)
```

```
##  [1] "lifted_d1_over_beta" "lambda[1]"
##  [3] "lambda[2]"           "lambda[3]"
##  [5] "lambda[4]"           "lambda[5]"
##  [7] "lambda[6]"           "lambda[7]"
##  [9] "lambda[8]"           "lambda[9]"
## [11] "lambda[10]"

pump$getNodeNames(stochOnly = TRUE)

##  [1] "alpha"     "beta"      "theta[1]"  "theta[2]"  "theta[3]"
##  [6] "theta[4]"  "theta[5]"  "theta[6]"  "theta[7]"  "theta[8]"
## [11] "theta[9]"  "theta[10]" "x[1]"      "x[2]"      "x[3]"
## [16] "x[4]"      "x[5]"      "x[6]"      "x[7]"      "x[8]"
## [21] "x[9]"      "x[10]"

pump$getNodeNames(dataOnly = TRUE)

##  [1] "x[1]"  "x[2]"  "x[3]"  "x[4]"  "x[5]"  "x[6]"  "x[7]"
##  [8] "x[8]"  "x[9]"  "x[10]"

pump$getVarNames()

## [1] "lifted_d1_over_beta" "beta"
## [3] "theta"               "alpha"
## [5] "lambda"              "x"
```

Note that some of the nodes may be "lifted" nodes introduced by NIMBLE as discussed in Section 5.2.4.

6.6.2 `getDependencies()`

Next we'll see how to determine the node dependencies in a model. There are a variety of arguments that allow one to specify whether to include the node itself, whether to include deterministic or stochastic or data dependents, etc. By default `getDependencies` returns descendants up to the next stochastic node on all edges of the graph. This is what would be needed to calculate a Metropolis-Hastings acceptance probability in MCMC, for example.

```
pump$getDependencies('alpha')

##  [1] "alpha"     "theta[1]"  "theta[2]"  "theta[3]"  "theta[4]"
##  [6] "theta[5]"  "theta[6]"  "theta[7]"  "theta[8]"  "theta[9]"
## [11] "theta[10]"

pump$getDependencies(c('alpha', 'beta'))
```

```
##  [1] "alpha"               "beta"
##  [3] "lifted_d1_over_beta" "theta[1]"
##  [5] "theta[2]"            "theta[3]"
##  [7] "theta[4]"            "theta[5]"
##  [9] "theta[6]"            "theta[7]"
## [11] "theta[8]"            "theta[9]"
## [13] "theta[10]"

pump$getDependencies('theta[1:3]', self = FALSE)

## [1] "lambda[1]" "lambda[2]" "lambda[3]" "x[1]"      "x[2]"
## [6] "x[3]"

pump$getDependencies('theta[1:3]', stochOnly = TRUE, self = FALSE)

## [1] "x[1]" "x[2]" "x[3]"

# get all dependencies, not just the direct descendants
pump$getDependencies('alpha', downstream = TRUE)

##  [1] "alpha"       "theta[1]"   "theta[2]"   "theta[3]"
##  [5] "theta[4]"    "theta[5]"   "theta[6]"   "theta[7]"
##  [9] "theta[8]"    "theta[9]"   "theta[10]"  "lambda[1]"
## [13] "lambda[2]"   "lambda[3]"  "lambda[4]"  "lambda[5]"
## [17] "lambda[6]"   "lambda[7]"  "lambda[8]"  "lambda[9]"
## [21] "lambda[10]"  "x[1]"       "x[2]"       "x[3]"
## [25] "x[4]"        "x[5]"       "x[6]"       "x[7]"
## [29] "x[8]"        "x[9]"       "x[10]"

pump$getDependencies('alpha', downstream = TRUE, dataOnly = TRUE)

##  [1] "x[1]"  "x[2]"  "x[3]"  "x[4]"  "x[5]"  "x[6]"  "x[7]"
##  [8] "x[8]"  "x[9]"  "x[10]"
```

6.6.3 `isData()`

Finally, you can query whether a node is a data node using the `isData` method applied to one or more nodes:

```
pump$isData('x[1]')

## [1] TRUE

pump$isData(c('x[1]', 'x[2]', 'alpha'))

## [1]  TRUE  TRUE FALSE
```

At the moment the `isData` method requires that each node be supplied as an individual element of the character vector, so `pump$isData('x[1:3]')` would throw an error.

You can also query variables to determine if the nodes that are part of a variable are data nodes.

```
pump$isData('x')

##  [1] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
```

6.7 The *modelValues* data structure

In the NIMBLE framework, *modelValues* are containers designed for storing values for models, although they can be used to store any type of information. They may be used for model outputs or model inputs. A modelValues object will contain *rows* of variables. Each row represents a single value of a variable from a model and will be an array (i.e. scalar, vector, matrix or three-dimensional array) from the same dimension[1]. The simplest way to build a modelValues object is from a model object. This will create a modelValues object with the same variables as the model.

```
pumpModelValues = modelValues(pumpModel, m = 2)
pumpModel$x

##  [1]  5  1  5 14  3 19  1  1  4 22

pumpModelValues$x

## [[1]]
##  [1] NA NA NA NA NA NA NA NA NA NA
##
## [[2]]
##  [1] NA NA NA NA NA NA NA NA NA NA
```

In this example, `pumpModelValues` has the same variables as `pumpModel`, although `pumpModelValues` has two rows because we set `m` to be 2. As you can see, the rows are stored as elements of a list.

Alternatively, one can define a modelValues object manually via the `ModelValuesSpec()` function. In this case, we will need to provide several arguments:

- `vars`, which is a character vector of variable names,
- `type`, which is a character vector of the data types for each variable ('double' for real numbers, 'integer' for integers) and

[1] In v0.3-1, NIMBLE is limited to three dimensions.

- `size`, which is a list of vectors of the sizes in each dimension of each variable. The names of the list elements must match the names provided in `vars`.

```
mvSpec = modelValuesSpec(vars = c('a', 'b', 'c'),
                         type = c('double', 'int', 'double'),
                         size = list( a = 2, b =c(2,2)  , c = 1) )

customMV = modelValues(mvSpec, m = 2 )
customMV$a

## [[1]]
## [1] NA NA
##
## [[2]]
## [1] NA NA
```

Note that in R execution, the types are not enforced. But they will be the types created in C++ code during compilation, so they should be specified carefully.

The object returned by `modelValues()` is an uncompiled modelValues. When a nimbleFunction is compiled, any modelValues objects it uses are also compiled. A NIMBLE model always contains a modelValues that it uses as a default location to store its variables.

Here is an example where the `customMV` created above is used as the setup argument for a nimbleFunction, which is then compiled. Its compiled mv is then accessed with `$`.

```
# Simple nimbleFunction that uses a modelValues object
resizeFunction_Gen <- nimbleFunction(
  setup = function(mv){},
  run = function(k = integer() ){
    resize(mv,k)})

rResize <- resizeFunction_Gen(customMV)
cResize <- compileNimble(rResize)
cCustomMV <- cResize$mv
# cCustomMV is a C++ modelValues object
```

Compiled modelValues objects can be accessed and altered in all the same ways as uncompiled ones. However, only uncompiled modelValues can be used as arguments to setup code in nimbleFunctions.

6.7.1 Accessing contents of modelValues

The values in a modelValues object can be accessed in several ways from R, and in fewer ways from NIMBLE.

```
# Sets the first row of a to (0, 1).  R only.
customMV[['a']][[1]] <- c(0,1)

# Sets the second row of a to (2, 3)
customMV['a', 2] <- c(2,3)

#Can access subsets of each row in standard R manner
customMV['a', 2][2] <- 4

# Accesses all values of 'a'. Output is a list.  R only.
customMV[['a']]

## [[1]]
## [1] 0 1
##
## [[2]]
## [1] 2 4

# Sets the first row of b to a matrix with values 1. R only.
customMV[['b']][[1]] <- matrix(1, nrow = 2, ncol = 2)

# Sets the second row of b.  R only.
customMV[['b']][[2]] <- matrix(2, nrow = 2, ncol = 2)

# Make sure the size of inputs is correct
# customMV['a', 1] <- 1:10
# Problem: dimension of 'a' is 2, not 10!
# Will cause problems when compiling nimbleFunction using customMV
```

Currently, only the syntax `customMV[‘a’, 2]` works in the NIMBLE language, not `customMV[[‘a’]][[2]]`. Also note that `c()` does not work in NIMBLE, but one can do `customMV[‘a’, 2] <- X[1:2]`.

Every row of a modelValues object is expected to be of the same dimension. As with types, this is not enforced in R, but writing code that changes dimensionality in R will lead to an error during compilation.

We can query and change the number of rows using `getsize()` and `resize()`, respectively. These work in both R and NIMBLE. Note that we don’t specify the variables in this case: all variables in a modelValues object will have the same number of rows.

```
getsize(customMV)

## [1] 2

resize(customMV, 3)
getsize(customMV)
```

```
## [1] 3

customMV$a

## [[1]]
## [1] 0 1
##
## [[2]]
## [1] 2 4
##
## [[3]]
## [1] NA NA
```

Often it is practical to convert a modelValues object to a matrix for use in R, such as with MCMC output for use with the tools provided by the `coda` package. This can be done with the `as.matrix` method for modelValues objects. This will generate column names by 'flattening' the variable names and indices. The rows of the modelValues will be the rows of the matrix, with any matrices or arrays converted to a vector based on column-major ordering.

```
as.matrix(customMV, 'a')   # convert 'a'

##      a[1] a[2]
## [1,]    0    1
## [2,]    2    4
## [3,]   NA   NA

as.matrix(customMV)        # convert all variables

##      a[1] a[2] b[1, 1] b[2, 1] b[1, 2] b[2, 2]  c
## [1,]    0    1       1       1       1       1 NA
## [2,]    2    4       2       2       2       2 NA
## [3,]   NA   NA      NA      NA      NA      NA NA
```

If a variable is a scalar, using `unlist()` in R to extract all rows as a vector can be very useful.

```
customMV['c', 1] <- 1
customMV['c', 2] <- 2
customMV['c', 3] <- 3
unlist(customMV['c', ])

## [1] 1 2 3
```

Once we have a modelValues object, we can see the structure of object based on the `varNames` and `sizes` components of the object.

```
customMV$varNames

## [1] "a" "b" "c"

customMV$sizes

## $a
## [1] 2
##
## $b
## [1] 2 2
##
## $c
## [1] 1
```

It is very important to note that, as with most NIMBLE objects, modelValues are passed by reference, not by value. Any modifications of modelValues objects in either R or nimbleFunctions will persist outside of the function. This allows for more efficient computation, as stored values are immediately shared among nimbleFunctions.

```
alter_a <- function(mv){
  mv['a',1][1] <- 1
}
customMV['a', 1]

## [1] 0 1

alter_a(customMV)
customMV['a',1]

## [1] 1 1

#Note that the first row was changed
```

However, when you retrieve a variable from a modelValues object, the result is a standard R list, which is subsequently passed by value, as usual in R.

6.8 NIMBLE passes objects by reference

NIMBLE relies heavily on R's Reference Class system. When models, modelValues, and nimbleFunctions with setup code are created, NIMBLE generates a new, customized reference class definition for each. As a result, objects of these types are passed by reference and hence modified in place by most NIMBLE operations. This is necessary to avoid a great deal of copying and returning and having to reassign large objects, both in processing model and nimbleFunctions and in running algorithms.

One cannot generally copy NIMBLE models or nimbleFunctions (specializations or generators) in a safe fashion, because of the references to other objects embedded within NIMBLE objects. However, models provide a member function `newModel` that will create a new copy of the same model definition, like this:

```
newPump <- pumpModel$newModel()
```

This new model can then be used with newly instantiated nimbleFunctions.

The reliable way to create new copies of nimbleFunctions is to re-run the R function called `nimbleFunction()` and record the result in a new object.

Chapter 7

MCMC

Creation and execution of an MCMC algorithm in NIMBLE consists of several independent steps:

- Creating a specification for the MCMC algorithm for a specific model
- Building and compiling an executable MCMC function from the specification
- Running the MCMC function
- Extracting and analyzing the posterior samples

We'll also discuss:

- Sampling algorithms provided with the NIMBLE package
- A detailed example of using MCMC
- Higher level usage: MCMC Suite
- Advanced Topics

7.1 The MCMC specification

The MCMC specification contains the necessary information to fully specify an MCMC algorithm. This includes:

- The model on which the MCMC will operate
- The model nodes which will be sampled (updated) during execution of the MCMC
- The particular sampling algorithms for each of these nodes, including any control parameters required by each sampling algorithm
- The variables which will be monitored (recorded) during execution of the MCMC
- The thinning interval on which the monitored nodes will be recorded

An MCMC specification is created using `configureMCMC()`, and the resulting MCMC specification object will generally be denoted as `mcmcspec` in this Chapter. The only required argument to `configureMCMC()` is the original model object, which is the object resulting from a call to `nimbleModel()`.

We've already seen a basic example of an MCMC in the introductory example in Section 2.1.

7.1.1 Default MCMC specification

Assuming we have a model named `Rmodel`, the following will generate a default MCMC specification:

```
mcmcspec <- configureMCMC(Rmodel)
```

The default specification will contain a single sampler for each *stochastic, non-data* node in the model, and the samplers will be ordered by the topological dependencies of the model.

`configureMCMC()` creates an *MCMCspec* reference class object. The *MCMCspec* reference class has a number of methods, such as `addSampler()` that will be described in this Chapter.

An MCMC function corresponding to the default MCMC specification for `model` may also be created directly using the call `buildMCMC(model)`; see section 7.2 for more information.

Default assignment of sampler algorithms

The particular sampling algorithm assigned to each stochastic node is determined by the following, in order of precedence:

1. If the node has no stochastic dependents, a predictive *end* sampler is assigned. The *end* sampling algorithm merely calls `simulate()` on the particular node, since this simulates identically from the conditional posterior distribution.

2. The node is checked for presence of a conjugate relationship between its prior distribution and the distributions of its stochastic dependents. If it is determined to be in a conjugate relationship, then the corresponding *conjugate* sampler is assigned.

3. If the node is discrete-valued, then a *slice* sampler is assigned.

4. If the node is vectorized (specified using a multivariate distribution), then a single *RW_block* sampler is assigned to jointly sample all scalar components of the multivariate node. This sampler performs multi-dimensional Metropolis-Hastings random walk sampling.

5. If none of the above criteria are satisfied, then the default, scalar random walk *RW* sampler is assigned. This algorithm performs Metropolis-Hastings sampling with a normal proposal distribution.

The control parameters governing each of the default sampling algorithms are dictated by the system-level variable `controlDefaultList`. These default values are described in Section 7.5, along with the related sampling algorithms.

Additional control arguments

The following optional control arguments to `configureMCMC()` may be used to override the default assignment of sampler algorithms:

useConjugacy (default `TRUE`) If `TRUE`, conjugate samplers will be assigned to nodes determined to be in conjugate relationships. If `FALSE`, no conjugate samplers will be assigned.

onlyRW (default `FALSE`) If `TRUE`, `RW` samplers will be assigned to all non-terminal, continuous-valued stochastic nodes. Terminal stochastic nodes are still assigned `end` samplers.

onlySlice (default `FALSE`) If `TRUE`, `slice` samplers will be assigned to all non-terminal stochastic nodes. Terminal stochastic nodes are still assigned *end* samplers.

multivariateNodesAsScalars (default `FALSE`) If `TRUE`, then independent scalar random walk Metropolis-Hastings samplers (`RW`) will be assigned to all scalar components comprising multivariate nodes. This contrasts the default behavior of a single block sampler being assigned to multivariate nodes. Regardless of the value of this argument, conjugate samplers will be assigned to conjugate (scalar and multivariate nodes), provided `useConjugacy = TRUE`.

Default monitors

The default MCMC specification includes monitors on all top-level stochastic nodes of the model.

7.1.2 Customizing the MCMC specification

The MCMC specification may be customized in a variety of ways, either through additional named arguments to `configureMCMC()` or by calling member methods of an existing `MCMCspec` object.

Default samplers for particular nodes

One can create an MCMC specification with default samplers on just a particular set of nodes using the `nodes` argument to `configureMCMC()`. The value for the `nodes` argument may be a character vector, containing particular node names, or variable names. In the case of a variable name, a default sampler will be added for all stochastic nodes contained within this particular variable. The choice of the particular sampling algorithm assigned to node follows the same order of precedence described in Section 7.1.1.

If the `nodes` argument is provided, default samplers are created only for the *stochastic* nodes specified by this argument (possibly including data nodes), and the ordering of these sampling algorithms respects the ordering within the `nodes` argument. It is worthwhile to note this is the *only* way in which a sampler may be placed on a data node, which upon execution of the MCMC will overwrite any value stored in the data node.

The `nodes` argument may also be provided with the value `NULL`, `character(0)`, or `list()`, any of which will result in an MCMC specification containing no samplers.

Overriding the default sampler control list values

The default values of control list elements for all sampling algorithms may be overridden through use of the `control` argument to `configureMCMC()`, which should be a named list. Named elements in the `control` argument will be used for all default samplers added. In addition, they are retained in the `MCMCspec` object, and will be used as defaults for any subsequent samplers added to this same `MCMCspec` object. For example, the following will create the default MCMC specification, except all `RW` samplers will have their initial `scale` set to 3, and none of the samplers (*RW*, or otherwise) will be adaptive.

```
mcmcspec <- configureMCMC(Rmodel, control = list(scale = 3, adaptive = FALSE))
```

Subsequent addition of samplers for particular nodes

Once an `MCMCspec` object has been created, additional samplers may be added to the specification, by calling the `addSampler` method on the `MCMCspec` object. The mandatory `type` argument is a character string, specifying the type of sampler to be added. For example, `type = 'RW'` specifies the Metropolis-Hastings random walk sampler, and `type = 'slice'` specifies a slice sampler.

The `type` argument must specify a valid sampling algorithm, which has been generated as the result of `nimbleFunction()`. If `type = 'typeStr'` is specified, then the sampling function `sampler_typeStr` must exist. If it does not exist, an error will result.

The optional `control` argument may be used to provide a list of additional control list elements for the sampler. When the `control` argument is provided in a call to `addSampler()`, the `control` list elements specified will have the highest priority. The hierarchy of precedence for control list elements for samplers is:

1. Those supplied in the `control` list argument to `addSampler()`
2. Those supplied in the `control` list argument in the preceding preceding call to `configureMCMC()`
3. Those in the system-level `controlDefaultList` variable

Note that every sampling algorithm will require either the `targetNode` element of the `control` list, or the `targetNodes` element in the case of multivariate samplers. There is no default value for the `targetNode` element, since it reflects a property of the particular sampler, rather than the sampling algorithm.

A call to `addSampler()` results in a single instance of the specified sampler being added at end of the current sampler ordering.

Printing, re-ordering, and removing samplers

The current, ordered, list of all samplers in the MCMC specification may be printed by calling the `getSamplers()` method. Each sampler is displayed, along with the value of all control parameters, and the index corresponding to its position in the sampler ordering. These indices are useful for removing and re-ordering the samplers.

The existing samplers may be re-ordered using the `setSamplers()` method. The `ind` argument is a vector of sampler indices. The samplers in the MCMC specification will be replaced by the samplers corresponding to the indices provided. A few examples of how this may operate (all examples assume the `MCMCspec` object initially contains 10 samplers; each example call is independent of the others) are as follows:

```
## Truncate the current list of samplers to the first 5
mcmcspec$setSamplers(ind = 1:5)

## Retain only the third sampler, which will subsequently
## become the first sampler
mcmcspec$setSamplers(ind = 3)

## Reverse the ordering of the samplers
mcmcspec$setSamplers(ind = 10:1)

## The new set of samplers becomes the
## {first, first, first, second, third} from the current list.
## Upon each iteration of the MCMC, the 'first' sampler will
## be executed 3 times, however each instance of the sampler
## will be independent in terms of scale, adaptation, etc.
mcmcspec$setSamplers(ind = c(1, 1, 1, 2, 3))
```

Samplers may be removed from the current sampler ordering through use of the `removeSamplers()` method. The following examples demonstrate this usage, where again each example assumes that `mcmcspec` initially contains 10 samplers, and each example is independent of the others:

```
## Remove the first sampler
mcmcspec$removeSamplers(ind = 1)

## Remove the last five samplers
mcmcspec$removeSamplers(ind = 6:10)

## Remove all samplers,
## resulting in an empty MCMC specification, containing no samplers
mcmcspec$removeSamplers(ind = 1:10)

## Special case: providing no argument removes all samplers
mcmcspec$removeSamplers()
```

Monitors and thinning intervals

An `MCMCspec` object contains two independent lists of variables to monitor, which correspond to two independent thinning intervals: `thin` corresponding to `monitors`, and `thin2`

corresponding to `monitors2`. Monitors operate at the *variable* level. Only entire model variables may be monitored. Specifying a monitor on a *node*, e.g., `x[1]`, will result in the entire variable `x` being monitored.

The variables specified in `monitors` will be recorded (with thinning interval `thin`) into the *modelValues* object `mvSamples`, which is a member data object of the MCMC algorithm object. Likewise, the variables specified in `monitors2` will be recorded (with thinning interval `thin2`) into the *modelValues* object `mvSamples2`. See Section 7.4 for information about extracting these *modelValues* objects from the MCMC algorithm object.

Monitors may be added to the MCMC specification either in the original call to `configureMCMC()` or using the `addMonitors()` method:

```
## Using an arguments to configureMCMC()
mcmcspec <- configureMCMC(Rmodel, monitors = c('alpha', 'beta'), monitors2 = 'x')

## Calling a member method of the mcmcspec object
## This results in the same monitors as above
mcmcspec$addMonitors(c('alpha', 'beta'))
mcmcspec$addMonitors2('x')
```

Similarly, either thinning interval may be set analogously:

```
## Using an argument to configureMCMC()
mcmcspec <- configureMCMC(Rmodel, thin = 1, thin2 = 100)

## Calling a member method of the mcmcspec object
## This results in the same thinning intervals as above
mcmcspec$setThin(1)
mcmcspec$setThin2(100)
```

The current lists of monitors, and thinning intervals, may be displayed using the `getMonitors()` method. Both sets of monitors (`monitors` and `monitors2`) may be reset to empty character vectors by calling the `resetMonitors()` method.

The preceding examples can be used to motivate the practical usage of the *two* separate monitor lists and thinning intervals. Consider the circumstance where `alpha` and `beta` are scalar model variables of interest, hence we wish to record all samples, which is possible without using much computer memory or, ultimately, disk storage. The `x` variable might represent a latent matrix of non-trivial dimensions, for which we desire a sparsely thinned record of samples, so as to limit memory or disk requirements.

7.2 Building and compiling the MCMC algorithm

Once the MCMC specification object has been created, and customized to one's liking, it may be used to build an executable MCMC function. The following call uses the specification `mcmcspec` to build an instance of the MCMC function for the model:

```
Rmcmc <- buildMCMC(mcmcspec)
```

The `buildMCMC()` function accepts only a single argument, which may be an MCMC specification object created from a call to `configureMCMC()`. The resulting MCMC function, `Rmcmc`, is an instance of a NIMBLE function specific to the model on which the specification was based.

The `buildMCMC()` function is overloaded to accept NIMBLE model object as its argument. In this case, it creates an MCMC function specified by the default MCMC specification (section 7.1.1) for the model. The following two MCMC functions will be identical:

```
mcmcspec <- configureMCMC(Rmodel)    ## default MCMC specification
Rmcmc1 <- buildMCMC(mcmcspec)

Rmcmc2 <- buildMCMC(Rmodel)    ## uses the default specification for Rmodel
```

For speed of execution, we usually desire to compile the MCMC function to C++ (as is the case for other NIMBLE functions). To do so, we use `compileNimble()`. Care must be taken to perform this compilation in the same project that contains the underlying model and compiled model objects. A typical compilation call looks like:

```
Cmcmc <- compileNimble(Rmcmc, project = Rmodel)
```

Alternatively, if the model has not already been compiled, they can be compiled together in one line:

```
Cmcmc <- compileNimble(Rmodel, Rmcmc)
```

7.3 Executing the MCMC algorithm

The MCMC function (either the compiled or uncompiled version) has one required argument, `niter`, representing the number of iterations to run the MCMC algorithm. We'll assume the function is called `mcmc`. Calling `mcmc(niter)` causes the full list of samplers (as determined from the input `MCMCspec` object) to be executed `niter` times, and the monitored variables to stored into the internal *modelValues* objects as governed by the corresponding thinning intervals.

The `mcmc()` function has an optional `reset` argument. When `reset = TRUE` (the default value), the following occurs at the onset of the call to `mcmc$run()`:

- All model nodes are checked that they contain values, and that model log-probabilities are up-to-date with the current node values. If a stochastic node is missing a value, it is populated using a call to `simulate()`. The values of deterministic nodes are calculated, to be consistent with their parent nodes. If any right-hand-side-only nodes are missing a value, an error results.

- All MCMC sampler functions are reset to their initial state: the initial values of any sampler control parameters (e.g., `scale`, `sliceWidth`, or `propCov`) are reset to their initial values, as were specified by the original MCMC specification.
- The internal *modelValues* objects `mvSamples` and `mvSamples2` are each resized to the appropriate length, for holding the required number of samples (`niter/thin`, and `niter/thin2`, respectively).

The aforementioned actions have the effect of "resetting" the entire MCMC algorithm to its initial state. This (default) functionality may be thought of as initializing separate, independent chains of the same MCMC algorithm.

When `mcmc$run(niter, reset = FALSE)` is called, the MCMC algorithm effectively picks up from where it left off. No values in the model are checked or altered, and sampler functions are not reset to their initial states. Further, the internal *modelValues* objects containing samples are each *increased in size to appropriately accommodate the additional samples*. This functionality may be used when the MCMC algorithm has already been run for some number of iterations, and one wishes to continue running the MCMC, exactly from where it left off, for some additional number of iterations.

The MCMC function has a second optional argument, `simulateAll`, with default value `FALSE`. When `mcmc(niter, simulateAll = TRUE)` is called, the `simulate()` method of all stochastic nodes in the model is called, prior to beginning MCMC iterations. This behavior may be thought of as generating a new set of random, initial values for all stochastic nodes in the model. Note that there is some danger in doing this when non-informative priors (such as normal distributions with very large variances or gamma distributions with small parameter values) are used for top-level nodes, as one may easily simulate an extreme value as the starting value for a given node.

7.4 Extracting MCMC samples

Samples may be extracted in the form of *modelValues* objects, from either the uncompiled or compiled MCMC functions. Note that the *modelValues* extracted from an uncompiled MCMC function will be an uncompiled *modelValues* object, while that extracted from the compiled MCMC function will be a compiled *modelValues* object. In either case, the *modelValues* object corresponding to `monitors` and `thin` will be named `mvSamples`, and that corresponding to the `monitors2` and `thin2` will be named `mvSamples2`. These objects may be extracted from either `mcmc()` function as:

```
mvSamples <- mcmc$mvSamples
mvSamples2 <- mcmc$mvSamples2
```

Subsequently, these *modelValues* objects may be transformed into a more convenient matrix object, using the `as.matrix()` method for *modelValues* objects:

```
samplesMatrix <- as.matrix(mvSamples)
samplesMatrix2 <- as.matrix(mvSamples2)
```

The resulting `samplesMatrix` matrix objects will have the *node names* of the monitored nodes as the column names. Thus, for example, the mean of the samples for node `x` could be calculated as:

```
mean(samplesMatrix[, 'x'])
```

7.5 Sampler Algorithms provided with NIMBLE

The NIMBLE package provides a variety of sampling algorithms available for use. Any of the following samplers may be added to an MCMC specification, using the `addSampler()`. Additional sampler functions may also be written using the NIMBLE language, as discussed in Chapter 9.

We now describe the samplers which are provided with the NIMBLE package. The MCMC specification for a model generated from the following model code will serve as our example for application of all samplers.

