NIMBLE User Manual

NIMBLE Development Team

Version 0.6-4

R-nimble.org

Contents

Part I

Introduction and Building Models in NIMBLE

Chapter 1

Welcome to NIMBLE

NIMBLE is a system for building and sharing analysis methods for statistical models from R, especially for hierarchical models and computationally-intensive methods. While NIMBLE is embedded in R, it goes beyond R by supporting separate programming of models and algorithms along with compilation for fast execution.

As of 0.6-4, NIMBLE has been around for a while and is reasonably stable, but we have a lot of plans to expand and improve it. The algorithm library provides MCMC with a lot of user control and ability to write new samplers easily. Other algorithms include particle filtering (sequential Monte Carlo) and Monte Carlo Expectation Maximization (MCEM).

But NIMBLE is about much more than providing an algorithm library. It provides a language for writing model-generic algorithms. We hope you will program in NIMBLE and make an R package providing your method. Of course, NIMBLE is open-source, so we also hope you'll contribute to its development.

Please 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. You can also follow and contribute to developer discussions on the wiki of our GitHub repository.

1.1 What does NIMBLE do?

NIMBLE makes it easier to program statistical algorithms that will run efficiently and work on many different models from R.

You can think of NIMBLE as comprising four 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 models written in BUGS.
4. A compiler that generates C++ for your models and algorithms, compiles that C++, and lets you use it seamlessly from R without knowing anything about C++.

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[1]See Section **??** for information about NIMBLE's version of BUGS.

NIMBLE stands for Numerical Inference for statistical Models for Bayesian and Likelihood Estimation.

Although NIMBLE was motivated by algorithms for hierarchical statistical models, it's useful for other goals too. You could use it for simpler models. And since NIMBLE can automatically compile R-like functions into C++ that use the Eigen library for fast linear algebra, you can use it to program fast numerical functions without any model 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.

1.2   How to use this manual

We suggest everyone start with the Lightning Introduction.

Then, if you want to jump into using NIMBLE's algorithms without learning about NIMBLE's programming system, go to Part **??** to learn how to build your model and Part **??** to learn how to apply NIMBLE's built-in algorithms to your model.

If you want to learn about NIMBLE programming (nimbleFunctions), go to Part **??**. This teaches how to program user-defined function or distributions to use in BUGS code, compile your R code for faster operations, and write algorithms with NIMBLE. These algorithms could be specific algorithms for your particular model (such as a user-defined MCMC sampler for a parameter in your model) or general algorithms you can distribute to others. In fact the algorithms provided as part of NIMBLE and described in Part **??** are written as nimbleFunctions.

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[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 R in a nimbleFunction and the NIMBLE compiler turns it into C++.

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]. We could load the model from the standard BUGS example file formats (Section **??**), but instead we'll show how to 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 configuration for the pump model.
4. Compile and run the MCMC
5. Customize the MCMC configuration 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.

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

---

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

```
  }
  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))
```

Here `x[i]` is the number of failures recorded during a time duration of length `t[i]` for the ith pump. `theta[i]` is a failure rate, and the goal is estimate parameters `alpha` and `beta`. 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)

## defining model...
## building model...
## setting data and initial values...
## running calculate on model (any error reports that follow may simply reflect
missing values in model variables) ...
##
## checking model sizes and dimensions...
##
## model building finished.

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$logProb_x

##  [1]  -2.998011  -1.118924  -1.882686  -2.319466  -4.254550
##  [6] -20.739651  -2.358795  -2.358795  -9.630645 -48.447798

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

pump$lambda

##  [1]  9.430  1.570  6.290 12.600  0.524  3.140  0.105  0.105
##  [9]  0.210  1.050
```

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, as can using a link function or a distribution argument that is an expression. 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).

```
pump$plotGraph()
```

You are in control of the model. By default, `nimbleModel` does its best to initialize a model, but let's say you want to re-initialize `theta`. To simulate from the prior for `theta` (overwriting the initial values previously in the model) we first need to be sure the parent nodes of all `theta[i]` nodes are fully initialized, including any non-stochastic nodes such as lifted nodes. We then use the `simulate` function to simulate from the distribution for `theta`. Finally we use the `calculate` function to calculate the dependencies of `theta`, namely `lambda` and the log probabilities of `x` to ensure all parts of the model are up to date.
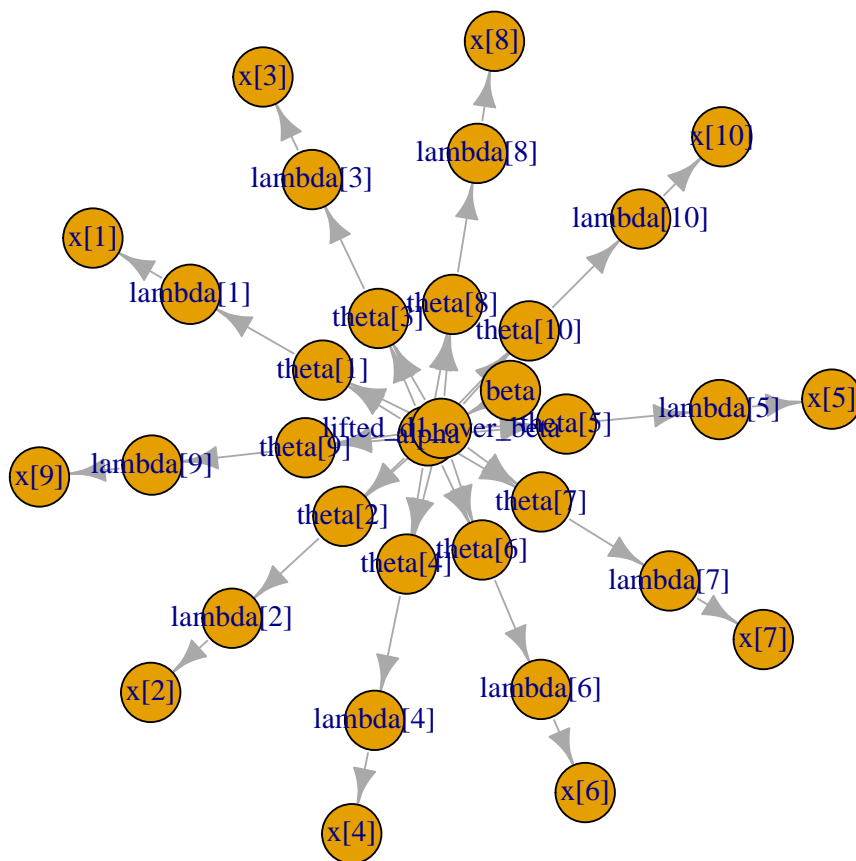
Figure 2.1: Directed Acyclic Graph plot of the pump model, thanks to the igraph package

First we show how to use the model's `getDependencies` method to query information about its graph.

```r
## Show all dependencies of alpha and beta terminating in stochastic nodes
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]"

## Now show only the deterministic dependencies
pump$getDependencies(c('alpha', 'beta'), determOnly = TRUE)

## [1] "lifted_d1_over_beta"

## Check that the lifted node was initialized.
pump[["lifted_d1_over_beta"]] ## It was.

## [1] 1

## Now let's simulate new theta values
set.seed(0) ## This makes the simulations here reproducible
pump$simulate('theta')
pump$theta    ## the new theta values

##  [1] 1.79180692 0.29592523 0.08369014 0.83617765 1.22254365
##  [6] 1.15835525 0.99001994 0.30737332 0.09461909 0.15720154

## lambda and logProb_x haven't been re-calculated yet
pump$lambda ## these are the same values as above

##  [1]  9.430  1.570  6.290 12.600  0.524  3.140  0.105  0.105
##  [9]  0.210  1.050

pump$logProb_x

##  [1]  -2.998011  -1.118924  -1.882686  -2.319466  -4.254550
##  [6] -20.739651  -2.358795  -2.358795  -9.630645 -48.447798

pump$getLogProb('x') ## The sum of logProb_x

## [1] -96.10932
```

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

## [1] -286.6951

pump$lambda  ## Now they have.

##  [1] 168.9673926    4.6460261    5.2641096 105.3583839    6.4061287
##  [6]  36.3723548    1.0395209    0.3227420   0.1987001    1.6506161

pump$logProb_x

##  [1] -148.106356   -3.110014   -1.747041  -65.346457   -2.626123
##  [6]   -7.429868   -1.000761   -1.453644   -9.840589  -39.096527
```

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. The call to `pump$simulate('theta')` expands 'theta' to include all nodes in `theta`. After simulating into `theta`, we can see that `lambda` and the log probabilities of `x` still reflect the old values of `theta`, so we `calculate` them and then see that they have been updated.

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)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_49_05.dll > dynamicRegistrations_03_08_15_49_05.log'
had status 1
## Error:  Failed to create the shared library

Cpump$theta

## Error in eval(expr, envir, enclos):  object 'Cpump' not found
```

Note that the compiled model is used when running any NIMBLE algorithms via C++, so the model needs to be compiled before (or at the same time as) any compilation of algorithms, such as the compilation of the MCMC done in the next section.

2.4 Creating, compiling and running a basic MCMC configuration

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 conjugate relationships are detected for all nodes except for `alpha`, on which the default sampler is a random walk Metropolis sampler.

```r
pumpConf <- configureMCMC(pump, print = TRUE)

## [1]  RW sampler: alpha
## [2]  conjugate_dgamma_dgamma sampler: beta
## [3]  conjugate_dgamma_dpois sampler: theta[1]
## [4]  conjugate_dgamma_dpois sampler: theta[2]
## [5]  conjugate_dgamma_dpois sampler: theta[3]
## [6]  conjugate_dgamma_dpois sampler: theta[4]
## [7]  conjugate_dgamma_dpois sampler: theta[5]
## [8]  conjugate_dgamma_dpois sampler: theta[6]
## [9]  conjugate_dgamma_dpois sampler: theta[7]
## [10] conjugate_dgamma_dpois sampler: theta[8]
## [11] conjugate_dgamma_dpois sampler: theta[9]
## [12] conjugate_dgamma_dpois sampler: theta[10]

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

## thin = 1: alpha, beta, theta

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

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_49_12.dll > dynamicRegistrations_03_08_15_49_12.log'
had status 1
## Error:  Failed to create the shared library

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

## Error in eval(expr, envir, enclos):  object 'CpumpMCMC' not found

samples <- as.matrix(CpumpMCMC$mvSamples)

## Error in as.matrix(CpumpMCMC$mvSamples):  object 'CpumpMCMC' not found
```

```
par(mfrow = c(1, 4), mai = c(.6, .5, .1, .2))
plot(samples[ , 'alpha'], type = 'l', xlab = 'iteration',
     ylab = expression(alpha))

## Error in plot(samples[, "alpha"], type = "l", xlab = "iteration", ylab = expression(a
object 'samples' not found

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

## Error in plot(samples[, "beta"], type = "l", xlab = "iteration", ylab = expression(be
object 'samples' not found

plot(samples[ , 'alpha'], samples[ , 'beta'], xlab = expression(alpha),
     ylab = expression(beta))

## Error in plot(samples[, "alpha"], samples[, "beta"], xlab = expression(alpha),
:  object 'samples' not found

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

## Error in plot(samples[, "theta[1]"], type = "l", xlab = "iteration", ylab =
expression(theta[1])):  object 'samples' not found

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

## Error in as.ts(x):  object 'samples' not found

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

## Error in as.ts(x):  object 'samples' not found
```

Notice the posterior correlation between `alpha` and `beta`. A measure of the mixing for each is the autocorrelation for each parameter, 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.

```
pumpConf$addSampler(target = c('alpha', 'beta'), type = 'RW_block',
                    control = list(adaptInterval = 100))

pumpMCMC2 <- buildMCMC(pumpConf)

# need to reset the nimbleFunctions in order to add the new MCMC
```

```
CpumpNewMCMC <- compileNimble(pumpMCMC2, project  = pump,
                              resetFunctions = TRUE)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_49_21.dll > dynamicRegistrations_03_08_15_49_21.log'
had status 1
## Error:  Failed to create the shared library

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

## Error in eval(expr, envir, enclos):  object 'CpumpNewMCMC' not found

samplesNew <- as.matrix(CpumpNewMCMC$mvSamples)

## Error in as.matrix(CpumpNewMCMC$mvSamples):  object 'CpumpNewMCMC' not found

par(mfrow = c(1, 4), mai = c(.6, .5, .1, .2))
plot(samplesNew[ , 'alpha'], type = 'l', xlab = 'iteration',
     ylab = expression(alpha))

## Error in plot(samplesNew[, "alpha"], type = "l", xlab = "iteration", ylab =
expression(alpha)):  object 'samplesNew' not found

plot(samplesNew[ , 'beta'], type = 'l', xlab = 'iteration',
     ylab = expression(beta))

## Error in plot(samplesNew[, "beta"], type = "l", xlab = "iteration", ylab =
expression(beta)):  object 'samplesNew' not found

plot(samplesNew[ , 'alpha'], samplesNew[ , 'beta'], xlab = expression(alpha),
     ylab = expression(beta))

## Error in plot(samplesNew[, "alpha"], samplesNew[, "beta"], xlab = expression(alpha),
:  object 'samplesNew' not found

plot(samplesNew[ , 'theta[1]'], type = 'l', xlab = 'iteration',
     ylab = expression(theta[1]))

## Error in plot(samplesNew[, "theta[1]"], type = "l", xlab = "iteration", :  object
'samplesNew' not found

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

## Error in as.ts(x):  object 'samplesNew' not found

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

## Error in as.ts(x):  object 'samplesNew' not found
```

We can see that the block sampler has decreased the autocorrelation for both `alpha` and `beta`. Of course these are just short runs, and what we are really interested in is the effective sample size of the MCMC per computation time, but that's not the point of this example.

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[2].

```
pumpMLE <- c(0.8221657, 1.2589865)

pumpMLE

## [1] 0.8221657 1.2589865
```

Both estimates are within 0.01 of the values reported by **?**][3]. Some discrepancy is to be expected since it is a Monte Carlo algorithm.

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. More details on programming in NIMBLE are in Part **??**.

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) {
            model$simulate(nodes)
            model$calculate(deps)
```

---

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

[3]Table 2 of the paper accidentally swapped the two estimates.

```
        copy(from = model, nodes = allNodes,
            to = mv, rowTo = i, logProb = TRUE)
      }
   })

simNodesTheta1to5 <- simNodesMany(pump, 'theta[1:5]')
simNodesTheta6to10 <- simNodesMany(pump, 'theta[6:10]')
```

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

1. The `setup` function is written in R. It creates relevant information specific to our model for use in the run-time code.
2. The `setup` code creates a `modelValues` object to hold multiple sets of values for variables in the model provided.
3. The `run` function 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.
4. The `run` 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.
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. Multiple instances, or "specializations", can be made by calling `simNodesMany` with different arguments. Above, `simNodesTheta1to5` has been made by calling `simNodesMany` with the `pump` model and nodes 'theta[1:5]' as inputs to the `setup` function, while `simNodesTheta6to10` differs by providing 'theta[6:10]' as an argument. The returned objects are objects of a uniquely generated R reference class with fields (member data) for the results of the `setup` code and a `run` method (member function).

By the way, `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]
## make sure to update deterministic dependencies of the altered nodes
pump$calculate(pump$getDependencies(c('alpha','beta'), determOnly = TRUE))

## [1] 0

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

```
## [[1]]
##   [1] 1.43768367 1.53151871 1.45080488 0.03706194 0.13290812
##   [6] 1.15835525 0.99001994 0.30737332 0.09461909 0.15720154
##
## [[2]]
##   [1] 0.34208243 3.46038459 0.82805935 0.08779673 0.34426137
##   [6] 1.15835525 0.99001994 0.30737332 0.09461909 0.15720154

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

## [[1]]
##   [1] -115.813490  -20.864923  -73.474796   -8.285386   -3.573525
##   [6]   -7.429868   -1.000761   -1.453644   -9.840589  -39.096527
##
## [[2]]
##   [1] -19.676977 -50.332998 -37.108047  -2.603897  -1.825787
##   [6]  -7.429868  -1.000761  -1.453644  -9.840589 -39.096527
```

In this code we have initialized the values of `alpha` and `beta` to their MLE and then recorded the `theta` values to use below. 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)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_49_24.dll > dynamicRegistrations_03_08_15_49_24.log'
had status 1
## Error:  Failed to create the shared library

Cpump$alpha <- pumpMLE[1]

## Error in Cpump$alpha <- pumpMLE[1]:  object 'Cpump' not found

Cpump$beta <- pumpMLE[2]

## Error in Cpump$beta <- pumpMLE[2]:  object 'Cpump' not found

Cpump$calculate(Cpump$getDependencies(c('alpha','beta'), determOnly = TRUE))

## Error in eval(expr, envir, enclos):  object 'Cpump' not found
```

```
Cpump$theta <- saveTheta

## Error in Cpump$theta <- saveTheta:  object 'Cpump' not found

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

## Error in eval(expr, envir, enclos):  object 'CsimNodesTheta1to5' not found

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

## Error in eval(expr, envir, enclos):  object 'CsimNodesTheta1to5' not found

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

## Error in eval(expr, envir, enclos):  object 'CsimNodesTheta1to5' not found
```

Given the same initial values and the same random number generator seed, we got identical results for `theta[1:5]` and their dependencies, 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.

One of the most important concepts behind NIMBLE is to allow a combination of high-level processing in R and low-level processing in 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 C++. This separation between *setup* and *run* steps will become clearer as we go.

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 became widely used 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.

NIMBLE extends BUGS by:

1. allowing you to write new functions and distributions and use them in BUGS models;
2. allowing you to define multiple models in the same code using conditionals evaluated when the BUGS code is processed;
3. supporting a variety of more flexible syntax such as R-like named parameters and more general algebraic expressions.

By supporting new functions and distributions, NIMBLE makes BUGS an extensible language, which is a major departure from previous packages that implement BUGS.

We adopted BUGS because it has been so successful, with over 30,000 users by the time they stopped counting [?]. Many papers and books provide BUGS code as a way to document their statistical models. We describe NIMBLE's version of BUGS later. The web sites for WinBUGS, OpenBUGS and JAGS provide other useful documntation on writing models in BUGS. For the most part, if you have BUGS code, you can try NIMBLE.

NIMBLE does several things with BUGS code:

1. NIMBLE creates a *model definition* object that knows everything about the variables and their relationships written in the BUGS code. Usually you'll ignore the *model definition* and let NIMBLE's default options take you directly to the next step.
2. NIMBLE creates a model object[1]. 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. When you're ready, NIMBLE can generate customized C++ code representing the model, compile the C++, load it back into R, and provide a new model object that uses the compiled model internally. We use the word "compile" to refer to all of these steps together.

As an example of how radical a departure NIMBLE is from previous BUGS implementations, consider a situation where you want to simulate new data from a model written in BUGS code. Since NIMBLE creates model objects that you can control from R, simulating new data is trivial. With previous BUGS-based packages, this isn't possible.

More information about specifying and manipulating models is in Chapters **??** and **??**.

3.2 nimbleFunctions for writing algorithms

NIMBLE provides *nimbleFunction*s for writing functions that can (but don't have to) use BUGS models. The main ways they can use BUGS models are:

1. inspecting the structure of a model, such as determining the dependencies between variables, in order to do the right calculations with each model;
2. accessing values of the model's variables;
3. controlling execution of the model's probability calculations or corresponding simulations;
4. managing *modelValues* data structures for multiple sets of model values and probabilities.

In fact, the calculations of the model are themselves constructed as nimbleFunctions, as are the algorithms provided in NIMBLE's algorithm library[2].

Programming with nimbleFunctions involves a fundamental distinction between two stages of processing:

1. A *setup* function within a nimbleFunction gives the steps that need to happen only once for each new situation (e.g., for each new model). Typically such steps include inspecting the model's variables and their relationships, such as determining which parts of a model will need to be calculated for a MCMC sampler. *setup* functions are executed in R and never compiled.

---

[1]or multiple model objects

[2]That's why it's easy to use new functions and distributions written as nimbleFunctions in BUGS code.

2. One or more *run* functions within a nimbleFunction give steps that need to happen multiple times using the results of the *setup* function, such as the iterations of a MCMC sampler. Formally, *run* code is written in the NIMBLE language, which you can think of as a small subset of R along with features for operating models and related data structures. The NIMBLE language is what the NIMBLE compiler can automatically turn into C++ as part of a compiled nimbleFunction.

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`. This is most useful for debugging.
2. When you are ready, NIMBLE can generate C++ code, compile it, load it back into R and give you new objects that use the compiled C++ internally. Again, we refer to these steps all together as "compilation." The behavior of compiled `nimbleFunctions` is usually very similar, but not identical, to their uncompiled counterparts.

More about writing algorithms is in Chapter **??**.

If you are familiar with object-oriented programming, you can think of a nimbleFunction as a class definition. The *setup* function initializes a new object and *run* functions are class methods. Member data are determined automatically as the objects from a *setup* function needed in *run* functions. If no `setup` function is provided, the nimbleFunction corresponds to a simple (compilable) function rather than a class.

3.3 The NIMBLE algorithm library

In Version 0.6-4, the NIMBLE algorithm library includes:

1. MCMC with samplers including conjugate (Gibbs), slice, adaptive random walk (with options for reflection or sampling on a log scale), adaptive block random walk, and elliptical slice. You can modify sampler choices and configurations from R before compiling the MCMC. You can also write new samplers as nimbleFunctions.
2. A set of particle filter (sequential Monte Carlo) methods including a basic bootstrap filter, auxiliary particle filter, and Liu-West filter.
3. An ascent-based Monte Carlo Expectation Maximization (MCEM) algorithm.
4. A variety of basic algorithms that can be used as programming tools for larger algorithms. These include:
   (a) A likelihood function for arbitrary parts of any model.
   (b) Functions to simulate one or many sets of values for arbitrary parts of any model.
   (c) Functions to calculate the summed log probability (density) for one or many sets of values for arbitrary parts of any model along with stochastic dependencies in the model structure.
   (d) Other functions described in Chapter **??**.

Add references where appropriate..

CJP - so is the only difference between calculate and calcNodes (and similarly for simNodes, getLogProbNodes) that calcNodes etc. include operations on dependencies? If so, I propose we extend calculate, simulate, getLogProb to have an argument includeDependencies with default FALSE. PdV - There were a couple of things conflated here, but the question is still valid. The suggestion seems like a slippery slope towards trying to make calculate (etc.) smarter, which could get away from the core design ideas.

More about the NIMBLE algorithm library is in Chapter **??**.

Chapter 4

Installing NIMBLE

4.1 Requirements to run NIMBLE

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

The following are required to run NIMBLE.

1. R, of course.
2. The igraph and coda R packages.
3. A working C++ compiler that NIMBLE can use from R on your system. There are standard open-source C++ compilers that the R community has already made easy to install. See Section ?? for instructions. You don't need to know anything about C++ to use NIMBLE. This must be done before installing 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 Installing a C++ compiler for NIMBLE to use

NIMBLE needs a C++ compiler and the standard utility *make* in order to generate and compile C++ for models and algorithms. [1]

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[1] This differs from most packages, which might need a C++ compiler only when the package is built. If you normally install R packages using `install.packages` on Windows or OS X, the package arrives already built to your system.

4.2.1 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 Apple developer site and the App Store.

PdV – Is this link to App Store really stable?

For the compiler to work correctly for OS X, the installed R must be for the correct version of OS X. For example, R for Snow Leopard (OS X version 10.8) will attempt to use an incorrect C++ compiler if the installed OS X is actually version 10.9 or higher.

PdV – rewrote this – need to check example.

In the somewhat unlikely event you want to install from the source package rather than the CRAN binary package, the easiest approach is to use the source package provided at R-nimble.org. If you do want to install from the source package provided by CRAN, you'll need to install this gfortran package.

4.2.2 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
```

4.2.3 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 (and follow the urge to update your version of R if you notice it is not the most recent). This installer leads you through several "pages". We think you can accept the defaults with one exception: check the PATH checkbox (page 5) so that the installer will add the location of the C++ compiler and related tools to your system's PATH, ensuring that R can find them. After you click "Next", you will get a page with a window for customizing the new PATH variable. You shouldn't need to do anything there, so you can simply click "Next" again.

The checkbox for the "R 2.15+ toolchain" (page 4) must be checked (in order to have *gcc/g++*, *make*, etc. installed). This should be checked by default.

4.3 Installing the NIMBLE package

Since NIMBLE is an R package, you can install it in the usual way, via `install.packages('nimble')` in R or using the `R CMD INSTALL` method if you download the package source directly.

NIMBLE can also be obtained from the NIMBLE website. To install from our website, please see our Download page for the specific invocation of `install.packages`.

4.3.1 Problems with installation

We have tested the installation on the three commonly used platforms – OS X, Linux, Windows[2]. 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`.

Add links to nimble-users and nimble.stats@gmail.com

4.4 Customizing your installation

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

4.4.1 Using your own copy of Eigen

NIMBLE uses the Eigen C++ template library for linear algebra. 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_VERSION.tar.gz`
   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/include/eigen3`. It is not the full path to the Eigen directory itself, i.e., NOT `/usr/include/eigen3/Eigen`.

4.4.2 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 the library code is compiled once as a linkable library - *libnimble.so*. This single instance of the library is then linked with the code for each generated model. In contrast, the default for Windows and Mac OS X is to compile the library code as a static library - *libnimble.a* - that is compiled into each model's and each algorithm'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. If one would like to enable the linkable library in place of the

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[2]We've tested NIMBLE on Windows 7, 8 and 10

static library (do this only on Mac OS X and other UNIX variants and not on Windows), one can install the source package with the configuration argument `--enable-dylib` set to true. First obtain the NIMBLE source package (which will have the extension `.tar.gz` from our website and then install as follows, replacing `VERSION` with the appropriate version number:

```
R CMD INSTALL --configure-args='--enable-dylib=true' nimble_VERSION.tar.gz
```

4.4.3   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 available on CRAN for more details on providing a fast BLAS for your R installation.

4.4.4   Customizing compilation of the NIMBLE-generated C++

For each model or nimbleFunction, NIMBLE can generate and compile C++. To compile generated C++, NIMBLE makes system calls starting with `R CMD SHLIB` and therefore uses 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 as usual.

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. Such an alternative file 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*.

Advanced users can also change their default compilers by editing the *Makevars* file, see Section 1.2.1 of the Writing R Extensions manual available on CRAN.

PdV – Can we combine the final Makevars point, which I moved here, with the previous paragraph.

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.

Part II

Models in NIMBLE

Chapter 5

Writing models in NIMBLE's dialect of BUGS

Models in NIMBLE are written using a variation on the BUGS language. From BUGS code, NIMBLE creates a model object. This chapter describes NIMBLE's version of BUGS. The next chapter explains how to build and manipulate model objects.

5.1 Comparison to BUGS dialects supported by Win-BUGS, OpenBUGS and JAGS

Many users will come to NIMBLE with some familiarity with WinBUGS, OpenBUGS and/or JAGS, so we start by summarizing how NIMBLE is similar and different to those before documenting NIMBLE's version of BUGS more completely. In general, NIMBLE aims to be compatible with the original BUGS language and also JAGS' version. However, at this point, there are some features not supported by NIMBLE, and there are some extensions that are planned but not implemented.

5.1.1 Supported features of BUGS and JAGS

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 4 dimensions.
7. Truncation and censoring as in JAGS using the `T()` notation and `dinterval`.

5.1.2 NIMBLE's Extensions to BUGS and JAGS

NIMBLE extends the BUGS language in the following ways:

---

[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.

1. User-defined functions and distributions – written as `nimbleFunctions` – can be used in model code. See Chapter **??**.
2. Multiple parameterizations for distributions, similar to those in R, can be used.
3. Named parameters for distributions and functions, similar to R function calls, can be used.
4. Linear algebra, including for vectorized calculations of simple algebra, can be used in deterministic declarations.
5. Distribution parameters can be expressions, as in JAGS but not in WinBUGS. Caveat: parameters to *multivariate* distributions (*e.g.,* `dmnorm`) cannot be expressions.
6. Alternative models can be defined from the same model code by using if-then-else statements that are evaluated when the model is defined.
7. More flexible indexing of vector nodes within larger variables is allowed. For example one can place a multivariate normal vector arbitrarily within a higher-dimensional object, not just in the last index.
8. More general constraints can be declared using `dconstraint`, which extends the concept of JAGS' `dinterval`.
9. Link functions can be used in stochastic, as well as deterministic, declarations.[2]
10. Data values can be reset, and which parts of a model are flagged as data can be changed, allowing one model to be used for different data sets without rebuilding the model each time.

5.1.3   Not-yet-supported features of BUGS and JAGS

In this release, the following are not supported.