```
code <- nimbleCode({
    a ~ dgamma(1, 1)
    b ~ dgamma(1, 1)
    p ~ dbeta(a, b)
    y1 ~ dbinom(prob = p, size = 10)
    y2 ~ dbinom(prob = p, size = 20)
})
```

7.5.1 Terminal node *end* Sampler

The *end* sampler is only appropriate for use on terminal stochastic nodes (that is, those having no stochastic dependencies). This sampler functions by calling the `simulate()` method of relevent node, then updating model probabilities, deterministic dependent nodes, and internal MCMC state variables. The application of an *end* sampler to any non-terminal node will result in invalid posterior inferences. The *end* sampler will automatically be assigned to all terminal, non-data stochastic nodes in a model by the default MCMC specification, so it is uncommon to manually assign this sampler.

The *end* sampler accepts only a single control list element:

targetNode The name of the node on which to operate. This is a required element with no default.

Example usage:

```
mcmcspec$addSampler(type = 'end',
     control = list(targetNode = 'y1'))
```

7.5.2 Scalar Metropolis-Hastings random walk *RW* sampler

The *RW* sampler executes the Metropolis-Hastings algorithm, with a normal proposal distribution. This sampler is optionally adaptive, this behavior being controlled by a control list element. When adaptive, the `scale` (proposal standard deviation) adapts throughout the course of the MCMC execution, to achieve a desirable acceptance rate. This sampler may be applied to any scalar continuous-valued stochastic model node.

The *RW* sampler accepts the following control list elements:

targetNode The name of the scalar node on which to operate. This is a required element with no default.

adaptive (default = `TRUE`) A logical argument, specifying whether or not the sampler should adapt the `scale` (proposal standard deviation) throughout the course of MCMC execution.

adaptInterval (default = 200) The interval on which to perform adaptation. Every `adaptInterval` MCMC iterations, the `RW` sampler will perform its adaptation procedure. This updates the `scale` variable, based upon the sampler's achieved acceptance rate over the past `adaptInterval` iterations.

scale (default = 1) The initial value of the normal proposal standard deviation. If `adaptive = FALSE`, `scale` will never change.

Example usage:

```
mcmcspec$addSampler(type = 'RW',
     control = list(targetNode = 'a', adaptive = FALSE, scale = 3))

mcmcspec$addSampler(type = 'RW',
     control = list(targetNode = 'b', adaptive = TRUE, adaptInterval = 200))
```

Note that because we use a simple normal proposal distribution on all nodes, negative proposals may be simulated for non-negative random variables. These will be rejected, so the only downsides to this are some inefficiency and the presence of warnings in your R session indicating `NA` or `NaN` values.

7.5.3 Multivariate Metropolis-Hastings *RW_block* sampler

The *RW_block* sampler performs a simultaneous update of one or more model nodes, using the Metropolis-Hastings algorithm with a multivarite normal proposal distribution. This sampler is optionally adaptive, which causes `scale` to adapt throughout the course of the

MCMC execution to achieve a desirable acceptance rate, and the `propCov` (multivariate normal proposal covariance matrix) to adapt to emulate the empirical covariance of the sampled nodes, calculated from the MCMC samples. In addition, the adaptation routine may be specified to *only* adapt the proposal `scale`, but not the proposal covariance matrix. This sampler may be applied to any set of continuous-valued model nodes, to any single continuous-valued multivariate model node, or to any combination thereof.

The *RW_block* sampler accepts the following control list elements:

targetNodes A character vetor of model nodes or variables, on which the multivariate sampling will operate. This is a required element with no default.

adaptive (default = `TRUE`) A logical argument, specifying whether or not the sampler should adapt the `scale` and `propCov` (multivariate normal proposal covariance matrix) throughout the course of MCMC execution. If only the `scale` should undergo adaptation, this argument should be specified as `TRUE`.

adaptScaleOnly (default = `FALSE`) A logical argument. This argument is only relevant when `adaptive = TRUE`. When this argument is `FALSE`, both `scale` and `propCov` undergo adaptation; the sampler tunes the scaling to achieve an optimal acceptance rate, and the proposal covariance to mimic that of the empirical samples. When this argument is `TRUE` and `adaptive = TRUE`, only the proposal `scale` is adapted. This allows for specification of a fixed proposal covariance matrix.

adaptInterval (default = 200) The interval on which to perform adaptation. Every `adaptInterval` MCMC iterations, the `RW_block` sampler will perform its adaptation procedure. This updates the `scale` variable, based upon the sampler's achieved acceptance rate over the past `adaptInterval` MCMC iterations, and updates the `propCov` variable towards the empirical covariance of `targetNodes`.

scale (default = 1) The initial value of the scalar multiplier for `propCov`. If `adaptive = FALSE`, `scale` will never change.

propCov (default = "identity") The initial covariance matrix for the multivariate normal proposal distribution. This element may be equal to the character string ``identity'', in which case the identity matrix of the appropriate dimension will be used for the initial proposal covariance matrix. Alternatively, this element may be provided as any positive definite matrix of the appropriate dimensions.

Example usage:

```
mcmcspec$addSampler(type = 'RW_block',
    control = list(targetNodes = c('a', 'b')))
```

7.5.4 Slice sampler

The *slice* sampler performs slice sampling of the scalar node to which it is applied. This is a particular useful sampler, since it can operate on either continuous-valued or discrete-valued scalar nodes. The slice sampler performs a "stepping out" procedure, in which the slice is iteratively expanded to the left or right by an amount `sliceWidth`. When sampling from the posterior slice, a "shrinkage" procedure is employed to improve sampling efficiency. This sampler is optionally adaptive, governed by a control list element, whereby the value of `sliceWidth` is adapted towards the observed absolute difference between successive samples.

The *slice* sampler accepts the following control list elements:

targetNode The name of the scalar node on which to operate. This is a required element with no default.

adaptive (default = `TRUE`) A logical argument, specifying whether or not the sampler will adapt the value of `sliceWidth` throughout the course of MCMC execution.

adaptInterval (default = 200) The interval on which to perform adaptation.

sliceWidth (default = 1) The initial value of the width of each slice, and also the width of the expansion during the iterative "stepping out" procedure.

sliceMaxSteps (default = 100) The maximum number of expansions which may occur during the "stepping out" procedure.

Example usage:

```
mcmcspec$addSampler(type = 'slice', control = list(targetNode = 'y1',
                                    adaptive = FALSE, sliceWidth = 3))

mcmcspec$addSampler(type = 'slice', control = list(targetNode = 'y2',
                                   adaptive = TRUE, sliceMaxSteps = 1))
```

7.5.5 Hierarchical *crossLevel* sampler

This sampler is constructed to perform simultaneous updates across two levels of stochastic dependence in the model structure. This is possible when all stochastic dependents of the top-level nodes appear in conjugate relationships. In this situation, a Metropolis-Hastings algorithm may be used, in which a multivariate normal proposal distribution is used for the top-level nodes, and the corresponding proposals for the lower-level nodes are determined using their conjugate relationships. The joint proposal for the top-level and lower-level nodes is either accepted or rejected, based upon the Metropolis-Hastings ratio.

The *crossLevel* sampler accepts the following control list elements:

topNodes A character vetor of model nodes or variables, for which the multivariate normal proposal distribution will be used. All stochastic dependents of `topNodes` must appear in conjugate relationships in the model structure. This requirement is checked at the

time of building the MCMC, and will produce an error if not satisfied. This is a required element with no default.

adaptive (default = TRUE) Logical argument, dictates the adaptation of the multivariate normal proposal distribution on `topNodes`.

adaptInterval (default = 200) The interval on which to perform adaptation.

scale (default = 1) The initial value of the scalar multiplier for `propCov`.

propCov (default = "identity") The initial covariance matrix for the multivariate normal proposal distribution. This element may be equal to the character string ``identity'', or any positive definite matrix of the appropriate dimensions.

Example usage:

```
mcmcspec$addSampler(type = 'crossLevel',
     control = list(topNodes = c('a', 'b')))
```

Note that this sampler amounts to sampling from the marginal posterior distribution of the top-level nodes, having integrated over the lower-level nodes, without having to analytically integrate over those nodes. This sampler is useful when there is strong dependence across the levels of a model that causes problems with convergence or mixing.

7.5.6 *RW_llFunction* sampler using a specified log-likelihood function

The *RW_llFunction* sampler performs a Metropolis-Hastings algorithm using a normal proposal distribution. However, the log-likelihood of the dependent nodes is calculated using a log-likelihood function (`llFunction`) which is provided as a control list element. The `llFunction` for calculating log-likelihoods must accurately produce the total log-likelihood for all stochastic dependent nodes of `targetNode`, optionally including the log-likelihood of `targetNode` itself; if not, incorrect inferences will result. This sampler is useful when the model likelihood can be directly calculated through analytical integration over latent model nodes. In this case, the log-likelihood function can be implemented as a nimbleFunction, and used to instantiate this sampler.

targetNode The name of the scalar node on which to operate. This is a required element with no default.

adaptive (default = TRUE) A logical argument, specifying whether or not the sampler should adapt the `scale` (proposal standard deviation) throughout the course of MCMC execution.

adaptInterval (default = 200) The interval on which to perform adaptation.

scale (default = 1) The initial value of the normal proposal standard deviation.

llFunction A specialized nimbleFunction, which accepts no arguments, and has return value equal to the total log-likelihood for all stochastic dependents of `topNodes`, given the current values of all model nodes. Optionally, the return value of `llFunction` may also include the log-likelihood associated with `targetNode`. This behavior is dictated by the control list element `includesTarget`. This is a required element with no default.

includesTarget Logical variable. If `TRUE`, the return value of `llFunction` must include the log-likelihood for `targetNode`. If `FALSE`, the return value of `llFunction` must not include the log-likelihood for `targetNode`. This is a required element with no default.

Example usage:

```
mcmcspec$addSampler(type = 'RW_llFunction',
    control = list(targetNode = 'p', llFunction = logLiky1y2, includesTarget = FALSE))
```

7.5.7 Conjugate samplers

Conjugate sampler functions are provided for nodes in conjugate relationships, as specified by the system-level `conjugacyRelationshipsInputList`. Conjugate samplers should not, in general, be manually added or modified by a user, since the control list requisites and syntax are lengthy, and determing conjugacy and assigning conjugate samplers is fully handled by the default MCMC specification.

In this release, conjugacies involving multivariate distributions as well as some additional conjugate relationships are not detected.

7.6 Detailed MCMC example: *litters*

The following is a self-contained full example of specifying, building, compiling, and running two MCMC algorithms. We use the *litters* example from the BUGS examples.