1. Stochastic indices (but see Chapter **??** for a description of how you could handle some cases with user-defined functions or distributions).
2. The appearance of the same node on the left-hand side of both a `<-` and a $\sim$ declaration (used in WinBUGS for data assignment for the value of a stochastic node).
3. Multivariate nodes must appear with brackets, even if they are empty. E.g., `x` cannot be multivariate but `x[]` or `x[2:5]` can be.
4. 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[])`, and if the dimensions of the variable are not clearly defined in other declarations, NIMBLE currently requires that the dimensions of `x` be provided when the model object is created (via `nimbleModel`).

5.2   Writing models

Here we introduce NIMBLE's version of BUGS. The WinBUGS, OpenBUGS and JAGS manuals are also useful resources for writing BUGS models, including many examples.

---

[2]But beware of the possibility of needing to set values for "lifted" nodes created by NIMBLE.
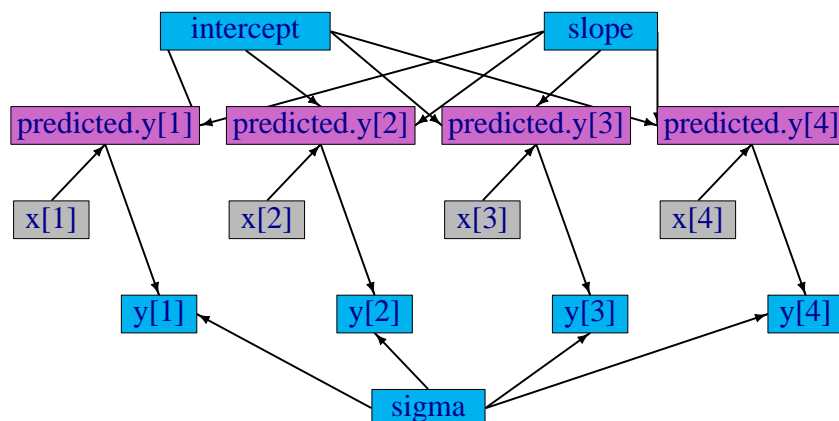
Figure 5.1: Graph of a linear regression model

5.2.1 Declaring stochastic and deterministic nodes

BUGS is a declarative language for graphical (or hierarchical) models. Most programming languages are imperative, which means a series of commands will be executed in the order they are written. A declarative language like BUGS is more like building a machine before using it. Each line declares that a component should be plugged into the machine, but it doesn't matter in what order they are declared as long as all the right components are plugged in by the end of the code.

The machine in this case is a graphical model[3]. A *node* (sometimes called a *vertex*) holds one value, which may be a scalar or a vector. *Edges* define the relationships between nodes. A huge variety of statistical models can be thought of as graphs.

For example, a simple linear regression with four observations is shown in figure **??**. Each observation, y[i], is a node whose edges say that it follows a normal distribution depending on a predicted value, predicted.y[i], and standard deviation, sigma, which are each nodes. Each predicted value is a node whose edges say how it is calculated from slope, intercept, and one value of an explanatory variable, x[i], which are each nodes.

This graph is created from the following BUGS code:

```
{
    intercept ~ dnorm(0, sd = 1000)
    slope ~ dnorm(0, sd = 1000)
    sigma ~ dunif(0, 100)
    for(i in 1:4) {
        predicted.y[i] <- intercept + slope * x[i]
```

---

[3]Technically, a *directed acyclic graph*

```
        y[i] ~ dnorm(predicted.y[i], sd = sigma)
    }
}
```

In this code, stochastic relationships are declared with "~" and deterministic relationships are declared with "<-". For example, each `y[i]` follows a normal distribution with mean `predicted.y[i]` and standard deviation `sigma`. Each `predicted.y[i]` is the result of `intercept + slope * x[i]`. The for-loop yields the equivalent of writing four lines of code, each with a different value of `i`. It does not matter in what order the nodes are declared. Imagine that each line of code draws part of figure **??**, and all that matters is that the everything gets drawn in the end. Available distributions, default and alternative parameterizations, and functions are listed in section **??**

An equivalent graph can be created by this BUGS code:

```
{
    intercept ~ dnorm(0, sd = 1000)
    slope ~ dnorm(0, sd = 1000)
    sigma ~ dunif(0, 100)
    for(i in 1:4) {
        y[i] ~ dnorm(intercept + slope * x[i], sd = sigma)
    }
}
```

In this case, the `predicted.y[i]` nodes in figure **??** will be created automatically by NIMBLE and will have a different name, generated by NIMBLE.

5.2.2   More kinds of BUGS declarations

Here are some examples of valid lines of BUGS code. This code does not describe a sensible or complete model, and it includes some arbitrary indices (e.g. `mvx[8:10, i]`) to illustrate flexibility. Instead the purpose of each line is to illustrate a feature of NIMBLE's version of BUGS.

```
{
    ## 1. normal distribution with BUGS parameter order
    x ~ dnorm(a + b * c, tau)
    ## 2. normal distribution with a named parameter
    y ~ dnorm(a + b * c, sd = sigma)
    ## 3. For-loop and nested indexing
    for(i in 1:N) {
        for(j in 1:M[i]) {
            z[i,j] ~ dexp(r[ blockID[i] ])
        }
    }
```

```
    ## 4. multivariate distribution with arbitrary indexing
    for(i in 1:3)
        mvx[8:10, i] ~ dmnorm(mvMean[3:5], cov = mvCov[1:3, 1:3, i])
    ## 5. User-provided distribution
    w ~ dMyDistribution(hello = x, world = y)
    ## 6. Simple deterministic node
    d1 <- a + b
    ## 7. Vector deterministic node with matrix multiplication
    d2[] <- A[ , ] %*% mvMean[1:5]
    ## 8. Deterministic node with user-provided function
    d3 <- foo(x, hooray = y)
}
```

When a variable appears only on the right-hand side, it must be provided in the `data` or `constants` argument to `nimbleModel`, covered in chapter **??**.

Notes on the comment-numbered lines are:

1. `x` follows a normal distribution with mean `a + b*c` and precision `tau` (default BUGS second parameter for `dnorm`).
2. `y` follows a normal distribution with the same mean as `x` but a named standard deviation parameter instead of a precision parameter (sd = 1/sqrt(precision)).
3. `z[i, j]` follows an exponential distribution with parameter `r[blockID[i] ]`. This shows how for-loops can be used for indexing of variables containing multiple nodes. Nested indexing can be used if the nested indices (`blockID`) are provided as constants when the model is defined (via `nimbleModel` or `readBUGSmodel`). Variables that define for-loop indices (`N` and `M`) must be provided as constants.
4. The arbitrary block `mvx[8:10, i]` follows a multivariate normal distribution, with a named covariance matrix instead of BUGS' default of a precision matrix. As in R, curly braces for for-loop contents are only needed if there is more than one line.
5. `w` follows a user-defined distribution. See Chapter **??**.
6. `d1` is a scalar deterministic node that, when calculated, will be set to `a + b`.
7. `d2` is a vector deterministic node using matrix multiplication in R's syntax.
8. `d3` is a deterministic node using a user-provided function. See Chapter **??**.

More about indexing

Examples of allowed indexing include:

- `x[i]` # a single index
- `x[i:j]` # a range of indices
- `x[i:j,k:l]` # multiple single indices or ranges for higher dimensional arrays
- `x[i:j, ]` # blank indices indicating the full range
- `x[3*i+7]` # computed indices
- `x[(3*i):(5*i+1)]` # computed lower and upper ends of an index range

NIMBLE does not allow multivariate nodes to be used 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[])` (if `x` is a vector) or `xbar <- mean(x[,])` (if `x` is a matrix) for NIMBLE. [4]. Ways to provide NIMBLE with dimensions of `x` in such cases, if necessary, is covered in section **??**.

Generally NIMBLE supports R-like linear algebra expressions and attempts to follow the same rules as R about dimensions (although in some cases this is not possible). For example, `x[1:3] %*% y[1:3]` converts `x[1:3]` into a row vector and thus computes the inner product, which is returned as a 1×1 matrix (use `inprod` to get it as a scalar, which it typically easier). Like in R, a scalar index will result in dropping a dimension unless the argument `drop=FALSE` is provided. For example, `mymatrix[i, 1:3]` will be a vector of length 3, but `mymatrix[i, 1:3, drop=FALSE]` will be a 1×3 matrix. More about indexing and dimensions is discussed in section (**??**).

5.2.3 Vectorized versus scalar declarations

Suppose you need nodes `logY[i]` that should be the log of the corresponding `Y[i]`, say for `i` from 1 to 10. Conventionally this would be created with a for loop:

```
{
    for(i in 1:10) {
        logY[i] <- log(Y[i])
    }
}
```

Since NIMBLE supports R-like algebraic expressions, an alternative in NIMBLE's dialect of BUGS is to use a vectorized declaration like this:

```
{
    logY[1:10] <- log(Y[1:10])
}
```

Supported functions from BUGS and JAGS are listed in Section **??**. Support for more general R expressions is covered in Chapter **??** about programming with nimbleFunctions.

There is an important difference between the models that are created by the above two methods. The first creates 10 scalar nodes, `logY[1]` ... `logY[10]`. The second creates one vector node, `logY[1:10]`. If each `logY[i]` is used separately by an algorithm, it may be beneficial to declare them as scalars. If they are all used together, it will often make sense to declare them as a vector.

---

[4]In `nimbleFunctions` explained in later chapters, square brackets with blank indices are not necessary for multivariate objects.

5.2.4 Available distributions

Distributions

NIMBLE supports most of the distributions allowed in BUGS and JAGS. Table **??** lists the distributions that are currently supported, with their default parameterizations, which match those of BUGS[5]. NIMBLE also allows one to use alternative parameterizations for a variety of distributions as described next. See section **??** to learn how to write new distributions using nimbleFunctions.

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

	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)` $a > 0, b > 0$	$\dfrac{x^{a-1}(1-x)^{b-1}}{\beta(a,b)}$	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)` $p \in (\mathbb{R}^+)^N$	$\dfrac{p_x}{\sum_i p_i}$	1	N
Chi-square	`dchisq(df = k)` $k > 0$	$\dfrac{x^{\frac{k}{2}-1}\exp(-x/2)}{2^{\frac{k}{2}}\Gamma(\frac{k}{2})}$	0	
Dirichlet	`ddirch(alpha = `α`)` $\alpha_j \geq 0$	$\Gamma(\sum_i \alpha_i)\prod_j \dfrac{x_j^{\alpha_j-1}}{\Gamma(\alpha_j)}$	0	
Exponential	`dexp(rate = `λ`)` $\lambda > 0$	$\lambda\exp(-\lambda x)$	0	
Gamma	`dgamma(shape = r, rate = `λ`)` $\lambda > 0, r > 0$	$\dfrac{\lambda^r x^{r-1}\exp(-\lambda x)}{\Gamma(r)}$	0	
Logistic	`dlogis(location = `μ`, rate = `τ`)` $\tau > 0$	$\dfrac{\tau\exp\{(x-\mu)\tau\}}{[1+\exp\{(x-\mu)\tau\}]^2}$		
Log-normal	`dlnorm(meanlog = `μ`, taulog = `τ`)` $\tau > 0$	$\left(\frac{\tau}{2\pi}\right)^{\frac{1}{2}}x^{-1}\exp\left\{-\tau(\log(x)-\mu)^2/2\right\}$	0	
Multinomial	`dmulti(prob = p, size = n)` $\sum_j x_j = n$	$n!\prod_j \dfrac{p_j^{x_j}}{x_j!}$		
Multivariate normal	`dmnorm(mean = `μ`, prec = `Λ`)` Λ positive definite	$(2\pi)^{-\frac{d}{2}}|\Lambda|^{\frac{1}{2}}\exp\{-\frac{(x-\mu)^T\Lambda(x-\mu)}{2}\}$		
Multivariate Student t	`dmvt(mu = `μ`, prec = `Λ`, df = `ν`)` Λ positive definite	$\frac{\Gamma(\frac{\nu+d}{2})}{\Gamma(\frac{\nu}{2})(\nu\pi)^{d/2}}|\Lambda|^{1/2}(1+\frac{(x-\mu)^T\Lambda(x-\mu)}{\nu})^{-\frac{\nu+d}{2}}$		
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(mean = `μ`, tau = `τ`)`	$\left(\frac{\tau}{2\pi}\right)^{\frac{1}{2}}\exp\{-\tau(x-\mu)^2/2\}$		

---

[5]Note that the same distributions are available for writing `nimbleFunctions`, but in that case the default parameterizations and function names match R's when possible. Please see Section **??** for how to use distributions in `nimbleFunctions`.

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

Name	Usage	Density	Lower	Upper
	$\tau > 0$			
Poisson	dpois(lambda = λ)	$\dfrac{\exp(-\lambda)\lambda^x}{x!}$	0	
	$\lambda > 0$			
Student t	dt(mu = μ, tau = τ, df = k)	$\dfrac{\Gamma(\frac{k+1}{2})}{\Gamma(\frac{k}{2})}\left(\dfrac{\tau}{k\pi}\right)^{\frac{1}{2}}\left\{1+\dfrac{\tau(x-\mu)^2}{k}\right\}^{-\frac{(k+1)}{2}}$		
	$\tau > 0, k > 0$			
Uniform	dunif(min = a, max = b)	$\dfrac{1}{b-a}$	a	b
	$a < b$			
Weibull	dweib(shape = v, lambda = λ)	$v\lambda x^{v-1}\exp(-\lambda x^v)$	0	
	$v > 0, \lambda > 0$			
Wishart	dwish(R = R, df = k)	$\dfrac{|x|^{(k-p-1)/2}|R|^{k/2}\exp\{-\mathrm{tr}(Rx/2)\}}{2^{pk/2}\Gamma_p(k/2)}$		
	$R\ p \times p$ pos. def., $k \geq p$			

Alternative parameterizations for distributions

NIMBLE allows one to specify distributions in model code using a variety of parameterizations, including the BUGS parameterizations. Available parameterizations is listed in Table **??**. 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[6]. 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 gamma, NIMBLE provides both (shape, rate) and (mean, sd) parameterization and creates nodes to calculate (shape, scale) from either (shape, rate) or (mean, sd). In the case of gamma, the BUGS parameterization is also an *alternative* parameterization.

Since NIMBLE provides compatibility with existing BUGS and JAGS code, the order of parameters places the BUGS parameterization first. For example, the order of parameters for dgamma 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).

---

[6]Usually this is the parameterization in the Rmath header of R's C implementation of distributions.

Table 5.2: Distribution parameterizations allowed in NIMBLE. The first column indicates the supported parameterizations for distributions given in Table **??**. The second column indicates the relationship to the *canonical* parameterization used in NIMBLE.

Parameterization	NIMBLE re-parameterization
dbern(prob)	dbin(size = 1, prob)
dbeta(shape1, shape2)	canonical
dbeta(mean, sd)	dbeta(shape1 = mean^2 * (1-mean) / sd^2 - mean, shape2 = mean * (1 - mean)^2 / sd^2 + mean - 1)
dbin(prob, size)	canonical
dcat(prob)	canonical
dchisq(df)	canonical
ddirch(alpha)	canonical
dexp(rate)	canonical
dexp(scale)	dexp(rate = 1/scale)
dgamma(shape, scale)	canonical
dgamma(shape, rate)	dgamma(shape, scale = 1 / rate)
dgamma(mean, sd)	dgamma(shape = mean^2/sd^2, scale = sd^2/mean)
dlogis(location, scale)	canonical
dlogis(location, rate)	dlogis(location, scale = 1 / rate
dlnorm(meanlog, sdlog)	canonical
dlnorm(meanlog, taulog)	dlnorm(meanlog, sdlog = 1 / sqrt(taulog)
dlnorm(meanlog, varlog)	dlnorm(meanlog, sdlog = sqrt(varlog)
dmulti(prob, size)	canonical
dmnorm(mean, cholesky, prec_param=1)	canonical (precision)
dmnorm(mean, cholesky, prec_param=0)	canonical (covariance)
dmnorm(mean, prec)	dmnorm(mean, cholesky = chol(prec), prec_param=1)
dmnorm(mean, cov)	dmnorm(mean, cholesky = chol(cov), prec_param=0)
dmvt(mu, cholesky, df, prec_param=1)	canonical (precision/inverse scale)
dmvt(mu, cholesky, df, prec_param=0)	canonical (scale)
dmvt(mu, prec, df)	dmvt(mu, cholesky = chol(prec), df, prec_param=1)
dmvt(mu, scale, df)	dmvt(mu, cholesky = chol(scale), df, prec_param=0)
dnegbin(prob, size)	canonical
dnorm(mean, sd)	canonical
dnorm(mean, tau)	dnorm(mean, sd = 1 / sqrt(var))
dnorm(mean, var)	dnorm(mean, sd = sqrt(var))
dpois(lambda)	canonical
dt(mu, sigma, df)	canonical
dt(mu, tau, df)	dt(mu, sigma = 1 / sqrt(tau), df)
dt(mu, sigma2, df)	dt(mu, sigma = sqrt(sigma2), df)
dunif(min, max)	canonical
dweib(shape, scale)	canonical
dweib(shape, rate)	dweib(shape, scale = 1 / rate)
dweib(shape, lambda)	dweib(shape, scale = lambda^(- 1 / shape)
dwish(R, df)	dwish(cholesky = chol(R), df, scale_param = 0)

Table 5.2: Distribution parameterizations allowed in NIMBLE. The first column indicates the supported parameterizations for distributions given in Table **??**. The second column indicates the relationship to the *canonical* parameterization used in NIMBLE.

Parameterization	NIMBLE re-parameterization
`dwish(S, df)`	`dwish(cholesky = chol(S), df, scale_param = 1)`

Note that for multivariate normal, multivariate t, and Wishart, the canonical parameterization uses the Cholesky decomposition of one of the precision/inverse scale or covariance/scale matrix. For example, for the multivariate normal, if `prec_param=TRUE`, the `cholesky` argument is treated as the Cholesky decomposition of a precision matrix. Otherwise it is treated as the Cholesky decomposition of a covariance matrix.

In addition, NIMBLE supports alternative distribution names, known as aliases, as in JAGS, as specified in Table **??**.

Distribution	Canonical name	Alias
Binomial	dbin	dbinom
Chi-square	dchisq	dchisqr
Dirichlet	ddirch	ddirich
Multinomial	dmulti	dmultinom
Negative binomial	dnegbin	dnbinom
Weibull	dweib	dweibull
Wishart	dwish	dwishart

Table 5.3: Distributions with alternative names (aliases).

We plan to, but do not currently, include the following distributions as part of core NIMBLE: double exponential (Laplace), beta-binomial, Dirichlet-multinomial, F, inverse gamma, Pareto, inverse Wishart, or forms of the multivariate t other than the standard one provided.

5.2.5   Available BUGS language functions

Tables **??**-**??** show the available operators and functions. This table needs updating.

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. Note that we provide distribution functions for use in calculations, namely the "p", "q", and "d" functions. See Section **??** for details on the syntax for using distribution functions as functions in deterministic calculations, as only some parameterizations are allowed and the names of some distributions differ from those used to define stochastic nodes in a model.

Table 5.4: 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	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; vector x and scalar y ok	✓	✓
`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	$\lceil (x) \rceil$	✓	✓

Table 5.4: 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	Accepts vector input
`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	$log(x + 1)$	✓	✓
`qDIST(x, PARAMS)`	"q" distribution functions	canonical parameterization	✓	
`pDIST(x, PARAMS)`	"p" distribution functions	canonical parameterization	✓	
`rDIST(1, PARAMS)`	"r" distribution functions	canonical parameterization	✓	
`dDIST(x, PARAMS)`	"d" distribution functions	canonical parameterization	✓	
`sort(x)`				
`rank(x, s)`				
`ranked(x, s)`				
`order(x)`				

Table 5.5: Functions operating on 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	✓
`t(x)`	matrix transpose	$x^\top$	✓
`x%*%y`	matrix multiply	xy; x, y conformant	✓
`inprod(x, y)`	dot product	$x^\top y$; x and y vectors	✓
`solve(x, y)`	solve system of equations	$x^{-1}y$; y matrix or vector	✓
`forwardsolve(x, y)`	solve lower-triangular system of equations	$x^{-1}y$; x lower-triangular	✓
`backsolve(x, y)`	solve upper-triangular system of equations	$x^{-1}y$; x upper-triangular	✓
`logdet(x)`	log matrix determinant	$\log |x|$	✓
`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		
`eigen(x)$values`	matrix eigenvalues	x symmetric, positive definite	✓
`eigen(x)$vectors`	matrix eigenvectors	x symmetric, positive definite	✓
`svd(x)$d`	matrix singular values		✓
`svd(x)$u`	matrix left singular vectors		✓

Table 5.5: Functions operating on vectors and matrices. Status column indicates if the function is currently provided in NIMBLE.

Usage	Description	Comments	Status
`svd(x)$v`	matrix right singular vectors		✓

5.2.6 Available link functions

NIMBLE allows the link functions listed in Table **??**.

Table 5.6: Link functions

	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)`

Link functions are specified as functions applied to a node on the left hand side of a BUGS expression. To handle link functions in deterministic declarations, NIMBLE converts the declaration into an equivalent inverse declaration. For example, `log(y) <- x` is converted into `y <- exp(x)`. In other words, the link function is just a simple variant for conceptual clarity.

To handle link functions in a stochastic declaration, NIMBLE does some processing that inserts an additional node into the model. For example, the declaration `logit(p[i])` $\sim$ `dnorm(mu[i],1)`, is equivalent to the follow two declarations:

- `logit_p[i]` $\sim$ `dnorm(mu[i], 1)`,
- `p[i] <- expit(logit_p[i])`

where `expit` is the inverse of `logit`.

Note that NIMBLE does not provide an automatic way of initializing the additional node (`logit_p` in this case), which is a parent node of the explicit node (`p[i]`), without explicitly referring to the additional node by the name that NIMBLE generates.

5.2.7 Truncation, censoring, and constraints

NIMBLE provides three ways to declare boundaries on the value of a variable, each for different situations. We introduce these and comment on their relationships to related features of JAGS and BUGS. The three methods are:

Truncation

Either of the following forms,

- x ~ dnorm(0, sd = 10) T(0, a), or
- x ~ T(dnorm(0, sd = 10), 0, a),

declares that x follows a normal distribution between 0 and a (inclusive of 0 and a). Either boundary may be omitted or may be another node, such as a in this example. The first form is compatible with JAGS, but in NIMBLE it can only be used when reading code from a text file. When writing model code in R, the second version must be used.

Truncation means the possible values of x are limited a priori, hence the probability density of x must be normalized. In this example it would be the normal probability density divided by its integral from 0 to a. Like JAGS, NIMBLE also provides I as a synonym for T to accommodate older BUGS code, but T is preferred because it disambiguates multiple usages of I in BUGS.

Censoring

Censoring refers to the situation where one datum gives the lower or upper bound on an unobserved random variable. This is common in survival analysis, when for individuals still surviving at the end of a study, their age of death is not known and hence is "censored" (right-censoring). NIMBLE adopts JAGS syntax for censoring, as follows (using right-censoring as an example):

```
censored[i] ~ dinterval(t[i], c[i])
t[i] ~ dweib(r, mu[i])
```

where censored[i] should be given as data with a value of 1 if t[i] is right-censored (t[i] > c[i]) and 0 if it is observed. The data vector for t should have NA (indicating missing data) for any censored t[i] entries. (As a result, these nodes will be sampled in an MCMC.) The data vector for c should give the censoring times corresponding to censored entries and a value below the observed times for uncensored entries (e.g., 0, assuming t[i] > 0). Left-censoring would be specified by setting censored[i] to 0 and t[i] to NA.

The dinterval is not really a distribution but rather a trick: in the above example when censored[i] = 1 it gives a "probability" of 1 if t[i] > c[i] and 0 otherwise. This means that t[i] ≤ c[i] is treated as impossible. More generally than simple right- or left-censoring, censored[i] ~ dinterval(t[i], c[i,]) is defined such that for a vector of increasing cutpoints, c[i,], t[i] is enforced to fall within the censored[i]-th cutpoint interval. This is done by setting data censored[i] as follows:

$$\text{censored[i]} = 0 \quad \text{if} \quad \text{t[i]} \leq \text{c[i, 1]}$$
$$\text{censored[i]} = m \quad \text{if} \quad \text{c[i, m]} < \text{t[i]} \leq \text{c[i, m+1]} \text{ for } 1 <= m <= M$$
$$\text{censored[i]} = M \quad \text{if} \quad \text{c[i, M]} < \text{t[i]}.$$

(The i index is provided only for consistency with the previous example.) The most common uses of dinterval will be for left- and right-censored data, in which case c[i,] will be a single value (and typically given as simply c[i]), and for interval-censored data, in which case c[i,] will be a vector of two values.

Nodes following a `dinterval` distribution should normally be set as `data` with known values. Otherwise, the node may be simulated during initialization in some algorithms (e.g., MCMC) and thereby establish a permanent, perhaps unintended, constraint.

Censoring differs from truncation because censoring an observation involves bounds on a random variable that could have taken any value, while in truncation we know a priori that a datum could not have occurred outside the truncation range.

Constraints and ordering

NIMBLE provides a more general way to enforce constraints using `dconstraint(cond)`. For example, we could specify that the sum of `mu1` and `mu2` must be positive like this:

```
mu1 ~ dnorm(0, 1)
mu2 ~ dnorm(0, 1)
constraint_data ~ dconstraint( mu1 + mu2 > 0 )
```

with `constraint_data` set (as `data`) to 1. This is equivalent to a half-normal distribution on the half-plane $\mu_1 + \mu_2 > 0$. Nodes following `dconstraint` should be provided as data for the same reason of avoiding unintended initialization described above for `dinterval`.

Formally, `dconstraint(cond)` is a probability distribution on $\{0, 1\}$ such that $P(1) = 1$ if `cond` is `TRUE` and $P(0) = 1$ if `cond` is `FALSE`.

Of course, in many cases, parameterizing the model so that the constraints are automatically respected may be a better strategy than using `dconstraint`. One should be cautious about constraints that would make it hard for an MCMC or optimization to move through the parameter space (such as equality constraints that involve two or more parameters). For such restrictive constraints, general purpose algorithms that are not tailored to the constraints may fail or be inefficient. If constraints are used, it will generally be wise to ensure the model is initialized with values that satisfy them.

Ordering   To specify an ordering of parameters, such as $\alpha_1 <= \alpha_2 <= \alpha_3$ one can use `dconstraint` as follows:

```
constraint_data ~ dconstraint( alpha1 <= alpha2 & alpha2 <= alpha3 )
```

Note that unlike in BUGS, one cannot specify prior ordering using syntax such as

```
alpha[1] ~ dnorm(0, 1) I(, alpha[2])
alpha[2] ~ dnorm(0, 1) I(alpha[1], alpha[3])
alpha[3] ~ dnorm(0, 1) I(alpha[2], )
```

as this does not represent a directed acyclic graph.

Also note that specifying prior ordering using `T(,)` can result in possibly unexpected results. For example:

```
alpha1 ~ dnorm(0, 1)
alpha2 ~ dnorm(0, 1) T(alpha1, )
alpha3 ~ dnorm(0, 1) T(alpha2, )
```

will enforce `alpha1` $\leq$ `alpha2` $\leq$ `alpha3`, but it does not treat the three parameters symmetrically. Instead it puts a marginal prior on `alpha1` that is standard normal and then constrains `alpha2` and `alpha3` to follow truncated normal distributions. This is not equivalent to a symmetric prior on the three `alpha`s that assigns 0 probability density when values are not in order.

NIMBLE does not support the JAGS `sort` syntax.

moved subsection on defining nodes/vars to chap 6

Chapter 6

Building and using models

This chapter explains how to build and manipulate model objects starting from BUGS code.

6.1 Creating model objects

NIMBLE provides two functions for creating model objects: `nimbleModel` and `readBUGSmodel`. The first, `nimbleModel`, is more general and was illustrated in Chapter **??**. The second, `readBUGSmodel` provides compatibility with BUGS file formats for models, variables, data, and initial values for MCMC. In addition one can create new model objects from existing model objects.

6.1.1 Using `nimbleModel` to create a model

`nimbleModel` processes BUGS code to determine all the nodes, variables, and their relationships in a model. Any constants must be provided at this step. Data and initial values can optionally be provided. BUGS code passed to `nimbleModel` must go through `nimbleCode`.