```
################################
##### model specification #####
################################

## define our model using BUGS syntax
litters_code <- nimbleCode({
    for (i in 1:G) {
        a[i] ~ dgamma(1, .001)
        b[i] ~ dgamma(1, .001)
        for (j in 1:N) {
            r[i,j] ~ dbin(p[i,j], n[i,j])
            p[i,j] ~ dbeta(a[i], b[i])
        }
        mu[i] <- a[i] / (a[i] + b[i])
```

```
        theta[i] <- 1 / (a[i] + b[i])
    }
})

## list of fixed constants
constants <- list(G = 2,
                  N = 16,
                  n = matrix(c(13, 12, 12, 11, 9, 10, 9,  9, 8, 11, 8, 10, 13,
                      10, 12, 9, 10,  9, 10, 5,  9,  9, 13, 7, 5, 10, 7,  6,
                      10, 10, 10, 7), nrow = 2))

## list specifying model data
data <- list(r = matrix(c(13, 12, 12, 11, 9, 10,  9, 9, 8, 10, 8, 9, 12, 9,
                11, 8, 9,  8,  9,  4, 8,  7, 11, 4, 4, 5 , 5, 3,  7, 3,
                7, 0), nrow = 2))

## list specifying initial values
inits <- list(p = matrix(0.5, nrow = 2, ncol = 16))

## build the R model object
Rmodel <- nimbleModel(litters_code,
                      constants = constants,
                      data      = data,
                      inits     = inits)


###########################################
##### MCMC specification and building #####
###########################################

## generate the default MCMC specification;
## only wish to monitor the derived quantity 'mu'
mcmcspec <- configureMCMC(Rmodel, monitors = 'mu')

## check the samplers assigned by default MCMC specification
mcmcspec$getSamplers()
## [1] RW sampler;   targetNode: a[1],  adaptive: TRUE,  adaptInterval: 200,  scale: 1
## [2] RW sampler;   targetNode: a[2],  adaptive: TRUE,  adaptInterval: 200,  scale: 1
## [3] RW sampler;   targetNode: b[1],  adaptive: TRUE,  adaptInterval: 200,  scale: 1
## [4] RW sampler;   targetNode: b[2],  adaptive: TRUE,  adaptInterval: 200,  scale: 1
## [5] conjugate_dbeta sampler;   targetNode: p[1, 1],  dependents_dbin: r[1, 1]
## [6] conjugate_dbeta sampler;   targetNode: p[1, 2],  dependents_dbin: r[1, 2]
## [7] conjugate_dbeta sampler;   targetNode: p[1, 3],  dependents_dbin: r[1, 3]
## [8] conjugate_dbeta sampler;   targetNode: p[1, 4],  dependents_dbin: r[1, 4]
```

```
## [9] conjugate_dbeta sampler;   targetNode: p[1, 5],  dependents_dbin: r[1, 5]
## [10] conjugate_dbeta sampler;   targetNode: p[1, 6],  dependents_dbin: r[1, 6]
## [11] conjugate_dbeta sampler;   targetNode: p[1, 7],  dependents_dbin: r[1, 7]
## [12] conjugate_dbeta sampler;   targetNode: p[1, 8],  dependents_dbin: r[1, 8]
## [13] conjugate_dbeta sampler;   targetNode: p[1, 9],  dependents_dbin: r[1, 9]
## [14] conjugate_dbeta sampler;   targetNode: p[1, 10],  dependents_dbin: r[1, 10]
## [15] conjugate_dbeta sampler;   targetNode: p[1, 11],  dependents_dbin: r[1, 11]
## [16] conjugate_dbeta sampler;   targetNode: p[1, 12],  dependents_dbin: r[1, 12]
## [17] conjugate_dbeta sampler;   targetNode: p[1, 13],  dependents_dbin: r[1, 13]
## [18] conjugate_dbeta sampler;   targetNode: p[1, 14],  dependents_dbin: r[1, 14]
## [19] conjugate_dbeta sampler;   targetNode: p[1, 15],  dependents_dbin: r[1, 15]
## [20] conjugate_dbeta sampler;   targetNode: p[1, 16],  dependents_dbin: r[1, 16]
## [21] conjugate_dbeta sampler;   targetNode: p[2, 1],  dependents_dbin: r[2, 1]
## [22] conjugate_dbeta sampler;   targetNode: p[2, 2],  dependents_dbin: r[2, 2]
## [23] conjugate_dbeta sampler;   targetNode: p[2, 3],  dependents_dbin: r[2, 3]
## [24] conjugate_dbeta sampler;   targetNode: p[2, 4],  dependents_dbin: r[2, 4]
## [25] conjugate_dbeta sampler;   targetNode: p[2, 5],  dependents_dbin: r[2, 5]
## [26] conjugate_dbeta sampler;   targetNode: p[2, 6],  dependents_dbin: r[2, 6]
## [27] conjugate_dbeta sampler;   targetNode: p[2, 7],  dependents_dbin: r[2, 7]
## [28] conjugate_dbeta sampler;   targetNode: p[2, 8],  dependents_dbin: r[2, 8]
## [29] conjugate_dbeta sampler;   targetNode: p[2, 9],  dependents_dbin: r[2, 9]
## [30] conjugate_dbeta sampler;   targetNode: p[2, 10],  dependents_dbin: r[2, 10]
## [31] conjugate_dbeta sampler;   targetNode: p[2, 11],  dependents_dbin: r[2, 11]
## [32] conjugate_dbeta sampler;   targetNode: p[2, 12],  dependents_dbin: r[2, 12]
## [33] conjugate_dbeta sampler;   targetNode: p[2, 13],  dependents_dbin: r[2, 13]
## [34] conjugate_dbeta sampler;   targetNode: p[2, 14],  dependents_dbin: r[2, 14]
## [35] conjugate_dbeta sampler;   targetNode: p[2, 15],  dependents_dbin: r[2, 15]
## [36] conjugate_dbeta sampler;   targetNode: p[2, 16],  dependents_dbin: r[2, 16]

## double-check our monitors, and thinning interval
mcmcspec$getMonitors()

## thin = 1: mu

## build the executable R MCMC function
mcmc <- buildMCMC(mcmcspec)

## let's try another MCMC, as well,
## this time using the crossLevel sampler for top-level nodes

## generate an empty MCMC specification
## we need a new copy of the model to avoid compilation errors
Rmodel2 <- Rmodel$newModel()
mcmcspec_CL <- configureMCMC(Rmodel2, nodes = NULL, monitors = 'mu')
```

```
## add two crossLevel samplers
mcmcspec_CL$addSampler(type = 'crossLevel',
     control = list(topNodes = c('a[1]', 'b[1]')))

## [1] crossLevel sampler;   topNodes: a[1], b[1],  adaptive: TRUE,  adaptScaleOnly: FAL

mcmcspec_CL$addSampler(type = 'crossLevel',
     control = list(topNodes = c('a[2]', 'b[2]')))

## [2] crossLevel sampler;   topNodes: a[2], b[2],  adaptive: TRUE,  adaptScaleOnly: FAL

## let's check the samplers
mcmcspec_CL$getSamplers()

## [1] crossLevel sampler;   topNodes: a[1], b[1],  adaptive: TRUE,  adaptScaleOnly: FAL
## [2] crossLevel sampler;   topNodes: a[2], b[2],  adaptive: TRUE,  adaptScaleOnly: FAL

## build this second executable R MCMC function
mcmc_CL <- buildMCMC(mcmcspec_CL)


###################################
##### compile to C++, and run #####
###################################

## compile the two copies of the model
Cmodel <- compileNimble(Rmodel)
Cmodel2 <- compileNimble(Rmodel2)

## compile both MCMC algorithms, in the same
## project as the R model object
## NOTE: at this time, we recommend compiling ALL
## executable MCMC functions together
Cmcmc <- compileNimble(mcmc, project = Rmodel)
Cmcmc_CL <- compileNimble(mcmc_CL, project = Rmodel2)

## run the default MCMC function,
## and example the mean of mu[1]
Cmcmc$run(1000)

## NULL

cSamplesMatrix <- as.matrix(Cmcmc$mvSamples)
mean(cSamplesMatrix[, 'mu[1]'])

## [1] 0.6153
```

```
## run the crossLevel MCMC function,
## and examine the mean of mu[1]
Cmcmc_CL$run(1000)

## NULL

cSamplesMatrix_CL <- as.matrix(Cmcmc_CL$mvSamples)
mean(cSamplesMatrix_CL[, 'mu[1]'])

## [1] 0.877
```

7.7 Higher level usage: MCMC Suite

This section introduces the higher level MCMC analysis capabilities of the MCMC Suite. We re-analyze the same *litters* example from Section 7.6, using an MCMC Suite. Subsequently, additional details of the Suite are given.

7.7.1 MCMC Suite example: *litters*

The following code executes the following MCMC algorithms on the *litters* example:

1. WinBUGS
2. JAGS
3. NIMBLE default specification
4. NIMBLE specification with argument `onlySlice = TRUE`
5. NIMBLE custom specification using two crossLevel samplers

```
litters_suite <- MCMCsuite(
    model = litters_code,
    constants = constants,
    data = data,
    inits = inits,
    monitors = 'mu',
    MCMCs = c('bugs', 'jags', 'nimble', 'nimble_slice', 'nimble_CL'),
    MCMCdefs = list(
        nimble_CL = quote({
            mcmcspec <- configureMCMC(Rmodel, nodes = NULL)
            mcmcspec$addSampler(type = 'crossLevel', control = list(topNodes = c('a[1]',
            mcmcspec$addSampler(type = 'crossLevel', control = list(topNodes = c('a[2]',
            mcmcspec
```

```
        })),
    plotName = 'littersSuite'
)

output <- litters_suite$output
```

7.7.2 MCMC Suite outputs

Executing the MCMC Suite generates a single `output` variable, which is a named list containing three objects, as well as several plots.

Samples

`output$samples` is a three-dimensional array, containing all MCMC samples from each algorithm. The first dimension of the `samples` array corresponds to each MCMC algorithm, and may be indexed by the name of the algorithm. The second dimension of the `samples` array corresponds to each node which was monitored, and may be indexed by the node name. The third dimension of `samples` contains the MCMC samples, and has length `niter/thin`.

Summary

The MCMC suite output contains a variety of pre-computed summary statistics, which are stored in the `output$summary` matrix. For each monitored node and each MCMC algorithm, the following default summary statistics are calculated: *mean*, *median*, *sd*, the 2.5% quantile, and the 97.5% quantile. These summary statistics are easily viewable, as:

```
litters_suite$output$summary
# , , mu[1]
#                   mean    median         sd  quant025  quant975
# bugs         0.8795868 0.8889000 0.04349589 0.7886775 0.9205025
# jags         0.8872778 0.8911989 0.02911325 0.8287991 0.9335317
# nimble       0.8562232 0.8983763 0.12501395 0.4071524 0.9299781
# nimble_slice 0.8975283 0.9000483 0.02350363 0.8451926 0.9367147
# nimble_CL    0.8871314 0.8961146 0.05243039 0.7640730 0.9620532
#
# , , mu[2]
#                   mean    median         sd  quant025  quant975
# bugs         0.7626974 0.7678000 0.04569705 0.6745975 0.8296025
# jags         0.7635539 0.7646913 0.03803033 0.6824946 0.8313314
# nimble       0.7179094 0.7246935 0.06061116 0.6058669 0.7970130
# nimble_slice 0.7665562 0.7683093 0.04051432 0.6641368 0.8350716
# nimble_CL    0.7605938 0.7655945 0.09138471 0.5822785 0.9568195
```

Timing

`output$timing` contains a named vector of timing information for each algorithm, and the compile time for NIMBLE (in minutes).

Plots

Executing the MCMC Suite provides and saves several plots. These include traceplots and posterior density plots for each monitored node, under each algorithm.

Note that the generation of MCMC Suite plots *specifically in Rstudio* may result in several warning messages from R (regarding graphics devices), but will function without any problems.

7.7.3 Custom arguments to MCMC Suite

An MCMC Suite is highly customizable, in terms of all of the following:

- Nodes to monitor
- Number of MCMC iterations
- Thinning interval
- Burn-in
- Summary statistics
- MCMC algorithms

argument: `monitors`

Character vector specifying the nodes and/or vectors to monitor.

argument: `niter`

Integer specifying the number of MCMC iterations to run.

argument: `thin`

Integer specifying the thinning interval.

argument: `burnin`

Integer specifying the number of samples to discard from all chains of MCMC samples. Samples are discarded prior to thinning.

argument: `summaryStats`

A character vector, providing the name of any function which operates on a numeric vector, and returns a numeric scalar. Likewise, a character string defining such a function is admissible, for example `'function(x) mean(abs(x))'`. The default value for `summaryStats` is the set: `mean`, `median`, `sd`, the 2.5% quantile, and the 97.5% quantile.

argument: `MCMCs`

A character vector, defining the MCMC algorithms to run. The default value for MCMCs includes the following algorithms:

`'bugs'` The standard WinBUGS algorithm

`'jags'` The standard JAGS algorithm

`'nimble'` NIMBLE using the default specification

`'nimble_RW'` NIMBLE using the default specification with `onlyRW = TRUE`

`'nimble_slice'` NIMBLE using the default MC specification with `onlySlice= TRUE`

The names of additional, custom, MCMC algorithms may also be provided in the `MCMCs` argument, so long as these custom algorithms are defined in the `MCMCdefs` argument. An example of this usage was given with the `crossLevel` algorithm in the *litters* MCMC Suite example.

argument: `MCMCdefs`

A named list of definitions, for any custom MCMC algorithms specified in the `MCMCs` argument. If `MCMCs` specified an algorithm called `'myMCMC'`, then `MCMCdefs` must contain an element named `'myMCMC'`. The contents of this element must be a block of code that, when executed, returns the desired MCMC specification object. This block of code may assume the existence of the R model object, `Rmodel`. Further, this block of code need not worry about adding monitors to the MCMC specification; it need only specify the samplers.

As a final important point, execution of this block of code must *return* the MCMC specification object. Therefore, elements supplied in the `MCMCdefs` argument should usually take the form:

```
MCMCdefs = list(
     myMCMC = quote({
          mcmcspec <- configureMCMC(Rmodel, ....)
          mcmcspec$addSampler(.....)
          mcmcspec     ## returns the MCMC specification object
     })
)
```

argument: `bugs_directory`

A character string giving the path to the directory containing the WinBUGS executable. The default value is `'C:/WinBUGS14'`.

argument: `bugs_program`

A character string giving the name of the WiBUGS program to execute. This will be passed directly to the `bugs()` function. The default value is `'WinBUGS'`.

argument: `makePlot`

A logical specifying whether to generate the traceplots and posterior density plots. Default value is `TRUE`.

argument: `savePlot`

A logical specifying whether to save the generated plots. Only used if `makePlot = TRUE`. Default value is `TRUE`.

argument: `plotName`

A character string giving the filename for saving plots. Only used if `savePlot = TRUE`. Default value is `'MCMCsuite'`.

7.8 Advanced topics

7.8.1 Custom sampler functions

The following code illustrates how a NIMBLE developer would concisely implement, and instantiate a Metropolis-Hastings random walk sampler with fixed proposal standard deviation. The comments accompanying the code explain the necessary characteristics of all sampler functions.