We look again at the pump example from the introduction:

```
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))

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

Data and constants

NIMBLE makes a distinction between data and constants:

- *Constants* can never be changed and must be provided when a model is defined. For example, a vector of known index values, such as for block indices, helps define the model graph itself and must be provided as constants. Variables used in the index ranges of for-loops must also be provided as constants.
- *Data* is a label for 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 (see `simulate` in Chapter **??**), but it is possible to over-ride that default or to change their values by direct assignment. This allows an algorithm to be applied to many data sets in the same model without re-creating the model each time. It also allows simulation of data in a model.

WinBUGS, OpenBUGS and JAGS do not allow data values to be changed or different nodes to be labeled as data without starting from the beginning again. Hence they do not distinguish between constants and data.

For compatibility with BUGS and JAGS, NIMBLE allows both to be provided in the `constants` argument to `nimbleModel`, in which case NIMBLE handles values for stochastic nodes as data and everything else as constants.

Values for nodes that appear only on the right-hand side of BUGS declarations (e.g., covariates/predictors) can be provided as data or constants.

Providing data and initial values to an existing model

Whereas constants must be provided during the call the `nimbleModel`, data and initial values can be provided later via the model member functions `setData` and `setInits`. For example, if `pumpData` is a named list of data values (as above), then `pump$setData(pumpData)` sets the named variables to the values in the list.

`setData` does two things: it sets the values of the data nodes, and it flags those nodes as containing data. `nimbleFunction` programmers can then use that information to control whether an algorithm should over-write data or not. For example, NIMBLE's `simulate` functions by default do not overwrite data values but can be told to do so. Values of data variables can be replaced, 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

Sometimes one needs a model variable to have a mix of data and non-data, often due to missing data values. In NIMBLE, when data values are provided, any nodes with `NA` values will *not* be labeled as data. 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. Some of the steps in this example are documented more below. NIMBLE's default MCMC configuration 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)

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

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

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

## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_49_33.dll > dynamicRegistrations_03_08_15_49_33.log'
had status 1
## Error:  Failed to create the shared library

niter <- 10
set.seed(0)
Cobj$pumpMissMCMC$run(niter)

## Error in eval(expr, envir, enclos):  object 'Cobj' not found

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

## Error in as.matrix(Cobj$pumpMissMCMC$mvSamples):  object 'Cobj' not found

samples[1:5, 13:17]

## Error in eval(expr, envir, enclos):  object 'samples' not found
```

Missing values may also occur in explanatory variables. Values for such variables should be passed in via the `data` argument to `nimbleModel`, with `NA` for the missing values. In some contexts, one would want to specify distributions for such explanatory variables, for example so that an MCMC would impute the missing values.

Defining alternative models with the same code

Avoiding code duplication is a basic principle of good programming. In NIMBLE, one can use definition-time if-then-else statements to create different models from the same code. As a simple example, say we have a linear regression model and want to consider including or omitting x[2] as an explanatory variable:

```
regressionCode <- nimbleCode({
    intercept ~ dnorm(0, sd = 1000)
    slope1 ~ dnorm(0, sd = 1000)
    if(includeX2) {
        slope2 ~ dnorm(0, sd = 1000)
        for(i in 1:N)
            predictedY[i] <- intercept + slope1 * x1[i] + slope2 * x2[i]
    } else {
        for(i in 1:N) predictedY[i] <- intercept + slope1 * x1[i]
    }
    sigmaY ~ dunif(0, 100)
    for(i in 1:N) Y[i] ~ dnorm(predictedY[i], sigmaY)
})

includeX2 <- FALSE
modelWithoutX2 <- nimbleModel(regressionCode, constants = list(N = 30),
                              check=FALSE)
modelWithoutX2$getVarNames()

## [1] "intercept"
## [2] "slope1"
## [3] "predictedY"
## [4] "sigmaY"
## [5] "lifted_d1_over_sqrt_oPsigmaY_cP"
## [6] "Y"
## [7] "x1"

includeX2 <- TRUE
modelWithX2 <- nimbleModel(regressionCode, constants = list(N = 30),
                           check = FALSE)
modelWithX2$getVarNames()

## [1] "intercept"
## [2] "slope1"
## [3] "slope2"
## [4] "predictedY"
## [5] "sigmaY"
## [6] "lifted_d1_over_sqrt_oPsigmaY_cP"
## [7] "Y"
```

```
## [8] "x1"
## [9] "x2"
```

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 generated from the same *model definition*. The `setData` and `setInits` described above can be used for each copy of the model.

Providing dimensions via `nimbleModel`

`nimbleModel` can usually determine the dimensions of every variable from the declarations in the BUGS code. However, it is possible to use a multivariate object only with empty indices (e.g. `x[,]`), in which case the dimensions must be provided as an argument to `nimbleModel`.

Here's an example with multivariate nodes. The first provides indices, so no `dimensions` argument is needed, while the second omits the indices and provides a `dimensions` argument instead.

```
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)),
                     check = FALSE)

## Adding alpha0,R as data for building model.

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),
                     check = FALSE)

## Adding alpha0,R as data for building model.
```

6.1.2 Creating a model from standard BUGS and JAGS input files

Users with BUGS and JAGS experience may have files set up in standard formats for use in BUGS and JAGS. `readBUGSmodel` can read in the model, data/constant values and initial values in those formats. It can also take information directly from R objects somewhat more flexibly than `nimbleModel`, specifically allowing inputs set up similarly to those for BUGS and JAGS. In either case, after processing the inputs, it calls `nimbleModel`. Note that unlike BUGS and JAGS, only a single set of initial values can be specified in creating a model. Please see `help(readBUGSmodel)` for argument details.

As an example of 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)

## Detected x as data within 'constants'.
## Adding x as data for building model.
```

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. Also note that if `data` and `inits` are provided as files, the files 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 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.

Note that 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'`.

6.1.3 Making multiple instances from the same model definition

Sometimes it is useful to have more than one copy of the same model. For example, an algorithm (i.e., `nimbleFunction`) such as an MCMC will be bound to a particular model before it is run. A user could build multiple algorithms to use the same model instance, or they may want each algorithm to have its own instance of the model.

There are two ways to create new instances of a model, shown in this example:

```
simpleCode <- nimbleCode({
    for(i in 1:N) x[i] ~ dnorm(0, 1)
    })

## Return the model definition only, not a built model
```

```
simpleModelDefinition <- nimbleModel(simpleCode, constants = list(N = 10),
                                     returnDef = TRUE, check = FALSE)
## Make one instance of the model
simpleModelCopy1 <- simpleModelDefinition$newModel(check = FALSE)
## Make another instance from the same definition
simpleModelCopy2 <- simpleModelDefinition$newModel(check = FALSE)
## Ask simpleModelCopy2 for another copy of itself
## small bug in version 0.6-1 means we need to set 'data' to an
## empty list for this to work; this will be fixed in 0.6-2
simpleModelCopy3 <- simpleModelCopy2$newModel(check = FALSE, data =
   list())
```

LET'S CHECK THE STATUS OF THE BUG DESCRIBED IN THE COMMENTS.

Each copy of the model can have different nodes flagged as data and different values in any nodes. They cannot have different values of N because that is a constant; it must be a constant because it helps define the model.

6.2 NIMBLE models are objects you can query and manipulate

NIMBLE models are objects that can be modified and manipulated from R. In this section we introduce some basic ways to use a model object. Chapter ?? covers more topics for writing algorithms that use models.

6.2.1 What are variables and nodes?

This section discusses some basic concepts and terminology to be able to speak about NIMBLE models clearly.

Suppose we have created a model from the following BUGS code.

```
mc <- nimbleCode({
    a ~ dnorm(0, 0.001)
    for(i in 1:5) {
        y[i] ~ dnorm(a, sd = 0.1)
        for(j in 1:3)
            z[i,j] ~ dnorm(y[i], tau)
    }
    tau ~ dunif(0, 20)
    y.squared[1:5] <- y[1:5]^2
})

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

In NIMBLE terminology:

- The *variables* of this model are `a`, `y`, `z`, and `y.squared`.
- The *nodes* of this model are `a`, `y[1]` ... `y[5]`, `z[1,1]` ... `z[5, 3]`, and `y.squared[1:5]`. In graph terminology, nodes are vertices in the model graph.
- the *node functions* of this model are `a ~ dnorm(0, 0.001)`, `y[i] ~ dnorm(a, 0.1)`, `z[i,j] ~ dnorm(y[i], sd = 0.1)`, and `y.squared[1:5] <- y[1:5]^2`. Each node's calculations are handled by a node function. Sometimes the distinction between nodes and node functions is important, but when it is not important we may refer to both simply as *nodes*.
- The *scalar elements* of this model include all the scalar nodes as well as the scalar elements `y.squared[1]` ... `y.squared[5]` of the multivariate node `y.squared[1:5]`.

6.2.2 Determining the nodes and variables in a model

One can determine the variables in a model using `getVarNames` and the nodes in a model using `getNodeNames`, with optional arguments allowing you to select only certain types of nodes.

```
model$getVarNames()
```

```
## [1] "a"                           "y"
## [3] "lifted_d1_over_sqrt_oPtau_cP" "z"
## [5] "tau"                         "y.squared"
```

```
model$getNodeNames()
```

```
##  [1] "a"
##  [2] "tau"
##  [3] "y[1]"
##  [4] "y[2]"
##  [5] "y[3]"
##  [6] "y[4]"
##  [7] "y[5]"
##  [8] "lifted_d1_over_sqrt_oPtau_cP"
##  [9] "y.squared[1:5]"
## [10] "z[1, 1]"
## [11] "z[1, 2]"
## [12] "z[1, 3]"
## [13] "z[2, 1]"
## [14] "z[2, 2]"
## [15] "z[2, 3]"
## [16] "z[3, 1]"
## [17] "z[3, 2]"
## [18] "z[3, 3]"
## [19] "z[4, 1]"
## [20] "z[4, 2]"
```

```
## [21] "z[4, 3]"
## [22] "z[5, 1]"
## [23] "z[5, 2]"
## [24] "z[5, 3]"

model$getNodeNames(determOnly = TRUE)

## [1] "lifted_d1_over_sqrt_oPtau_cP" "y.squared[1:5]"

model$getNodeNames(stochOnly = TRUE)

##  [1] "a"        "tau"     "y[1]"    "y[2]"    "y[3]"    "y[4]"
##  [7] "y[5]"    "z[1, 1]" "z[1, 2]" "z[1, 3]" "z[2, 1]" "z[2, 2]"
## [13] "z[2, 3]" "z[3, 1]" "z[3, 2]" "z[3, 3]" "z[4, 1]" "z[4, 2]"
## [19] "z[4, 3]" "z[5, 1]" "z[5, 2]" "z[5, 3]"

model$getNodeNames(dataOnly = TRUE)

##  [1] "z[1, 1]" "z[1, 2]" "z[1, 3]" "z[2, 1]" "z[2, 2]" "z[2, 3]"
##  [7] "z[3, 1]" "z[3, 2]" "z[3, 3]" "z[4, 1]" "z[4, 2]" "z[4, 3]"
## [13] "z[5, 1]" "z[5, 2]" "z[5, 3]"
```

Note that some of the nodes may be "lifted" nodes introduced by NIMBLE (Section **??**). In this case `lifted_d1_over_sqrt_oPtau_cP` (this is a node for the standard deviation of the `z` nodes using NIMBLE's canonical parameterization of the normal distribution) is the only lifted node in the model.

To determine the dependencies of one or more nodes in the model, you can use `getDependencies` as discussed in Section **??**.

moved expandNodeNames stuff to chapter 11

moved getDependencies stuff to chapter 11

6.2.3   Accessing nodes

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 -0.4115108   0.2522234 -0.8919211           NA

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

## [1]   0.4356833 -0.4115108   0.2522234 -0.8919211 -1.2375384

model$z[1,]

## [1]   1.2629543 -1.5399500   0.7635935
```

While nodes that are part of a variable can be accessed as above, each node also has its own name that can 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] -0.4115108

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

## [1]   0.4356833 -5.0000000   0.2522234 -0.8919211 -1.2375384

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

## [1] -0.7990092

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

## [1] -0.928567

model$z[2, 2]

## [1] -0.928567
```

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, such as `model[['z[2:4, 1:2]']][1, 2]`.

6.2.4   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 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)), calculate = FALSE)

multiVarModel$getNodeNames()

## [1] "lifted_chol_oPcov_oB1to5_1to5_cB_cP[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 multi-variate normal nodes.

In the event you need to ensure that a name is formatted correctly, you can use the `expandNodeNames` method. For example, to get the spaces correctly inserted into "X[1,1:5]":

```
multiVarModel$expandNodeNames("X[1,1:5]")

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

Alternatively, for those inclined to R's less commonly used features, a nice trick is to use its `parse` and `deparse` functions.

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

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

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

6.2.5   Why use node names?

Syntax like `model[["z[2, 3]"]]` may seem strange at first, because the natural habit of an R user would be `model[["z"]][2,3]`. To see its utility, consider the example of writing the nimbleFunction given in Section **??**. 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, regardless of the dimensionality of the variable in which it is embedded. This is particularly useful for NIMBLE, which resolves how to access a particular node during the compilation process.

6.2.6   Checking if a node holds data

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

```
model$isData('z[1]')

## [1] TRUE

model$isData(c('z[1]', 'z[2]', 'a'))

## [1]  TRUE  TRUE FALSE

model$isData('z')

##  [1] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
## [13] TRUE TRUE TRUE

model$isData('z[1:3, 1]')

## [1] TRUE TRUE TRUE
```

Part III

Algorithms in NIMBLE

Chapter 7

MCMC

Configuring, building and running an MCMC algorithm for a NIMBLE model involves the following steps:

1. Optionally create and customize an MCMC configuration for a particular model:
   (a) Use `configureMCMC` to create an MCMC configuration (see Chapters **??**-**??**). The configuration contains a list of samplers with the node(s) they will sample.
   (b) Customize the MCMC configuration:
       i. add, remove, or re-order the list of samplers (section **??** and `help(samplers)` in R for details), including adding your own samplers (section **??**);
       ii. change the tuning parameters or adaptive properties of individual samplers;
       iii. change the variables to monitor (record for output) and thinning intervals for MCMC samples.
2. Use `buildMCMC` to build the MCMC object and its samplers either from the model (using default MCMC configuration) or from a customized MCMC configuration.
3. Compile the MCMC object (and the model), unless one is debugging and wishes to run the uncompiled MCMC.
4. Run the MCMC and extract the samples (sections **??** and **??**).

NIMBLE provides several functions to simplify running one or multiple MCMCs:

- `runMCMC` simplifies the steps of modifying initial values, removing burn-in samples, returning samples in the form of a `coda mcmc` object, and running multiple chains for the same MCMC (section **??**).
- `MCMCsuite` can run multiple, different MCMCs for the same model. These can include multiple NIMBLE MCMCs from different configurations as well as external MCMCs such as from WinBUGS, OpenBUGS, JAGS or Stan (section **??**).
- `compareMCMCs` manages multiple calls to `MCMCsuite` and generates html pages comparing performance of different MCMCs.

End-to-end examples of MCMC in NIMBLE have been shown in sections **??**, **??** and **??**.

7.1   The MCMC configuration

The MCMC configuration contains information needed for building an MCMC. When no customization is needed, one can jump directly to the `buildMCMC` step below. An MCMC configuration is an object of class `MCMCconf`, which includes:

- the model on which the MCMC will operate;
- the model nodes which will be sampled (updated) by the MCMC;
- the samplers and their internal configurations, called control parameters;
- two sets of variables that will be monitored (recorded) during execution of the MCMC and thinning intervals for how often each set will be recorded. Two sets are allowed because it can be useful to monitor different variables at different intervals.

7.1.1   Default MCMC configuration

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

```
mcmcConf <- configureMCMC(Rmodel)
```

The default configuration will contain a single sampler for each node in the model, and the default ordering follows the topological ordering of the model.

Default assignment of sampler algorithms

The default sampler assigned to a stochastic node is determined by the following, in order of precedence:

1. If the node has no stochastic dependents, a `posterior_predictive` sampler is assigned. This sampler sets the new value for the node simply by simulating from its distribution.
2. If the node has a conjugate relationship between its prior distribution and the distributions of its stochastic dependents, a `conjugate` (Gibbs) sampler is assigned.
3. If the node is binary-valued (strictly taking values 0 or 1), then a `binary` sampler is assigned. This sampler calculates the conditional probability for both possible node values and draws the new node value from the conditional distribution, in effect making a Gibbs sampler.
4. If the node follows a multinomial distribution, then a `RW_multinomial` sampler is assigned. This is a discrete random-walk sampler in the space of multinomial outcomes.
5. If the node is otherwise discrete-valued, then a `slice` sampler is assigned [?].
6. If a node follows a Dirichlet distribution, then a `RW_dirichlet` sampler is assigned. This is a random walk sampler in the space of the simplex defined by the Dirichlet.
7. If the node follows a multivariate distribution, then a `RW_block` sampler is assigned for all elements. This is a Metropolis-Hastings adaptive random-walk sampler with a multivariate normal proposal [?].

8. If none of the above criteria are satisfied, then a `RW` sampler is assigned. This is a Metropolis-Hastings adaptive random-walk sampler with a univariate normal proposal distribution.

The default control parameters governing each of these samplers can be inspected and modified with `nimbleOptions('MCMCcontrolDefaultList')`.

Details of each sampler and its control parameters can be found by `help(samplers)` in R with `nimble` loaded.

Modifying the default sampler assignments

`configureMCMC` can take control arguments `useConjugacy`, `onlyRW`, `onlySlice`, and `multivariateNodesAsScalars` to modify default sampler assignments. These tell `configureMCMC` whether to assign conjugate sampler when possible, whether to use only random walk or only slice samplers, and whether to sample scalar elements of multivariate nodes individually, respectively. See `help(configureMCMC)` for usage details.

Default monitors

The default MCMC configuration includes monitors on all top-level stochastic nodes of the model. MCMC configurations include two sets of monitors, each with different thinning intervals. By default, the second set of monitors (`monitors2`) is empty.

Automated parameter blocking

The default configuration may be replaced by one generated from an automated parameter blocking algorithm. This algorithm determines groupings of model nodes that, when jointly sampled with a `RW_block` sampler, increase overall MCMC efficiency. Overall efficiency is defined as the effective sample size of the slowest-mixing node divided by computation time. This is done by:

```
autoBlockConf <- configureMCMC(Rmodel, autoBlock = TRUE)
```

Note that this using `autoBlock = TRUE` compiles and runs MCMCs, progressively exploring different sampler assignments, so it takes some time and generates some output. It is most useful for determining effective blocking strategies that can be re-used for later runs. The additional control argument `autoIt` may also be provided to indicate the number of MCMC samples to be used in each trial of the automated blocking procedure (default 20,000).

7.1.2 Customizing the MCMC configuration

The MCMC configuration may be customized in a variety of ways, either through additional named arguments to `configureMCMC` or by calling methods of an existing `MCMCconf` object.

Controlling which nodes to sample

One can create an MCMC configuration 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 node and/or variable names. In the case of a variable name, a default sampler will be added for all stochastic nodes in the variable. The order of samplers will match the order of `nodes`. Any deterministic nodes will be ignored.

If a data node is included in `nodes`, *it will be assigned a sampler*. This is the only way in which a default sampler may be placed on a data node and will result in overwriting data values in the node.

Creating an empty configuration

If you plan to customize the choice of all samplers, it can be useful to obtain a configuration with no sampler assignments at all. This can be done by `nodes = NULL`, `nodes = character()`, or `nodes = list()`.

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 and any subsequent sampler added via `addSampler` (see below). For example, the following will create the default MCMC configuration, except all `RW` samplers will have their initial `scale` set to 3, and none of the samplers (`RW`, or otherwise) will be adaptive.

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

When adding samplers to a configuration, the default control list can be over-ridden.

Adding samplers to the configuration: `addSampler`

Samplers may be added to a configuration using the `addSampler` method of the `MCMCconf` object. The frst argument gives the node(s) to be sampled, called the `target`, as a character vector. The second argument gives the type of sampler, which may be provided as a character string or a `nimbleFunction` object. Valid character strings include 'posterior_predictive', 'RW', 'RW_block', 'slice', 'RW_multinomial', 'RW_dirichlet', 'binary', 'ess', 'crossLevel', and 'RW_llFunction'. Added samplers can be labeled with a `name` argument, which is used in output of `printSamplers`.

Question from PdV: Isn't 'conjugate' now a valid sampler type?

Writing a new sampler as a `nimbleFunction` is covered in section **??**.

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 to `configureMCMC`;
3. the defaults, which are in `nimbleOptions('MCMCcontrolDefaultList')`.

Samplers added by `addSampler` will be appended to the end of current sampler list. Adding a sampler for a node will *not* automatically remove any existing samplers on that node.

Printing, re-ordering, modifying and removing samplers: `printSamplers`, `cdget-SamplerDefinition`, and `removeSamplers`

The current, ordered, list of all samplers in the MCMC configuration may be printed by calling the `printSamplers` method. When you want to see only samplers acting on specific model nodes or variables, provide those names as an argument to `printSamplers`.

The `nimbleFunction` definition underlying a particular sampler may be viewed using the `getSamplerDefinition` method, using the sampler index as an argument. A node name argument may also be supplied, in which case the definiton of the first sampler acting on that node is returned. In all cases, `getSamplerDefinition` only returns the definition of the *first* sampler specified either by index or node name.

```
## Return the definition of the third sampler in the mcmcConf object
mcmcConf$getSamplerDefinition(3)

## Return the definition of the first sampler acting on node 'x',
## or the first of any indexed nodes comprising the variable 'x'
mcmcConf$getSamplerDefinition('x')
```

The existing samplers may be re-ordered using the `setSamplers` method. The `ind` argument is a vector of sampler indices, or a character vector of model node or variable names. Here are a few examples. Each example assumes the `MCMCconf` object initially contains 10 samplers, and each example is independent of the others.

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

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

## Reverse the ordering of the samplers
mcmcConf$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.
mcmcConf$setSamplers(ind = c(1, 1, 1, 2, 3))
```

```
## Set the list of samplers to only those acting on model node 'alpha'
mcmcConf$setSamplers('alpha')

## Set the list of samplers to those acting on any components of the
## model variables 'x', 'y', or 'z'.
mcmcConf$setSamplers(c('x', 'y', 'z'))
```

Samplers may be removed from the current sampler ordering with the `removeSamplers` method. The following examples again assume that `mcmcConf` initially contains 10 samplers, and each example is independent of the others. `removeSamplers` accepts a vector of numeric indices of samplers to be removed or a character vector. In the latter case, all samplers acting on the named target model nodes will be removed.

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

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

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

## Remove all samplers acting on 'x' or any component of it
mcmcConf$removeSamplers('x')

## Default: providing no argument removes all samplers
mcmcConf$removeSamplers()
```

Customizing individual sampler configurations: `getSamplers`, `setSamplers`, `setName`, `setSamplerFunction`, `setTarget`, **and** `setControl`

PdV suggests this new subsubsection. Should getSamplerDefinition be moved here?

Each sampler in an `MCMCconf` object is represented by a sampler configuration as a `samplerConf` object. Each `samplerConf` is a reference class object containing the following (required) fields: name (a character string), samplerFunction (a valid nimbleFunction sampler), target (the model node to be sampled), and control (list of control arguments). The `MCMCconf` method `getSamplers` allows access to the `samplerConf` objects. These can be modified and then passed as an argument to `setSamplers` to over-write the current list of samplers in the MCMC configuration object. However, no checking of the validity of this modified list is performed; if the list of samplerConf objects is corrupted to be invalid, incorrect behavior will result at the time of calling `buildMCMC`. The fields of a `samplerConf` object can be modified using the access functions `setName(name)`, `setSamplerFunction(fun)`, `setTarget(target, model)`, and `setControl(control)`.

Here are some examples:

```r
## retrieve samplerConf list
samplerConfList <- mcmcConf$getSamplers()

## change the name of the first sampler
samplerConfList[[1]]$setName('newNameForThisSampler')

## change the sampler function of the second sampler,
## assuming existance of a nimbleFunction 'anotherSamplerNF',
## which represents a valid nimbleFunction sampler.
samplerConfList[[2]]$setSamplerFunction(anotherSamplerNF)

## change the 'adaptive' element of the control list of the third sampler
control <- samplerConfList[[3]]$control
control$adaptive <- FALSE
samplerConfList[[3]]$setControl(control)

## change the target node of the fourth sampler
samplerConfList[[4]]$setTarget('y', model)    ## model argument required

## use this modified list of samplerConf objects in the MCMC configuration
mcmcConf$setSamplers(samplerConfList)
```

Monitors and thinning intervals: `printMonitors`, `getMonitors`, `addMonitors`, `setThin`, and `resetMonitors`

An MCMC configuration object contains two independent lists of variables to monitor, each with their own thinning interval: `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` and `monitors2` will be recorded (with thinning interval `thin`) into objects called `mvSamples` and `mvSamples2`, contained within the MCMC object. These are both *modelValues* objects; *modelValues* are NIMBLE data structures used to store multiple sets of values of model variables. These can be accessed as the member data `mvSamples` and `mvSamples2` of the MCMC object, and they can be converted to matrices using `as.matrix` (see **??**).

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

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

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

Similarly, either thinning interval may be set at either step:

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

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

The current lists of monitors and thinning intervals may be displayed using the `printMonitors` method. Both sets of monitors (`monitors` and `monitors2`) may be reset to empty character vectors by calling the `resetMonitors` method. The methods `getMonitors` and `getMonitors2` return the currently specified `monitors` and `monitors2` as character vectors.

Monitoring model log-probabilities

To record model log-probabilities from an MCMC, one can add monitors for *logProb variables* (which begin with the prefix `logProb_`) that correspond to variables with (any) stochastic nodes. For example, to record and extract log-probabilities for the variables `alpha`, `sigma_mu`, and `Y`:

```
mcmcConf <- configureMCMC(Rmodel)
mcmcConf$addMonitors('logProb_alpha', 'logProb_sigma_mu', 'logProb_Y')
Rmcmc <- buildMCMC(mcmcConf)
Cmodel <- compileNimble(Rmodel)
Cmcmc <- compileNimble(Rmcmc, project = Rmodel)
Cmcmc$run(10000)
samples <- as.matrix(Cmcmc$mvSamples)
```

The `samples` matrix will contain both MCMC samples and model log-probabilities.

Measuring sampler computation times: `getTimes`

If you want to obtain the computation time spent in each sampler, you can set `time=TRUE` as a run-time argument and then use the method `getTimes()` obtain the times. For example,

```
Cmcmc$run(niter, time=TRUE)
Cmcmc$getTimes()
```

will return a vector of the total time spent in each sampler, measured in seconds.

7.2 Building and compiling the MCMC

Once the MCMC configuration object has been created, and customized to one's liking, it may be used to build an MCMC function:

```
Rmcmc <- buildMCMC(mcmcConf)
```

buildMCMC is a `nimbleFunction`. The returned object `Rmcmc` is an instance of the NIMBLE function specific to configuration `mcmcConf`.

When no customization is needed, one can skip `configureMCMC` and simply provide a model object to `buildMCMC`. The following two MCMC functions will be identical:

```
mcmcConf <- configureMCMC(Rmodel)   ## default MCMC configuration
Rmcmc1 <- buildMCMC(mcmcConf)

Rmcmc2 <- buildMCMC(Rmodel)   ## uses the default configuration 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`. If the model has already been compiled, it should be provided as the `project` argument so the MCMC will be part of the same compiled project. 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 Running the MCMC

The MCMC algorithm (either the compiled or uncompiled version) can be executed using the member method `mcmc$run()` (see `help(buildMCMC)` in R). The `run` method has one required argument, `niter`, the number of iterations to be run.

The `run` method has an optional `reset` argument. When `reset = TRUE` (the default value), the following occurs prior to running the MCMC:

- All model nodes are checked and filled or updated as needed, in valid (topological) order. If a stochastic node is missing a value, it is populated using a call to `simulate` and its log probability value is calculated. The values of deterministic nodes are calculated from their parent nodes. If any right-hand-side-only nodes (e.g. explanatory variables) 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 configuration.

- The internal *modelValues* objects `mvSamples` and `mvSamples2` are each resized to the appropriate length for holding the requested number of samples (`niter/thin`, and `niter/thin2`, respectively).

When `mcmc$run(niter, reset = FALSE)` is called, the MCMC picks up from where it left off, continuing the previous chain and expanding the output as needed. No values in the model are checked or altered, and sampler functions are not reset to their initial states.

The `run` method takes an optional `simulateAll` argument. When `simulateAll = TRUE`, the `simulate` method of all stochastic nodes is called before running the MCMC. This generates a new set of initial values. It should be used with caution since values drawn from priors may be extreme or invalid in some models.

The `run` method has an optional `time` argument. When `time = TRUE`, the net computation time spent in each sampler will be recorded. See Section **??**.

7.4 Extracting MCMC samples

After executing the MCMC, the output samples can be extracted as follows:

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

These *modelValues* objects can be converted into matrices using `as.matrix`:

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

The column names of the matrices will be the node names of nodes in the monitored variables. Then, for example, the mean of the samples for node `x[2]` could be calculated as:

```
mean(samplesMatrix[, 'x[2]'])
```

Obtaining samples as matrices is most common, but see section **??** for more about programming with `modelValues` objects, especially if you want to write nimbleFunctions to use the samples.