```
## the names of sampler functions must begin with 'sampler_'.
## the name of this sampler function, for the purposes of
## adding it to MCMC specifications, will be 'myRW'
sampler_myRW <- nimbleFunction(

    ## sampler functions must contain 'sampler_BASE'
    contains = sampler_BASE,

    ## sampler functons must have exactly these setup arguments:
    ## model, mvSaved, control
    setup = function(model, mvSaved, control) {
        ## first, extract the control list elements, which will
```

```
        ## dictate the behavior of this sampler.
        ## the setup code will be later processed to determine
        ## all named elements extracted from the control list.
        ## these will become the required elements for any
        ## control list argument to this sampler, unless they also
        ## appear in the system-level variable 'controlDefaultList'

        ## the name of the scalar node which we'll sample
        targetNode <- control$targetNode

        ## the random walk proposal standard deviation
        scale <- control$scale

        ## determine the list of all dependent nodes,
        ## up to the first layer of stochastic nodes, generally
        ## called 'calcNodes'.  The values, inputs, and logProbs
        ## of these nodes will be retrieved and/or altered
        ## by this algorithm.
        calcNodes <- model$getDependencies(targetNode)
    },

    ## the run function must accept no arguments, execute
    ## the sampling algorithm, leave the modelValues object
    ## 'mvSaved' as an exact copy of the updated values in model,
    ## and have no return value.  initially, mvSaved contains
    ## an exact copy of the values and logProbs in the model.
    run = function() {

        ## extract the initial model logProb
        model_lp_initial <- getLogProb(model, calcNodes)

        ## generate a proposal value for targetNode
        proposal <- rnorm(1, model[[targetNode]], scale)

        ## store this proposed value into targetNode.
        ## notice the double assignment operator, `<<-`,
        ## necessary because 'model' is a persistant member
        ## data object of this sampler.
        model[[targetNode]] <<- proposal

        ## calculate targetNode_logProb, propogate the
        ## proposed value through any deterministic dependents,
        ## and calculate the logProb for any stochastic
        ## dependnets.  The total (sum) logProb is returned.
```

```
        model_lp_proposed <- calculate(model, calcNodes)

        ## calculate the log Metropolis-Hastings ratio
        log_MH_ratio <- model_lp_proposed - model_lp_initial

        ## Metropolis-Hastings step: determine whether or
        ## not to accept the newly proposed value
        u <- runif(1, 0, 1)
        if(u < exp(log_MH_ratio)) jump <- TRUE
        else                      jump <- FALSE

        ## if we accepted the proposal, then store the updated
        ## values and logProbs from 'model' into 'mvSaved'.
        ## if the proposal was not accepted, restore the values
        ## and logProbs from 'mvSaved' back into 'model'.
        if(jump) nimCopy(from = model, to = mvSaved, row = 1,
                         nodes = calcNodes, logProb = TRUE)
        else     nimCopy(from = mvSaved, to = model, row = 1,
                         nodes = calcNodes, logProb = TRUE)
    },

    ## sampler functions must have a member method 'reset',
    ## which takes no arguments and has no return value.
    ## this function is used to reset the sampler to its
    ## initial state.  since this sampler function maintains
    ## no internal member data variables, reset() needn't
    ## do anything.
    methods = list(
        reset = function () {}
    )
)

## now, assume the existence of an R model object 'Rmodel',
## which has a scalar-valued stochastic node 'x'

## create an MCMC specification with no sampler functions
mcmcspec <- configureMCMC(Rmodel, nodes = NULL)

## add our custom-build random walk sampler on node 'x',
## with a fixed proposal standard deviation = 0.1
mcmcspec$addSampler(type = 'myRW',
     control = list(targetNode = 'x', scale = 0.1))

Rmcmc <- buildMCMC(mcmcspec)   ## etc...
```

Chapter 8

Other algorithms provided by NIMBLE

In v0.3-1, the NIMBLE algorithm library is quite limited beyond MCMC. It includes some basic utilities for calculating and simulating sets of nodes. And it includes a couple of algorithms, particle filters and MCEM, that illustrate the kind of programming with models that can be done with NIMBLE.

8.1 Basic Utilities

8.1.1 `simNodes`, `calcNodes`, and `getLogProbs`

`simNodes`, `calcNodes` and `getLogProb` are basic nimbleFunctions that simulate, calculate, or get the log probabilities (densities), respectively, of the same set of nodes each time they are called. Each of these takes a model and a character string of node names as inputs. If `nodes` is left blank, then all the nodes of the model are used.

For `simNodes`, the nodes provided are topologically sorted to simulate in the correct order. For `calcNodes` and `getLogProb`, the nodes are sorted and dependent nodes are included. Recall that the calculations must be up to date (from a calculate call) for `getLogProb` to return the values you are probably looking for.

```
simpleModelCode <- nimbleCode({
  for(i in 1:4){
    x[i] ~ dnorm(0,1)
    y[i] ~ dnorm(x[i], 1) #y depends on x
    z[i] ~ dnorm(y[i], 1) #z depends on y
    #z conditionally independent of x
  }
})

simpleModel <- nimbleModel(simpleModelCode)
cSimpleModel <- compileNimble(simpleModel)
```

```
#simulates all the x's and y's
rSimXY <- simNodes(simpleModel, nodes = c('x', 'y') )

#calls calculate on x and its dependents (y, but not z)
rCalcXDep <- calcNodes(simpleModel, nodes = 'x')

#calls getLogProb on x's and y's
rGetLogProbXDep <- getLogProbNodes(simpleModel,
                   nodes = 'x')

#compiling the functions
cSimXY <- compileNimble(rSimXY, project = simpleModel)
cCalcXDep <- compileNimble(rCalcXDep, project = simpleModel)
cGetLogProbXDep <- compileNimble(rGetLogProbXDep,
                           project = simpleModel)

cSimpleModel$x

## [1] NA NA NA NA

cSimpleModel$y

## [1] NA NA NA NA

#simulating x and y
cSimXY$run()

## NULL

cSimpleModel$x

## [1] -1.1992  0.6332  1.4244 -0.9829

cSimpleModel$y

## [1] -3.27693  1.11549  1.67456 -0.08521

cCalcXDep$run()

## [1] -12.48

#Gives correct answer because logProbs
#updated by 'calculate' after simulation
cGetLogProbXDep$run()

## [1] -12.48
```

```
cSimXY$run()

## NULL

#Gives old answer because logProbs
#not updated after 'simulate'
cGetLogProbXDep$run()

## [1] -12.48

cCalcXDep$run()

## [1] -12.67
```

8.1.2 simNodesMV, calcNodesMV, and getLogProbsMV

There is a similar trio of nimbleFunctions that does each job repeatedly for different rows of a modelValues object. For example, `simNodesMV` will simulate in the model multiple times and record each simulation in a row of its modelValues. `calcNodesMV` and `getLogProbsMV` iterate over the rows of a modelValues, copy the nodes into the model, and then do their job of calculating or collecting log probabilities (densities), respectively. Each of these returns a numeric vector with the summed log probabilities of the chosen nodes from each each row. `calcNodesMV` will save the log probabilities back into the modelValues object if `saveLP == TRUE`, a run-time argument.

Here are some examples:

```
mv <- modelValues(simpleModel)
rSimManyXY <- simNodesMV(simpleModel, nodes = c('x', 'y'), mv = mv)
rCalcManyXDeps <- calcNodesMV(simpleModel, nodes = 'x', mv = mv)
rGetLogProbMany <- getLogProbNodesMV(simpleModel,
                    nodes = 'x', mv = mv)

cSimManyXY <- compileNimble(rSimManyXY, project = simpleModel)
cCalcManyXDeps <- compileNimble(rCalcManyXDeps, project = simpleModel)
cGetLogProbMany <- compileNimble(rGetLogProbMany, project = simpleModel)

cSimManyXY$run(m = 5) # simulating 5 times

## NULL

cCalcManyXDeps$run(saveLP = TRUE) # calculating

## [1] -10.49 -13.98 -11.72 -12.75 -10.49

cGetLogProbMany$run() #

## [1] -10.49 -13.98 -11.72 -12.75 -10.49
```

8.2 Particle filter

NIMBLE includes an algorithm for a basic particle filter to be used for approximating the log likelihood of a state-space model. At this time, the particle filter only works with scalar states. A particle filter can be built around such a model by a call to `buildParticleFilter`. This nimbleFunction requires setup arguments `model` and `orderedNodeVector`, which is the properly ordered set of state nodes. Once this function is compiled, parameter values to the C-model should be set and then the particle filter can be run by specifying the number of particles.

Here is an example, using a linear state-space model for which we can easily calculate the likelihood using the Kalman Filter to verify if the particle filter seems to be working.

```
# Building a simple linear state-space model.
# x is latent space, y is observed data
timeModelCode <- nimbleCode({
  x[1] ~ dnorm(mu_0, 1)
        y[1] ~ dnorm(x[1], 1)
        for(i in 2:t){
                x[i] ~ dnorm(x[i-1] * a + b, 1)
                y[i] ~ dnorm(x[i] * c, 1)
        }

        a ~ dunif(0, 1)
        b ~ dnorm(0, 1)
        c ~ dnorm(1,1)
        mu_0 ~ dnorm(0, 1)
})

#simulate some data
t = 25; mu_0 = 1
x = rnorm(1 ,mu_0, 1)
y = rnorm(1, x, 1)
a = 0.5; b = 1; c = 1
for(i in 2:t){
        x[i] = rnorm(1, x[i-1] * a + b, 1)
        y[i] = rnorm(1, x[i] * c, 1)
}
## build and compile the model
rTimeModel <- nimbleModel(timeModelCode, constants = list(t = t), data = list(y = y) )
cTimeModel <- compileNimble(rTimeModel)

#Ordered list of hidden nodes. Equivalent to xTimeModel$expandNodeNames('x[1:t]')
xNodes = paste0('x[', 1:t, ']')

#Build the particle filter
```

```
rPF <- buildParticleFilter(rTimeModel, xNodes)
cPF = compileNimble(rPF,project = rTimeModel)

#Set parameter values
cTimeModel$mu_0 = 1
cTimeModel$a = 0.5
cTimeModel$b = 1
cTimeModel$c = 1
cTimeModel$mu_0 = 1

#Run particle filter with
#5000 particles
cPF$run(m = 5000)

## [1] -38.61
```

8.3 Monte Carlo Expectation Maximization (MCEM)

Suppose we have a model with missing data (or a layer of latent variables that can be treated as missing data) and we would like to maximize the marginal likelihood of the model, integrating over the missing data. A brute-force method for doing this is MCEM. This is an EM algorithm in which the missing data are simulated via Monte Carlo (often MCMC, when the full conditional distributions cannot be directly sampled from) at each iteration. MCEM can be slow, and there are other methods for maximizing marginal likelihoods that can be implemented in NIMBLE. The reason we started with MCEM is to explore the flexibility of NIMBLE and illustrate the combination of R and NIMBLE involved, with R managing the highest-level processing of the algorithm and calling nimbleFunctions for computations.

We will revisit the *pump* example to illustrate the use of NIMBLE's MCEM algorithm.

```
pumpMCEM <- buildMCEM(model = newPump,
                      latentNodes = 'theta',
                      burnIn = 100,
                      mcmcControl = list(adaptInterval = 20),
                      boxConstraints = list( list( c('alpha', 'beta'),
                          limits = c(0, Inf) ) ),
                      buffer = 1e-6)
```

The first argument, `model`, is a NIMBLE model, which can be either the uncompiled or compiled version. At the moment, the model provided cannot be part of another MCMC sampler.

The `latentNodes` argument should indicate the nodes that will be integrated over (sampled via MCMC), rather than maximized. These nodes must be stochastic, not deterministic! `latentNodes` will be expanded as described in section 6.4.1: e.g., either `latentNodes = 'x'`

or `latentNodes = c('x[1]', 'x[2]')` will treat `x[1]` and `x[2]` as latent nodes if `x` is a vector of two values. All other non-data nodes will be maximized over. Note that `latentNodes` can include discrete nodes, but the nodes to be maximized cannot.

The `burnIn` argument indicates the number of samples from the MCMC for the E-step that should be discarded when computing the expected likelihood in the M-step. Note that `burnIn` can be set to values lower than in standard MCMC computations, as each iteration will start off where the last left off.

The `mcmcControl` argument will be passed to `configureMCMC()` to define the MCMC to be used.

The MCEM algorithm allows for box constraints on the nodes that will be optimized, specified via the `boxConstraints` argument. This is highly recommended for nodes that have zero density on parts of the real line[1] Each constraint given should be a list in which the first element is the names of the nodes or variables that the constraint will be applied to and the second element is a vector of length 2, in which the first value is the lower limit and the second is the upper limit. Values of `Inf` and `-Inf` are allowed. If a node is not listed, it will be assumed that there are no constraints. These arguments are passed as `lower` and `upper` to R's `optim()` function, using `method = 'L-BFGS-B'`)

The value of the `buffer` argument shrinks the `boxConstraints` by this amount. This can help protect against non-finite values occuring when a parameter is on its boundary value.

Once the MCEM has been built for the model of interest using `buildMCEM()`, it can be run as follows.

```
pumpMCEM(maxit = 20, m1 = 250, m2 = 500)

##  alpha   beta
## 0.8419 1.3189

pumpMCEM(maxit = 50, m1 = 1000, m2 = 5000)

##  alpha   beta
## 0.8242 1.2696
```

There are three run-time arguments:

The `maxit` argument is the number of total iterations to run the algorithm. More advanced MCEM algorithms have a stopping criteria based on computing the MCMC error. Our current draft implementation of the algorithm merely runs `maxit` iterations and then terminates.

Halfway through the algorithm, the sample size used for the E-step switches from `m1` to `m2`. This provides smaller MCMC error as the algorithm converges. If `m1` or `m2` is less than or equal to `burnIn` as defined in `build_MCEM`, the MCEM algorithm will immediately quit.

When using the MCEM algorithm, we suggest first starting with small values of `m1` and `m2` to get an estimate of how long the algorithm will take for larger MCMC samples. The speed of the algorithm will be linear in `m2` (assuming that $m1 > m2$ as intended).

[1] Currently NIMBLE is not able to determine this automatically.

Chapter 9

Programming with models

9.1 Writing nimbleFunctions

When you write an R function, you say what the input arguments are, you provide the code for execution, and in that code you give the returned value[1]. Using the `function` keyword in R triggers the operation of creating an object that is the function.

Creating nimbleFunctions is a little more complicated because there are two kinds of code and two steps of execution:

1. `Setup` code is provided as a regular R function, but the programmer does not control what it returns. Normally the inputs to `setup` code are objects like a model, a vector of nodes, a modelValues object or modelValuesSpec, or another nimbleFunction. The `setup` code, as its name implies, sets up information for run-time code. It is executed in R, so it can use any aspect of R.

2. `Run` code is provided in the NIMBLE language. This is similar to a narrow subset of R, but it is important to remember that it is different and much more limited. `Run` code can use the objects created by the `setup` code. In addition, some information on variable types must be provided for input arguments, the return object, and in some circumstances for local variables. There are two kinds of `run` code:

   (a) There is always a primary function, given as an argument called `run`[2].

   (b) There can optionally be other functions, or `methods` in the language of object-oriented programming, that share the same objects created by the `setup` function.

To fix ideas, here is a small example to illustrate the two steps of executing a nimbleFunction:

```
logProbCalcPlus <- nimbleFunction(
    setup = function(model, node) {
        dependentNodes <- model$getDependencies(node)
```

[1] normally the value of the last evaluated code, or the argument to return().

[2] This can be empty, but why do that?

```
        valueToAdd <- 1
    },

    run = function(P = double(0)) {
        model[[node]] <<- P + valueToAdd
        return(calculate(model, dependentNodes))
        returnType(double(0))
    })

code <- nimbleCode({
    a ~ dnorm(0, 1); b ~ dnorm(a, 1)
})
testModel <- nimbleModel(code)
logProbCalcPlusA <- logProbCalcPlus(testModel, 'a')
testModel$b <- 1.5
logProbCalcPlusA$run(0.5)

## [1] -2.963

testModel$a  ## a was set to 0.5 + valueToAdd

## [1] 1.5
```

The call to the R function called `nimbleFunction` returns a function, similarly to defining a function in R. That function, `logProbCalcPlus`, takes arguments for its `setup` function, executes it, and returns an object, `logProbCalcPlusA`, that has a *run* member function (method) accessed by `$run`. In this case, the `setup` function obtains the stochastic dependencies of the `node` using the `getDependencies` member function of the model (see 6.6.2) and stores them in `dependentNodes`. In this way, `logProbCalcPlus` can adapt to any model. It also creates a variable, `valueToAdd`, that can be used by the nimbleFunction.

The object `logProbCalcPlusA`, returned by `logProbCalcPlus`, is permanently bound to the results of the processed `setup` function. In this case, `logProbCalcPlusA$run` takes a scalar input value, `P`, assigns `P + valueToAdd` to the given node in the model, and returns the sum of the log probabilities of that node and its stochastic dependencies[3]. We say `logProbCalcPlusA` is "specialized" or "bound" to the node `a` and the model `Rmodel`. Usually, the `setup` code will be where information about the model structure is determined, and then the `run` code can use that information without redundantly recomputing it. A nimbleFunction can be called repeatedly, each time returning a specialized nimbleFunction.

Readers familiar with object-oriented programming may find it useful to think in terms of class definitions and objects. nimbleFunction creates a class definition. Each specialized nimbleFunction is one object in the class. The setup arguments are used to define member data in the object.

[3]Note the use of the global assignment operator to assign into the model. This is necessary for assigning into variables from the `setup` function, at least if you want to void warnings from R. These warnings come from R's reference class system.

9.2 Using and compiling nimbleFunctions

To compile the nimbleFunction, together with its model, we use `compileNimble`:

```
CnfDemo <- compileNimble(testModel, logProbCalcPlusA)
CtestModel <- CnfDemo$testModel
ClogProbCalcPlusA <- CnfDemo$logProbCalcPlusA
```

These have been initialized with the values from their uncompiled versions and can be used in the same way:

```
CtestModel$a      ## values were initialized from testModel

## [1] 1.5

CtestModel$b

## [1] 1.5

lpA <- ClogProbCalcPlusA$run(1.5)
lpA

## [1] -5.463

## verify the answer:
dnorm(CtestModel$b, CtestModel$a, 1, log = TRUE) +
    dnorm(CtestModel$a, 0, 1, log = TRUE)

## [1] -5.463

CtestModel$a       ## a was modified in the compiled model

## [1] 2.5

testModel$a        ## the uncompiled model was not modified

## [1] 1.5
```

9.2.1 Accessing and modifying numeric values from setup

While models and nodes created during `setup` cannot be modified[4], numeric values and modelValues (see below) can be. For example:

[4] Actually, they can be, but only for uncompiled nimbleFunctions

```
logProbCalcPlusA$valueToAdd  ## uncompiled

## [1] 1

logProbCalcPlusA$valueToAdd <- 2
ClogProbCalcPlusA$valueToAdd  ## or compiled

## [1] 1

ClogProbCalcPlusA$valueToAdd <- 3
ClogProbCalcPlusA$run(1.5)

## [1] -16.46

CtestModel$a     ## a == 1.5 + 3

## [1] 4.5
```

9.3 Compiling numerical operations with no model: omitting `setup` code

The `setup` function is optional. If it is omitted, then `nimbleFunction` is more like `function`: it simply returns a function that can be executed and compiled. If there is no `setup` code, there is no specialization step. This is useful for doing math or the other kinds of processing available in NIMBLE when no model or modelValues is needed.

```
solveLeastSquares <- nimbleFunction(
    run = function(X = double(2), y = double(1)) {
        ans <- inverse(t(X) %*% X) %*% (t(X) %*% y)
        return(ans)
        returnType(double(2))
    } )

X <- matrix(rnorm(400), nrow = 100)
y <- rnorm(100)
solveLeastSquares(X, y)

##           [,1]
## [1,] -0.06953
## [2,] -0.02701
## [3,] -0.11505
## [4,] -0.07602
```

```
CsolveLeastSquares <- compileNimble(solveLeastSquares)
CsolveLeastSquares(X, y)

##           [,1]
## [1,] -0.06953
## [2,] -0.02701
## [3,] -0.11505
## [4,] -0.07602
```

This example shows the textbook calculation of a least squares solution for regression of 100 data points on 4 explanatory variables, all generated randomly. Such functions can be called from other nimbleFunctions. In the near future, they will be able to be used in BUGS code.[5]

When specifying a run-time member of a nimbleFunction, you need to specify the types of arguments and return values, described more below. Since nimbleFunctions take arguments by reference, they may modify their arguments. However, the R interface to a nimbleFunction performs a copy to protect the original R argument from modification. If you want to see arguments – potentially modified – as well as any return value, you can modify the `control` argument to compileNimble to include "`returnAsList = TRUE`". Then the returned object will be a list with the nimbleFunction's return value as the last element.

If one wants a nimbleFunction that does get specialized but has empty setup code, use `setup = function() {}` or `setup = TRUE`.

9.4 Useful tools for `setup` functions

The setup function is used to determine information on nodes in a model, set up any modelValues objects, set up any nimbleFunctions or nimbleFunctionLists, and set up any persistent numeric objects. The values of numeric objects created in `setup` will persist across calls to the specialized nimbleFunction.

Some of the useful tools and objects to create in `setup` functions include

vectors of node names Often these are obtained from the `getNodeNames` and `getDependencies` methods of a model, described in section 6.6.1.

modelValues objects These are discussed more below.

specializations of other nimbleFunctions A useful NIMBLE programming technique is to have one nimbleFunction contain other nimbleFunctions, which it can use in its run-time code.

lists of other nimbleFunctions In addition to containing single other nimbleFunctions, a nimbleFunction can contain a list of other nimbleFunctions, all defined with run-time

[5] On the machine this is being written on, the compiled version runs a few times faster than the uncompiled version. However we refrain from formal speed tests because have not, for example, optimized the BLAS & LAPACK available for R.

functions that use the same types of arguments and return values. These are discussed more below.

9.4.1 Control of `setup` outputs

Sometimes `setup` code may create variables that are not used in run-time code. By default, NIMBLE inspects run-time code and omits variables from `setup` that do not appear in run-time code from compilation. However, sometimes a programmer may want to force a numeric variable to be created in compilation, even if it is not used directly in run-time code. As shown below, such variables can be directly accessed in one nimbleFunction from another, and this provides a way of using nimbleFunctions as general data structures. To force NIMBLE to keep one or more numeric variables around during compilation, for example `X` and `Y`, simply include

```
setupOutputs(X, Y)
```

anywhere in the `setup` code.

9.5 NIMBLE language components

9.5.1 Basics

There are several general points that will be useful before describing the NIMBLE language in more detail.

- NIMBLE language functions are not R functions. In many cases we have used syntax identical or nearly so to R, and in most cases we have provided a matching R function, but it is important not to confuse the NIMBLE language definition with the behavior of the corresponding R function.
- NIMBLE language functions do not as a rule have named arguments, but some do.
- Like R, NIMBLE uses 1-based indexing. For example, the first element of a vector `x` is `x[1]`, not `x[0]`.
- To a large extent, NIMBLE functions can be executed in R (uncompiled) or can be compiled. Using them in R will be slow, and is intended for testing and debugging algorithm logic. At this time, the behavior in R will come close but will not perfectly match the behavior of the compiled function. We will try to note known differences in what follows.
- NIMBLE is the opposite of R for argument passing. R nearly always uses pass-by-value. NIMBLE nearly always uses pass-by-reference (or pointer). Thus it is possible to write a nimbleFunction that returns information by modifying an argument. That is one important behavior that is not yet implemented in R execution of nimbleFunctions.

- To understand NIMBLE compilation, it is helpful to know that anything labeled with a character string in R is resolved during NIMBLE compilation rather than being turned into a character string in C++. For example, model[[node]], if node == 'x', will access the variable 'x' in the model. However, this pairing of the model and node are resolved during compilation so that the C++ code makes direct access to the 'x' object without looking it up by the character string 'x' every time the code is executed. That means, for example, that model[[node[i]]] will not work, because it would take more work to resolve that during compilation. We intend to make that work in the future – a good example of a loose end in v0.3-1 – but for now it doesn't.

- BUGS model nodes are implemented as nimbleFunctions with member functions for `calculate`, `simulate`, and `getLogProb`. There are also member functions for obtaining the value of each parameter or alternative parameters (e.g. rate = 1/scale). Because we build BUGS models using the NIMBLE language, we anticipate it will be possible to allow BUGS models to call nimbleFunctions, and for new distributions to be defined using nimbleFunctions. In v0.3-1, we have not made that work yet.

9.5.2 Driving models: calculate, simulate, and getLogProb

These three functions are the primary ways to operate a model. Their syntax was explained in section 6.4. For calculate and simulate, it is usually important for the `nodes` object to be created in `setup` code such that they are sorted in topological order.

9.5.3 Accessing model and modelValues variables and using `copy`

The `modelValues` structure was introduced in section 6.7. Inside nimbleFunctions, modelValues are designed to easily save values from a model object during the running of a nimbleFunction. To access a modelValues object inside of a NIMBLE function, the object must exist in the setup code, either by passing the modelValues object in as a setup argument or creating the object in the setup code.

To illustrate this, we will create a nimbleFunction for computing importance weights for importance sampling. This function will use two modelValues objects. `propModelValues` will contain a set of values simulated from the importance sampling distribution and a field `propLL` for their log probabilities (densities). `savedWeights` will contain the difference in log probability (density) between the model and the `propLL` value provided for each set of values.