7.5 Running multiple MCMC chains

Once an MCMC algorithm has been created using `buildMCMC`, the function `runMCMC` can be used to run multiple chains and extract samples (see `help(runMCMC)` in R). `runMCMC` can be used to execute compiled or uncompiled algorithms, although uncompiled algorithms will be much slower. Specifically, `runMCMC` takes arguments to control:

- Number of iterations in each chain
- Number of chains

- Number of burnin samples to discard from each chain
- Inital values, or a function for generating initial values for each chain
- Setting the random number seed
- Supressing messages and output
- Returning the samples as a `coda mcmc` object

The following examples demonstrate some uses of `runMCMC`, and assume the existence of `Cmcmc`, a compiled MCMC algorithm.

```r
## run a single chain, return a matrix of samples
samplesMatrix <- runMCMC(Cmcmc)

## run three chains of 10,000 samples, discard a burnin of 1,000,
## and return of list of sample matrices
samplesList <- runMCMC(Cmcmc, niter=10000, nburnin=1000, nchains=3)

## run two chains, and provide inital values for each
initsList <- list(list(mu=1, sigma=1),
                  list(mu=2, sigma=10))
samplesList <- runMCMC(Cmcmc, nchains=3, inits=initsList)

## run ten chains of 100,000 iterations,
## using a function to generate inital valies
initsFunction <- function()
    list(mu=rnorm(1,0,1), sigma=runif(1,0,100))
samplesList <- runMCMC(Cmcmc, niter=100000, nchains=10, inits=initsFunction)

## run three chains, using a fixed random number seed for each chain
samplesList <- runMCMC(Cmcmc, nchains=3, setSeed=TRUE)

## run three chains, return a coda mcmc.list object
codaMCMClist <- runMCMC(Cmcmc, nchains=3, returnCodaMCMC=TRUE)
```

7.6 Samplers provided with NIMBLE

Most documentation of MCMC samplers provided with NIMBLE can be found by `help(samplers)` in R. Here we provide additional explanation of conjugate samplers and how complete customization can be achieved by making a sampler use an arbitrary log likelihood function, such as to build a particle MCMC algorithm.

PdV suggests cutting most of this since it is a copy of what is in the Rd pages. The example lines could be moved to the roxygen entries.

7.6.1 Conjugate (Gibbs) samplers

By default, `configureMCMC()` and `buildMCMC()` will assign conjugate samplers to all nodes satisfying a conjugate relationship, unless the option `useConjugacy = FALSE` is specified.

The current release of NIMBLE supports conjugate sampling of the relationships listed in Table ??[1].

Prior Distribution	Sampling (Dependent Node) Distribution	Parameter
Beta	Bernoulli	`prob`
	Binomial	`prob`
	Negative Binomial	`prob`
Dirichlet	Multinomial	`prob`
Gamma	Poisson	`lambda`
	Normal	`tau`
	Lognormal	`taulog`
	Gamma	`rate`
	Exponential	`rate`
Normal	Normal	`mean`
	Lognormal	`meanlog`
Multivariate Normal	Multivariate Normal	`mean`
Wishart	Multivariate Normal	`prec`

Table 7.1: Conjugate relationships supported by NIMBLE's MCMC engine.

Conjugate sampler functions may (optionally) dynamically check that their own posterior likelihood calculations are correct. If incorrect, a warning is issued. However, this functionality will roughly double the run-time required for conjugate sampling. By default, this option is disabled in NIMBLE. This option may be enabled by `nimbleOptions(verifyConjugatePosteriors = TRUE)`.

If one wants information about conjugate node relationships for other purposes, they can be obtained using `model$checkConjugacy()`. This returns a named list describing all conjugate nodes. The `checkConjugacy()` method can also accept a character vector argument specifying a subset of node names to check for conjugacy.

7.6.2 Customized log likelihood evaluations: `RW_llFunction` sampler

Sometimes it is useful to control the log likelihood calculations used for an MCMC updater instead of simply using the model. For example, one could use a sampler with a log likelihood that analytically (or numerically) integrates over latent model nodes. Or one could use a sampler with a log likelihood that comes from a stochastic approximation such as a particle filter (see below), allowing composition of a particle MCMC (PMCMC) algorithm [?]. The `RW_llFunction` sampler handles this by using a Metropolis-Hastings algorithm

---

[1]NIMBLE's internal definitions of these relationships can be viewed by `nimble:::conjugacyRelationshipsInputList`.

with a normal proposal distribution and a user-provided log-likelihood function. To allow compiled execution, the log-likelihood function must be provided as a specialized instance of a `nimbleFunction`. The log-likelihood function may use the same model as the MCMC as a setup argument (as does the example below), but if so the state of the model should be unchanged during execution of the function (or you must understand the implications otherwise).

The `RW_llFunction` sampler can be customized using the `control` list argument to set the initial proposal distribution scale and the adaptive properties for the Metropolis-Hastings sampling. In addition, the `control` list argument must contain a named `llFunction` element, which is specialized nimbleFunction that accepts no arguments and returns a scalar double number. The return value must be the total log-likelihood of all stochastic dependents of the `target` nodes – and, if `includesTarget = TRUE`, of the target node(s) themselves – or whatever surrogate is being used for the total log-likelihood. This is a required `control` list element with no default. See `help(samplers)` for details.

Complete example of correct usage:

```r
code <- nimbleCode({
    p ~ dunif(0, 1)
    y ~ dbin(p, n)
})

Rmodel <- nimbleModel(code, data = list(y=3), inits = list(p=0.5, n=10))

llFun <- nimbleFunction(
    setup = function(model) { },
    run = function() {
        y <- model$y
        p <- model$p
        n <- model$n
        ll <- lfactorial(n) - lfactorial(y) - lfactorial(n-y) +
                y * log(p) + (n-y) * log(1-p)
        returnType(double())
        return(ll)
    }
)

RllFun <- llFun(Rmodel)

mcmcConf <- configureMCMC(Rmodel, nodes = NULL)

mcmcConf$addSampler(target = 'p', type = 'RW_llFunction',
    control = list(llFunction = RllFun, includesTarget = FALSE))

Rmcmc <- buildMCMC(mcmcConf)
```

7.6.3   Particle MCMC `PMCMC` sampler

For state space models, a particle MCMC (PMCMC) sampler can be specified for top-level
parameters. This sampler is described in Section **??**.

7.7   Detailed MCMC example: `litters`

Here is a detailed example of specifying, building, compiling, and running two MCMC algo-
rithms. We use the `litters` example from the BUGS examples.

```
#############################
##### model configuration #####
#############################

## 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(a = c(1, 1),
              b = c(1, 1),
              p = matrix(0.5, nrow = 2, ncol = 16),
```

```
              mu    = c(.5, .5),
              theta = c(.5, .5))

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

## defining model...
## building model...
## setting data and initial values...
## running calculate on model (any error reports that follow may simply reflect
missing values in model variables) ...
##
## checking model sizes and dimensions...
##
## model building finished.

#########################################
##### MCMC configuration and building #####
#########################################

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

## check the samplers assigned by default MCMC configuration
mcmcConf$printSamplers()

## [1]  RW sampler: a[1]
## [2]  RW sampler: a[2]
## [3]  RW sampler: b[1]
## [4]  RW sampler: b[2]
## [5]  conjugate_dbeta_dbin sampler: p[1, 1]
## [6]  conjugate_dbeta_dbin sampler: p[1, 2]
## [7]  conjugate_dbeta_dbin sampler: p[1, 3]
## [8]  conjugate_dbeta_dbin sampler: p[1, 4]
## [9]  conjugate_dbeta_dbin sampler: p[1, 5]
## [10] conjugate_dbeta_dbin sampler: p[1, 6]
## [11] conjugate_dbeta_dbin sampler: p[1, 7]
## [12] conjugate_dbeta_dbin sampler: p[1, 8]
## [13] conjugate_dbeta_dbin sampler: p[1, 9]
## [14] conjugate_dbeta_dbin sampler: p[1, 10]
## [15] conjugate_dbeta_dbin sampler: p[1, 11]
```

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


## double-check our monitors, and thinning interval
mcmcConf$printMonitors()

## thin = 1: mu

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

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

## generate an empty MCMC configuration
## we need a new copy of the model to avoid compilation errors
Rmodel2 <- Rmodel$newModel()

## setting data and initial values...
## running calculate on model (any error reports that follow may simply reflect
missing values in model variables) ...
##
## checking model sizes and dimensions...
##

mcmcConf_CL <- configureMCMC(Rmodel2, nodes = NULL, monitors = 'mu')
```

```
## add two crossLevel samplers
mcmcConf_CL$addSampler(target = c('a[1]', 'b[1]'), type = 'crossLevel')

mcmcConf_CL$addSampler(target = c('a[2]', 'b[2]'), type = 'crossLevel')

## let's check the samplers
mcmcConf_CL$printSamplers()

## [1] crossLevel sampler: a[1], b[1]
## [2] crossLevel sampler: a[2], b[2]

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



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

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

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_49_48.dll > dynamicRegistrations_03_08_15_49_48.log'
had status 1
## Error:  Failed to create the shared library

Cmodel2 <- compileNimble(Rmodel2)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_49_54.dll > dynamicRegistrations_03_08_15_49_54.log'
had status 1
## Error:  Failed to create the shared library

## 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)
```

```
## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_50_00.dll > dynamicRegistrations_03_08_15_50_00.log'
had status 1
## Error:  Failed to create the shared library
```

```
Cmcmc_CL <- compileNimble(mcmc_CL, project = Rmodel2)
```

```
## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_50_07.dll > dynamicRegistrations_03_08_15_50_07.log'
had status 1
## Error:  Failed to create the shared library
## run the default MCMC function,
## and example the mean of mu[1]
Cmcmc$run(1000)
```

```
## Error in eval(expr, envir, enclos):  object 'Cmcmc' not found
```

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

```
## Error in as.matrix(Cmcmc$mvSamples):  object 'Cmcmc' not found
```

```
mean(cSamplesMatrix[, 'mu[1]'])
```

```
## Error in mean(cSamplesMatrix[, "mu[1]"]):  object 'cSamplesMatrix' not found
## run the crossLevel MCMC function,
## and examine the mean of mu[1]
Cmcmc_CL$run(1000)
```

```
## Error in eval(expr, envir, enclos):  object 'Cmcmc_CL' not found
```

```
cSamplesMatrix_CL <- as.matrix(Cmcmc_CL$mvSamples)
```

```
## Error in as.matrix(Cmcmc_CL$mvSamples):  object 'Cmcmc_CL' not found
```

```
mean(cSamplesMatrix_CL[, 'mu[1]'])
```

```
## Error in mean(cSamplesMatrix_CL[, "mu[1]"]):  object 'cSamplesMatrix_CL' not
found
################################
#### run multiple MCMC chains #####
################################

## run 3 chains of the crossLevel MCMC
samplesList <- runMCMC(Cmcmc_CL, niter=1000, nchains=3)
```

```
## Error in is.nfGenerator(f):  object 'Cmcmc_CL' not found
```

```
lapply(samplesList, dim)
```

```
## Error in lapply(samplesList, dim):  object 'samplesList' not found
```

7.8 Comparing different MCMCs with `MCMCsuite` and `compareMCMCs`

NIMBLE's `MCMCsuite` function automatically runs WinBUGS, OpenBUGS, JAGS, Stan, and/or multiple NIMBLE configurations on the same model. Note that the BUGS code must be compatible with whichever BUGS packages are included, and separate Stan code must be provided. NIMBLE's `compareMCMCs` manages calls to `MCMCsuite` for multiple sets of comparisons and organizes the output(s) for generating html pages summarizing results. It also allows multiple results to be combined and allows some different options for how results are processed, such as how effective sample size is estimated.

We show how to use `MCMCsuite` for the same `litters` example used in Section **??**. Subsequently, additional details of the `MCMCsuite` are given. Since use of `compareMCMCs` is similar, we refer readers to `help(compareMCMCs)` and the functions listed under "See also" on that R help page.

7.8.1 MCMC Suite example: `litters`

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

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

```r
output <- MCMCsuite(
    code = litters_code,
    constants = constants,
    data = data,
    inits = inits,
    monitors = 'mu',
    MCMCs = c('winbugs', 'jags', 'nimble', 'nimble_slice', 'nimble_CL'),
    MCMCdefs = list(
        nimble_CL = quote({
            mcmcConf <- configureMCMC(Rmodel, nodes = NULL)
            mcmcConf$addSampler(target = c('a[1]', 'b[1]'), type = 'crossLevel')
            mcmcConf$addSampler(target = c('a[2]', 'b[2]'), type = 'crossLevel')
            mcmcConf
        })),
    plotName = 'littersSuite'
)
```

7.8.2   MCMC Suite outputs

Executing the MCMC Suite returns a named list containing various outputs, as well as generates and saves traceplots and posterior density plots. The default elements of this return list object are:

Samples

`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 - burnin`.

Summary

The MCMC suite output contains a variety of pre-computed summary statistics, which are stored in the `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:

```
output$summary
# , , mu[1]
#                     mean     median         sd quant025  quant975
# winbugs        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
# winbugs        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

`timing` contains a named vector of the runtime for each MCMC algorithm, the total compile time for the NIMBLE model and MCMC algorithms, and the compile time for Stan (if specified). All run- and compile- times are given in seconds.

Efficiency

Using the MCMC Suite option `calculateEfficiency = TRUE` will also provide several measures of MCMC sampling efficiency. Additional summary statistics are provided for each node: the total number of samples collected (n), the effective sample size resulting from these samples (ess), and the effective sample size per second of algorithm runtime (*efficiency*).

In addition to these node-by-node measures of efficiency, an additional return list element is also provided. This element, *efficiency*, is itself a named list containing two elements: *min* and *mean*, which contain the minimal and mean efficiencies (effective sample size per second of algorithm runtime) across all monitored nodes, separately for each algorithm.