```
## Accepting modelValues as a setup argument
setupFunction = function(propModelValues, model){
    ## Building a modelValues in the setup function
    savedWeightsSpec <- modelValuesSpec(vars = 'w',
                                        types = 'double',
                                        sizes = 1)
    savedWeights <- modelValues(spec = savedWeightsSpec)
    ## List of nodes to be used in run function
```

```
    modelNodes <- model$getNodeNames(stochOnly = TRUE,
                                     includeData = FALSE)
}
```

The simplest way to pass values back and forth between models and modelValues inside of a nimbleFunction is with `nimCopy`, which has the synonym `copy`. This takes arguments

`from, to` which can either be models or modelValues

`row, rowTo` which refers to the rows of a modelValues object, if either `from` or `to` is a modelValues. If `rowTo` is omitted, it is assumed to be equal to `row` if necessary.

`nodes, nodesTo` which is a vector of the names of the nodes to be copied. The node names will be expanded when variable names are provided. If `nodesTo` is omitted it will be set equal to `nodes`.

Alternatively, the values may be accessed via indexing of individual rows, using the notation `mv[var, i]`, where `mv` is a modelValues object, `var` is a variable name (not a node name), and `i` is a row number. Likewise, the `getsize` and `resize` functions can be used as discussed previously. However the function `as.matrix` does not work in the NIMBLE language.

Here is a run-time function to use these modelValues:

```
runFunction = function(){
    ## gets the number of rows of propSamples
    m <- getsize(propModelValues)

    ## resized savedWeights to have the proper rows
    resize(savedWeights, m)
    for(i in 1:m){
        ## Copying from propSamples to model.
        ## Node names of propSamples and model must match!
        nimCopy(from = propModelValues, to = model, row = i,
                nodes = modelNodes, logProb = FALSE)
        ## calculates the log likelihood of the model
        targLL <- calculate(model)
        ## retreaves the saved log likelihood from the proposed model
        propLL <- propModelValues['propLL',i][1]
        ## saves the importance weight for the i-th sample
        savedWeights['w', i][1] <<- exp(targLL - propLL)
    }
    ## does not return anything
}
```

Once the nimbleFunction is built, the modelValues object can be accessed using using `$`, which is shown in more detail below. In fact, since modelValues, like most NIMBLE objects,

are reference class objects, one can get a reference to them before the function is executed and then use that reference afterwards.

```
##   Simple model and modelValue for example
targetModelCode <- nimbleCode({
    x ~ dnorm(0,1)
    for(i in 1:4)
        y[i] ~ dnorm(0,1)
})

## Code for proposal model
propModelCode <- nimbleCode({
        x ~ dnorm(0,2)
        for(i in 1:4)
                y[i] ~ dnorm(0,2)
})

## Building R models
targetModel = nimbleModel(targetModelCode)
propModel = nimbleModel(propModelCode)
cTargetModel = compileNimble(targetModel)
cPropModel = compileNimble(propModel)


sampleMVSpec = modelValuesSpec(vars = c('x', 'y', 'propLL'),
    types = c('double', 'double', 'double'),
    sizes = list(x = 1, y = 4, propLL = 1) )

sampleMV <- modelValues(sampleMVSpec)

##   nimbleFunction for generating proposal sample
PropSamp_Gen <- nimbleFunction(
    setup = function(mv, propModel){
        nodeNames <- propModel$getNodeNames()
    },
    run = function(m = integer() ){
        resize(mv, m)
        for(i in 1:m){
            simulate(propModel)
            nimCopy(from = propModel, to = mv, nodes = nodeNames, row = i)
            mv['propLL', i][1] <<- calculate(propModel)
        }
    }
    )
```

```
## nimbleFunction for calculating importance weights
## Recylcing setupFunction and runFunction as defined in earlier example
impWeights_Gen <- nimbleFunction(setup = setupFunction,
                                 run = runFunction)


## Making instances of nimbleFunctions
## Note that both functions share the same modelValues object
RPropSamp <- PropSamp_Gen(sampleMV, propModel)
RImpWeights <- impWeights_Gen(sampleMV, targetModel)

# Compiling
CPropSamp <- compileNimble(RPropSamp, project = propModel)
CImpWeights <- compileNimble(RImpWeights, project = targetModel)

#Generating and saving proposal sample of size 10
CPropSamp$run(10)

## NULL

## Calculating the importance weights and saving to mv
CImpWeights$run()

## NULL

## Retrieving the modelValues objects
## Extracted objects are C-based modelValues objects

savedPropSamp_1 = CImpWeights$propModelValues
savedPropSamp_2 = CPropSamp$mv

# Subtle note: savedPropSamp_1 and savedPropSamp_2
# both provide interface to the same compiled modelValues objects!
# This is because they were both built from sampleMV.

savedPropSamp_1['x',1]

## [1] 0.6048

savedPropSamp_2['x',1]

## [1] 0.6048

savedPropSamp_1['x',1] <- 0
savedPropSamp_2['x',1]
```

```
## [1] 0

## Viewing the saved importance weights
savedWeights <- CImpWeights$savedWeights
unlist(savedWeights[['w']])

##  [1] 0.4373 0.6318 0.2419 0.9155 0.6402 0.9237 0.4510 0.3657
##  [9] 0.9556 0.3641

#Viewing first 3 rows. Note that savedPropSsamp_1['x', 1] was altered
as.matrix(savedPropSamp_1)[1:3, ]

##      propLL       x    y[1]     y[2]    y[3]    y[4]
## [1,] -4.673  0.0000 -1.0117  0.03771 -0.5520 -0.3406
## [2,] -5.409  0.1145  1.5731 -0.06211  0.1899 -0.1402
## [3,] -3.489 -0.5080 -0.4271  0.09572  0.3552 -0.2277
```

Importance sampling could also be written using simple vectors for the weights, but we illustrated putting them in a modelValues object along with model variables.

9.5.4 Using model variables and modelValues in expressions

Each way of accessing a variable, node, or modelValues can be used amid mathematical expressions, including with indexing, or passed to another nimbleFunction as an argument. For example, the following two statements would be valid:

```
model[['x[2:8, ]']][2:4, 1:3] %*% Z
```

if Z is a vector or matrix, and

```
C[6:10] <- mv[v, i][1:5, k] + B
```

if B is a vector or matrix.

The NIMBLE language allows scalars, but BUGS models never have purely scalar nodes. Instead, a single node such as defined by `z ~ dnorm(0, 1)` is implemented as a vector of length 1, similar to R. When using z via `model$z` or `model[['z']]`, NIMBLE will try to do the right thing by treating this as a scalar. In the event of problems[6], a more explicit way to access z is `model$z[1]` or `model[['z']][1]`.

9.5.5 Getting and setting more than one model node or variable at a time

Sometimes it is useful to set a collection of nodes or variables at one time. For example, one might want a nimbleFunction that will serve as the objective function for an optimizer. The

[6] please tell us!

input to the nimbleFunction would be a vector, which should be used to fill a collection of nodes in the model before calculating their log probabilities. NIMBLE has two ways to do this, one of which was set up during development and may be deprecated in the future.

The recommended newer way is:

```
P <- values(model, nodes)
values(model, nodes) <- P
```

where the first line would assign the collection of values from nodes into P, and the second would to the inverse. In both cases, values from nodes with 2 or more dimensions are flattened into a vector in column-wise order.

The older syntax, which may be deprecated in the future, is

```
getValues(P, model, nodes)
setValues(P, model, nodes)
```

These are equivalent to the two previous lines. Note that `getValues` modifies P in the calling environment.

With the new notation, `values(model, nodes)` may appear as a vector in other expressions, e.g. `Y <- A %*% values(model, nodes) + b`.

9.5.6 Basic flow control: if-then-else, for, and while

These basic control flow structures use the same syntax as in R. However, `for`-loops are limited to sequential integer indexing. For example, `for(i in 2:5) {...}` works as it does in R. Decreasing index sequences are not allowed.

In v0.3-1, there is support for iterating over indices of a nimbleFunctionList using `seq_along` as in R. This is described below.

9.5.7 How numeric types work

Numeric types in NIMBLE are much less flexible than in R, a reflection of the fact that NIMBLE code can be compiled into C++[7]. In NIMBLE, the *type* of a numeric object refers to the number of dimensions and the numeric type of the elements. In v0.3-1, objects from 0 (scalar) to 3 dimensions are supported, and the numeric types integer and double are supported. In addition the type logical is supported for scalars only. While the number of dimensions cannot change during run-time, numeric objects can be resized using `setSize` or by full (non-indexed) assignment.

When possible, NIMBLE will determine the type of a variable for you. In other cases you must declare the type. The rules are as follows:

- For numeric variables from the `setup` function that appear in the `run` function or other member functions (or are declared in `setupOutputs`): the type is determined from the

[7] C++ is a statically typed language, which means the type of a variable cannot change.

values created by the `setup` code. Note that the types created by `setup` code must be consistent across all specializations of the nimbleFunction. For example if X is created as a matrix (2-dimensional double) in one specialization but as a vector (1-dimensional double) in another, there will be a problem during compilation. The sizes may differ in each specialization.

Treatment of vectors of length 1 presents special challenges because they could be treated as scalars or vectors. Currently they are treated as scalars. If you want a vector, ensure that the length is greater than 1 in the setup code and the use `setSize` in the run-time code.

- In `run` code, when a numeric variable is created by assignment, its type is determined by that assignment. Subsequent uses of that variable must be consistent with that type.

- If the first uses of a variable involve indexing, the type must be declared explicitly, using `declare`, before using it. In addition, its size must be set before assigning into it. Sizes can be included in the declare() statement, but if so they should not subsequently change. If a variable may have its size changed during execution, then the declare statement should omit the size argument, and a separate call to `setSize` should be used to set the initial size(s).

9.5.8 Declaring argument types and the return type

NIMBLE requires that types of arguments and a return type be explicitly declared.

The syntax for a type declaration is:

- `type(nDim, sizes)`

`type` can currently take values `double`, `integer`, or, for scalars only, `logical`. In a `returnType` statement, a type of `void()` is valid, but you won't usually include that because it is the default if no `returnType` statement is included. `nDim` is the number of dimensions, with 0 indicating scalar. `sizes` is an optional vector of fixed, known sizes. These should use R's `c` function if `nDim` > 1. If sizes are omitted, they will either be set when the entire object is assigned to, or an explicit call to `setSize` is needed.

9.5.9 Querying and changing sizes

Sizes can be queried as follows:

- `length()` behaves like R's `length()` function. It returns the *entire* length of X. That means if X is multivariate, `length` returns the product of the sizes in each dimension.

- `nimbleDim()` behaves like R's `dim()` function for matrices or arrays, and like R's `length()` function for vectors. In other words, regardless of whether the number of dimensions is 1 or more, it returns a vector of the sizes. The keyword `dim()` is a valid substitute for `nimbleDim()`, but if you use it you should recognize it behaves differently from R's `dim()`.

  - A quirky limitation in v0.3-1: It not currently possible to assign the results from `nimbleDim()` to another object using vector assignment. So the only practical way to use `nimbleDim()` is to extract elements immediately, such as `nimbleDim(X)[1]`, `nimbleDim(X)[2]`, etc.

Sizes can be changed using:

- setSize(X, sizes)

where `sizes` is a scalar if `X` is 1-dimensional and uses R's `c()` function to provide a vector of sizes if X is more than 1-dimensional.

9.5.10 Basic math and linear algebra

NIMBLE uses the *Eigen* library in C++ to accomplish linear algebra. In v0.3-1, we use a lot of Eigen's capabilities, but not all of them. The supported operations are given in tables 5.3-5.4.

No vectorized operations other than assignment are supported for more than two dimensions in v0.3-1. That means `A = B + C` will work only if B and C have dimensions $\leq$ 2.

Managing dimensions and sizes: asRow, asCol, and dropping dimensions

It can be tricky to determine the dimensions returned by a linear algebra expression. As much as possible, NIMBLE behaves like R, but in some cases this is not possible because R uses run-time information while NIMBLE must determine dimensions at compile-time.

Suppose v1 and v2 are vectors, and M1 is a matrix. Then

- `v1 + M1` generates a compilation error unless one dimension of M1 is known at compile-time to be 1. If so, then v1 is promoted to a 1-row or 1-column matrix to conform with M1, and the result is a matrix of the same sizes. This behavior occurs for all component-wise binary functions.
- `v1 %*% M1` defaults to promoting v1 to a 1-row matrix, unless it is known at compile-time that M1 has 1 row, in which case v1 is promoted to a 1-column matrix.
- `M1 %*% v1` defaults to promoting v1 to a 1-column matrix, unless it is known at compile time that M1 has 1 column, in which case v1 is promoted to a 1-row matrix.
- `v1 %*% v2` promotes v1 to a 1-row matrix and v2 to a 1-column matrix, so the returned values is a 1x1 matrix with the inner product of v1 and v2.
- `asRow(v1)` explicitly promotes v1 to a 1-row matrix. Therefore `v1 %*% asRow(v2)` gives the outer product of v1 and v2.
- `asCol(v1)` explicitly promotes v1 to a 1-column matrix.
- The default promotion for a vector is to a 1-column matrix. Therefore, `v1 %*% t(v2)` is equivalent to `v1 %*% asRow(v2)` .

- When indexing, dimensions with scalar indices will be dropped. For example, `M1[1,]` and `M1[,1]` are both vectors.
- The left-hand side of an assignment can use indexing, but if so it must already be correctly sized for the result. For example, `Y[5:10, 20:30] <- model$x` will not work – and could crash your R session with a segmentation fault – if Y is not already at least 10x30 in size.

Here are some examples to illustrate the above points, assuming M2 is a square matrix.

- `Y <- v1 + M2 %*% v2` will return a 1-column matrix. If Y is created by this statement, it will be a 2-dimensional variable. If Y already exists, it must already be 2-dimesional, and it will be automatically re-sized for the result.
- `Y <- v1 + (M2 %*% v2)[,1]` will return a vector. Y will either be created as a vector or must already exist as a vector and will be re-sized for the result.

Size warnings and the potential for crashes

For matrix algebra, NIMBLE cannot ensure perfect behavior because sizes are not known until run-time. Therefore, it is possible for you to write code that will crash your R session. In v0.3-1, NIMBLE attempts to issue warning if sizes are not compatible, but it does not halt execution. Therefore, if you execute `A <- M1 % * % M2`, and M1 and M2 are not compatible for matrix multiplication, NIMBLE will output a warning that the number of rows of M1 does not match the number of columns of M2. After that warning the statement will be executed and may result in a crash. Another easy way to write code that will crash is to do things like `Y[5:10, 20:30] <- model$x` without ensuring Y is at least 10x30. In the future we hope to prevent crashes, but in v0.3-1 we limit ourselves to trying to provide useful information.

9.5.11 Including other methods in a nimbleFunction

Other methods can be included with the `methods` argument to `nimbleFunction`. These methods can use the objects created in `setup` code in just the same ways as the `run` function. In fact, the `run` function is just a method that has the special status of executing when the specialized nimbleFunction object is used like a function. Within a nimbleFunction, other methods are called just like a regular function. When one nimbleFunction calls a method of another nimbleFunction other than `run`, it does so via `$`, as illustrated in the following.

```
methodsDemo <- nimbleFunction(
    setup = function() {sharedValue <- 1},
    run = function(x = double(1)) {
        print('sharedValues = ', sharedValue, '\n')
        increment()
        print('sharedValues = ', sharedValue, '\n')
        A <- times(5)
```

```
        return(A * x)
        returnType(double(1))
    },
    methods = list(
        increment = function() {
            sharedValue <<- sharedValue + 1
        },
        times = function(factor = double()) {
            return(factor * sharedValue)
            returnType(double())
        }))

methodsDemo1 <- methodsDemo()
methodsDemo1$run(1:10)

## sharedValues = 1
##
## sharedValues = 2
##  [1]  10  20  30  40  50  60  70  80  90 100

methodsDemo1$sharedValue <- 1
CmethodsDemo1 <- compileNimble(methodsDemo1)
CmethodsDemo1$run(1:10)

##  [1]  10  20  30  40  50  60  70  80  90 100
```

9.5.12 Using other nimbleFunctions

One nimbleFunction can use another nimbleFunction that was passed to it as a setup argument or was created in the setup function. This can be an effective way to program. When a nimbleFunction needs to access a setup variable or method of another nimbleFunction, use `$`.

```
usePreviousDemo <- nimbleFunction(
    setup = function(initialSharedValue) {
        myMethodsDemo <- methodsDemo()
    },
    run = function(x = double(1)) {
        myMethodsDemo$sharedValue <<- initialSharedValue
        A <- myMethodsDemo$run(x[1:5])
        print(A)
        B <- myMethodsDemo$times(10)
        return(B)
        returnType(double())
```

```
    })

usePreviousDemo1 <- usePreviousDemo(2)
usePreviousDemo1$run(1:10)

## sharedValues = 2
##
## sharedValues = 3
##
## 15 30 45 60 75
## [1] 30

CusePreviousDemo1 <- compileNimble(usePreviousDemo1)
CusePreviousDemo1$run(1:10)

## [1] 30
```

Note that the output from the `print` calls in the compiled function match those from the uncompiled function when run in an R session. It is not shown here due to how R and `knitr` manage such output.

9.5.13 Virtual nimbleFunctions and nimbleFunctionLists

Often it is useful for one nimbleFunction to have a list of other nimbleFunctions that have methods with the same arguments and return types. For example, NIMBLE's MCMC contains a list of samplers that are each nimbleFunctions.

To make such a list, NIMBLE provides a way to declare the arguments and return types of methods: virtual nimbleFunctions created by `nimbleFunctionVirtual`. Other nimbleFunctions can inherit from virtual nimbleFunctions, which in R is called containing them. Readers familiar with object oriented programming will recognize this as a simple class inheritance system. In v0.3-1 it is limited to simple, single-level inheritance.

Here is how it works:

```
baseClass <- nimbleFunctionVirtual(
    run = function(x = double(1)) {returnType(double())},
    methods = list(
        foo = function() {returnType(double())}
    ))

derived1 <- nimbleFunction(
    contains = baseClass,
    setup = function(){},
    run = function(x = double(1)) {
        print('run 1')
        return(sum(x))
```

```
        returnType(double())
    },
    methods = list(
        foo = function() {
        print('foo 1')
        return(rnorm(1, 0, 1))
        returnType(double())
    }))

derived2 <- nimbleFunction(
    contains = baseClass,
    setup = function(){},
    run = function(x = double(1)) {
        print('run 2')
        return(prod(x))
        returnType(double())
    },
    methods = list(
        foo = function() {
        print('foo 2')
        return(runif(1, 100, 200))
        returnType(double())
    }))

useThem <- nimbleFunction(
    setup = function() {
        nfl <- nimbleFunctionList(baseClass)
        nfl[[1]] <- derived1()
        nfl[[2]] <- derived2()
        val <- 0
    },
    run = function(x = double(1)) {
        for(i in seq_along(nfl)) {
            print( nfl[[i]]$run(x) )
            print( nfl[[i]]$foo() )
        }
    }
    )

useThem1 <- useThem()
set.seed(0)
useThem1$run(1:5)
```

```
## run 1
## 15
```

```
## foo 1
## 1.263
## run 2
## 120
## foo 2
## 137.2

CuseThem1 <- compileNimble(useThem1)
set.seed(0)
CuseThem1$run(1:5)

## NULL
```

As in R, the `seq_along` function is equivalent to `1:length(nimFunList)` if `length(nimFunList)` > 0, and it is an empty sequence if `length(nimFunList)` $== 0$.

Currently `seq_along` works only for nimbleFunctionLists.

Virtual nimbleFunctions cannot define `setup` values to be inherited.

9.5.14 print

As demonstrated above, the NIMBLE function `print`, or equivalently `nimPrint`, prints an arbitrary set of outputs in order. Again, this output is not able to be included in this document from compiled models due to how R and `knitr` work.

9.5.15 Alternative keywords for some functions

NIMBLE uses some keywords, such as `dim` and `print`, in ways similar to but not the same as R. In addition, there are some keywords in NIMBLE that have the same names as really different R functions. For example, `step` is part of the BUGS language, but it is also an R function for stepwise model selection. And `equals` is part of the BUGS language but is also used in the `testthat` package, which we use in testing NIMBLE.

The way NIMBLE handles this to try to avoid conflicts is to replace some keywords immediately upon creating a nimbleFunction. These replacements include

- `copy` → `nimCopy`
- `dim` → `nimbleDim`
- `print` → `nimPrint`
- `step` → `nimbleStep`
- `equals` → `nimbleEquals`

This system give programmers the choice between using the keywords like `nimPrint` directly, to avoid confusion in their own code about which "print" is being used, or to use the more intuitive keywords like `print` but remember that they are not the same as R's functions.

9.5.16 User-defined data structures

NIMBLE does not currently have user-defined data structures, but one can use nimbleFunctions to achieve a similar effect. To do so, one can define setup code with whatever variables are wanted and ensure they are compiled using `setupOutputs`. Here is an example:

```
dataNF <- nimbleFunction(
    setup = function() {
        X <- 1
        Y <- as.numeric(c(1, 2)) ## will be a scalar if all sizes are 1
        Z <- matrix(as.numeric(1:4), nrow = 2) ## will be a scalar is all sizes are 1
        setupOutputs(X, Y, Z)
    })

useDataNF <- nimbleFunction(
    setup = function(myDataNF) {},
    run = function(newX = double(), newY = double(1), newZ = double(2)) {
        myDataNF$X <<- newX
        myDataNF$Y <<- newY
        myDataNF$Z <<- newZ
    })

myDataNF <- dataNF()
myUseDataNF <- useDataNF(myDataNF)
myUseDataNF$run(as.numeric(100), as.numeric(100:110), matrix(as.numeric(101:120), nrow =
myDataNF$X

## [1] 100

myDataNF$Y

##  [1] 100 101 102 103 104 105 106 107 108 109 110

myDataNF$Z

##      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
## [1,]  101  103  105  107  109  111  113  115  117   119
## [2,]  102  104  106  108  110  112  114  116  118   120

myUseDataNF$myDataNF$X

## [1] 100

CmyUseDataNF <- compileNimble(myUseDataNF)
CmyUseDataNF$run(-100, -(100:110), matrix(-(101:120), nrow = 2))

## NULL
```

```
CmyDataNF <- CmyUseDataNF$myDataNF
CmyDataNF$X

## [1] -100

CmyDataNF$Y

##  [1] -100 -101 -102 -103 -104 -105 -106 -107 -108 -109 -110

CmyDataNF$Z

##      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
## [1,] -101 -103 -105 -107 -109 -111 -113 -115 -117  -119
## [2,] -102 -104 -106 -108 -110 -112 -114 -116 -118  -120
```

You'll notice that

- after execution of the compiled function, access to the `X`, `Y`, and `Z` is not yet quite the same as for the uncompiled case.
- We need to take care that at the time of compilation, the `X`, `Y` and `Z` values contains doubles via `as.numeric` so that they are not compiled as integer objects.
- The `myDataNF` could be created in the setup code. We just provided it as a setup argument to illustrate that option.

9.5.17 distribution functions

Distribution "d" and "r" functions can be used from nimbleFunctions, although at the moment they are neither as flexible nor as standard as in NIMBLE's processing of BUGS models. In particular, only one parameterization is used, and it is the canonical one used ultimately for compiling. These are listed next:

- `dbinom(size, prob)`
- `dcat(prob)`
- `dmulti(size, prob)`
- `dnbinom(prob, size)`
- `dpois(lambda)`
- `dbeta(shape1, shape2)`
- `dchisq(df)`
- `dexp(rate)`

- `dgamma(shape, scale)`
- `dlnorm(meanlog, sdlog)`
- `dlogis(location, scale)`
- `dnorm(mean, sd)`
- `dt_nonstandard(df, mu, sigma)`
- `dweibull(shape, scale)`
- `ddirch(alpha)`
- `dmnorm_chol(mean, chol, prec_param)`
- `dwish_chol(chol, df, scale_param)`

In the last two, chol stands for Cholesky decomposition; prec_param indicates whether the Cholesky is of a precision matrix or covariance matrix; and scale_param indicates whether the Cholesky is of a scale matrix or an inverse scale matrix.

To call a "d" function, the variable (usually "x" in R) must be included as the first argument. To call the "r" function, a 1 must be included as the first argument. We'll make these more standard and flexible, and include "q" and "p" functions, in the future.

Chapter 10

Additional and advanced topics

10.1 Cautions and suggestions

- When the value of a stochastic node changes, the values of any deterministics nodes that depend on that node are NOT automatically updated. In nimbleFunctions or when manipulating models from R, one must use `calculate()` (or `simulate()` called on the relevant deterministic nodes) to update the values of the dependent nodes.
- Similarly, `getLogProb` should only be used when one is sure the current log probabilities are up to date. If you assign new values to nodes, you must call `calculate` on them to update the log probabilities.
- We have tried to make NIMBLE's handling of multivariate objects flexible, but how you choose to set things up could affect computational efficiency. We'll explore that more in the future.

10.2 Parallel processing

Eigen and NIMBLE's distribution functions (which use BLAS and LAPACK) can use multiple threads if enabled on your system. In general one can control this using the *OMP_NUM_THREADS* environment variable. For parallelized distribution functions, one needs a threaded BLAS installed on your system, with R linked to that BLAS.

We will be exploring providing additional parallelization tools in NIMBLE, in particular parallel for loops, analogous to `foreach`.