Plots

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

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

7.8.3   Customizing MCMC Suite

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

- MCMC algorithms to execute, optionally including WinBUGS, OpenBUGS, JAGS, Stan, and various flavours of NIMBLE's MCMC
- Custom-configured NIMBLE MCMC algorithms
- Automated parameter blocking for efficienct MCMC sampling
- Nodes to monitor
- Number of MCMC iterations
- Thinning interval
- Burn-in
- Summary statistics to report
- Calculating sampling efficiency (effective sample size per second of algorithm runtime)
- Generating and saving plots

NIMBLE MCMC algorithms may be specified using the `MCMCs` argument to `MCMCsuite`, which is character vector defining the MCMC algorithms to run. The `MCMCs` argument may include any of the following algorithms:

'`winbugs`' WinBUGS MCMC algorithm
'`openbugs`' OpenBUGS MCMC algorithm
'`jags`' JAGS MCMC algorithm

'`Stan`' Stan MCMC algorithm

'`nimble`' NIMBLE MCMC using the default configuration

'`nimble_noConj`' NIMBLE MCMC using the default configuration with `useConjugacy = FALSE`

'`nimble_RW`' NIMBLE MCMC using the default configuration with `onlyRW = TRUE`

'`nimble_slice`' NIMBLE MCMC using the default configuration with `onlySlice= TRUE`

'`autoBlock`' NIMBLE MCMC algorithm with block sampling of dynamically determined parameter groups attempting to maximize sampling efficiency

The default value for the `MCMCs` argument is '`nimble`', which specifies only the default NIMBLE MCMC algorithm.

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 is given with the `crossLevel` algorithm in the `litters` MCMC Suite example.

The `MCMCdefs` may be provided as 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 configuration 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 configuration; it need only specify the samplers.

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

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

Full details of the arguments and customization of the MCMC Suite is available through the R help using `help(MCMCsuite)`.

Chapter 8

Sequential Monte Carlo and MCEM

The NIMBLE algorithm library is growing and as of version 0.5-1 includes a suite of Sequential Monte Carlo algorithms as well as a more robust MCEM.

8.1 Particle Filters / Sequential Monte Carlo

8.1.1 Filtering Algorithms

NIMBLE includes algorithms for four different types of sequential Monte Carlo (also known as particle filters), which can be used to sample from the latent states and approximate the log likelihood of a state space model. The particle filters currently implemented in NIMBLE are the bootstrap filter, the auxiliary particle filter, the Liu-West filter, and the ensemble Kalman filter, which can be built, respectively, with calls to `buildBootstrapFilter`, `buildAuxiliaryFilter`, `buildLiuWestFilter`, and `buildEnsembleKF`. Each particle filter requires setup arguments `model` and `nodes`, which is a character vector specifying latent model nodes. In addition, each particle filter can be customized using a `control` list argument. Details on the control options and specifics of the filtering algorithms can be found in the help pages for the functions.

Once built, each filter can be run by specifying the number of particles. Each filter has a model values object named `mvEWSamples` that is populated with equally-weighted samples from the posterior distribution of the latent states (and in the case of the Liu-West filter, the posterior distribution of the top level parameters as well) as the filter is run. The bootstrap, auxiliary, and Liu-West filters also have another model values object, `mvWSamples`, which has unequally-weighted samples from the posterior distribution of the latent states, along with weights for each particle. In addition, the bootstrap and auxiliary particle filters return estimates of the log likelihood of the given state space model.

We first create a linear state-space model to use as an example for our particle filter algorithms.

```
# 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 the model
rTimeModel <- nimbleModel(timeModelCode, constants = list(t = t),
                        data <- list(y = y), check = FALSE )

## defining model...
## building model...
## setting data and initial values...
## running calculate on model (any error reports that follow may simply reflect
missing values in model variables) ...
##
## checking model sizes and dimensions...
##  note that missing values (NAs) or non-finite values were found in model
variables:  x, lifted_x_oBi_minus_1_cB_times_a_plus_b, lifted_x_oBi_cB_times_c,
a, b, c, mu_0.  This is not an error, but some or all variables may need to
be initialized for certain algorithms to operate properly.
##
## model building finished.

#Set parameter values and compile the model
rTimeModel$a <- 0.5
rTimeModel$b <- 1
rTimeModel$c <- 1
```

```
rTimeModel$mu_0 <- 1

cTimeModel <- compileNimble(rTimeModel)

## compiling...   this may take a minute.   Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:   running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_50_20.dll > dynamicRegistrations_03_08_15_50_20.log'
had status 1
## Error:   Failed to create the shared library
```

Here is an example of building and running the bootstrap filter. Additional information about the bootstrap filter can be found with `help(buildBootstrapFilter)`.

```
#Build bootstrap filter
rBootF <- buildBootstrapFilter(rTimeModel, "x",
                                control = list(thresh = 0.8, saveAll = TRUE,
                                                smoothing = FALSE))
#Compile filter
cBootF <- compileNimble(rBootF,project = rTimeModel)

## compiling...   this may take a minute.   Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:   running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_50_27.dll > dynamicRegistrations_03_08_15_50_27.log'
had status 1
## Error:   Failed to create the shared library

#Set number of particles
parNum <- 5000
#Run bootstrap filter, which returns estimate of model log-likelihood
bootLLEst <- cBootF$run(parNum)

## Error in eval(expr, envir, enclos):   object 'cBootF' not found
```

Next, we provide an example of building and running the auxiliary particle filter. Additional information about the auxiliary particle filter can be found with `help(buildAuxiliaryFilter)`. Note that a filter cannot be built on a model that already has a filter specialized to it, so we create a new copy of our state space model first

```
#Copy our state-space model for use with the auxiliary filter
auxTimeModel <- rTimeModel$newModel(replicate = TRUE)

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

```
## checking model sizes and dimensions...
##  note that missing values (NAs) or non-finite values were found in model
variables:  x, y, lifted_x_oBi_minus_1_cB_times_a_plus_b, lifted_x_oBi_cB_times_c,
a, b, c, mu_0.  This is not an error, but some or all variables may need to
be initialized for certain algorithms to operate properly.
##

compileNimble(auxTimeModel)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_50_41.dll > dynamicRegistrations_03_08_15_50_41.log'
had status 1
## Error:  Failed to create the shared library

#Build auxiliary filter
rAuxF <- buildAuxiliaryFilter(auxTimeModel, "x",
                              control = list(thresh = 0.5, saveAll = TRUE))
#Compile filter
cAuxF <- compileNimble(rAuxF, project = auxTimeModel)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_50_46.dll > dynamicRegistrations_03_08_15_50_46.log'
had status 1
## Error:  Failed to create the shared library

#Run auxliary filter, which returns estimate of model log-likelihood
auxLLEst <- cAuxF$run(parNum)

## Error in eval(expr, envir, enclos):  object 'cAuxF' not found
```

Now we give an example of building and running the Liu and West filter, which can sample from the posterior distribution of top-level parameters as well as latent states. The Liu and West filter accepts an additional `params` argument, specifying the top-level parameters to be sampled. Additional information can be found with `help(buildLiuWestFilter)`.

```
#Copy model
LWTimeModel <- rTimeModel$newModel(replicate = TRUE)

## running calculate on model (any error reports that follow may simply reflect
missing values in model variables) ...
##
## checking model sizes and dimensions...
```

```
##  note that missing values (NAs) or non-finite values were found in model
variables:  x, y, lifted_x_oBi_minus_1_cB_times_a_plus_b, lifted_x_oBi_cB_times_c,
a, b, c, mu_0.  This is not an error, but some or all variables may need to
be initialized for certain algorithms to operate properly.
##

compileNimble(LWTimeModel)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_50_57.dll > dynamicRegistrations_03_08_15_50_57.log'
had status 1
## Error:  Failed to create the shared library

#Build Liu-West filter, also
#specifying which top level parameters to estimate
rLWF <- buildLiuWestFilter(LWTimeModel, "x", params = c("a", "b", "c"),
                           control = list(saveAll = FALSE))
#Compile filter
cLWF <- compileNimble(rLWF,project = LWTimeModel)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_51_06.dll > dynamicRegistrations_03_08_15_51_06.log'
had status 1
## Error:  Failed to create the shared library

#Run Liu-West filter
cLWF$run(parNum)

## Error in eval(expr, envir, enclos):  object 'cLWF' not found
```

Below we give an example of building and running the ensemble Kalman filter, which can sample from the posterior distribution of latent states. Additional information can be found with `help(buildEnsembleKF)`.

```
#Copy model
ENKFTimeModel <- rTimeModel$newModel(replicate = TRUE)

## running calculate on model (any error reports that follow may simply reflect
missing values in model variables) ...
##
## checking model sizes and dimensions...
##  note that missing values (NAs) or non-finite values were found in model
variables:  x, y, lifted_x_oBi_minus_1_cB_times_a_plus_b, lifted_x_oBi_cB_times_c,
```

```
a, b, c, mu_0.   This is not an error, but some or all variables may need to
be initialized for certain algorithms to operate properly.
##

compileNimble(ENKFTimeModel)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_51_20.dll > dynamicRegistrations_03_08_15_51_20.log'
had status 1
## Error:  Failed to create the shared library

#Build and compile ensemble Kalman filter
rENKF <- buildEnsembleKF(ENKFTimeModel, "x",
                         control = list(saveAll = FALSE))
cENKF <- compileNimble(rENKF,project = ENKFTimeModel)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_51_28.dll > dynamicRegistrations_03_08_15_51_28.log'
had status 1
## Error:  Failed to create the shared library

#Run ensemble Kalman filter
cENKF$run(parNum)

## Error in eval(expr, envir, enclos):  object 'cENKF' not found
```

Once each filter has been run, we can extract samples from the posterior distribution of our latent states as follows:

```
#Equally-weighted samples (available from all filters)
bootEWSamp <- as.matrix(cBootF$mvEWSamples)
auxEWSamp <- as.matrix(cAuxF$mvEWSamples)
LWFEWSamp <- as.matrix(cLWF$mvEWSamples)
ENKFEWSamp <- as.matrix(cENKF$mvEWSamples)

#Unequally-weighted samples, along with weights (available
#from bootstrap, auxiliary, and Liu and West filters)
bootWSamp <- as.matrix(cBootF$mvWSamples, 'x')
bootWts <- as.matrix(cBootF$mvWSamples, 'wts')
auxWSamp <-  as.matrix(xAuxF$mvWSamples, 'x')
auxWts <- as.matrix(cAuxF$mvWSamples, 'wts')
```

```
#Liu and West filter also returns samples
#from posterior distribution of top-level parameters:
aEWSamp <- as.matrix(cLWF$mvEWSamples, 'a')
```

8.1.2 Particle MCMC (PMCMC)

In addition to our four particle filters, NIMBLE also has particle MCMC samplers implemented. These sample top-level parameters by using either a bootstrap filter or auxiliary particle filter to obtain estimates of the likelihood of a model for use in a Metropolis-Hastings MCMC step. The `RW_PF` sampler uses a univariate normal proposal distribution, and should be used to sample scalar top-level parameters. The `RW_PF_block` sampler uses a multivariate normal proposal distribution for vectors of top-level parameters. Each PMCMC sampler also includes an optional algorithm to estimate the optimal number of particles to use in the particle filter at each iteration, based on a trade off between computational time and efficiency. The PMCMC samplers can be specified with a call to `addSampler` with `type = 'RW_PF'` or `type = 'RW_PF_block'`, a syntax similar to the other MCMC samplers listed in **??**.

The `RW_PF` sampler and `RW_PF_block` sampler can be customized using the `control` list argument to set the adaptive properties of the sampler and options for the particle filter algorithm to be run. In addition, setting the `pfOptimizeNparticles` control list option to `TRUE` will allow the sampler to estimate the optimal number of particles for the bootstrap filter. See `help(samplers)` for details. The MCMC configuration for the `timeModel` in the previous section will serve as an example for the use of our PMCMC sampler. Here we use the identity matrix as our proposal covariance matrix.

```
timeConf <- configureMCMC(rTimeModel)   # default MCMC configuration

# Add random walk pmcmc sampler with particle number optimization.
timeConf$addSampler(target = c('a', 'b', 'c', 'mu_0'), type = 'RW_PF_block',
                    control <- list(propCov= diag(4), adaptScaleOnly = FALSE,
                                    latents = 'x', pfOptimizeNparticles = TRUE))
```

8.2 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. NIMBLE provides an ascent-based MCEM algorithm that automatically determines when the algorithm has converged by examining the size of the changes in the likelihood between each iteration (`buildMCEM`).

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

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


compileNimble(pump)

#build an MCEM algorithm with Ascent-based convergence criterion
pumpMCEM <- buildMCEM(model = pump,
                    latentNodes = 'theta', burnIn = 300,
                    mcmcControl = list(adaptInterval = 100),
                    boxConstraints = list( list( c('alpha', 'beta'),
                                                limits = c(0, Inf) ) ),
                    buffer = 1e-6)
```

The first argument to the MCEM, `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 ascent-based MCEM algorithm has a number of control options:

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 **??**: 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 automatically detects box constraints for the nodes that will be optimized, using NIMBLE's getBounds() function. It is also possible for a user to manually specify constraints via the `boxConstraints` argument. 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 two, 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, its constraints will be automatically determined by NIMBLE. These constraint

arguments are passed as the `lower` and `upper` arguments to R's `optim` function, using `method = 'L-BFGS-B'`. Note that NIMBLE will give a warning if a user-provided constraint is more extreme than the constraint determined by NIMBLE.

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

In addition, the MCEM has some extra control options that can be used to further tune the convergence criterion. See `help(buildMCEM)` for more information.

Once an MCEM has been built for the model of interest, it can be run as follows. There is only one run-time argument, `initM`, which is the number of MCMC iterations to use when the algorithm is initialized.

```
pumpMLE <- pumpMCEM(initM = 1000)
pumpMLE
```

Direct maximization after analytically integrating over the latent nodes (possible for this model but often not feasible) gives estimates of $\hat{\alpha} = 0.823$ and $\hat{\beta} = 1.261$, so the MCEM seems to do pretty well.

Part IV

Programming with NIMBLE

Part **??** is the programmer's guide to NIMBLE. At the heart of programming in NIM-BLE are nimbleFunctions, which are written using the NIMBLE language (also called the NIMBLE DSL).

In Chapter **??**, we describe how to write simple nimbleFunctions (nimbleFunctions that don't interact with models) to compile parts of R for fast calculations. We then show how to use these simple nimbleFunctions to write user-defined distributions and user-defined functions that you can use within the BUGS code of a model to extend the distributions and functions build into NIMBLE (Chapter **??**).

We then move into the functionality in NIMBLE that allows one to program with models, namely writing nimbleFunctions that interact with models. We first describe how one interacts with models by querying model structure and carrying out model calculations (Chapter **??**). We then discuss the `modelValues` and `nimbleList` data structures in Chapter **??**. The functionality for interacting with models and `modelValues` is central to writing nimbleFunctions that operate on models, described in Chapter **??**. In particular one will often query model structure within nimbleFunction setup code and then carry out model calculations based on that structural information within nimbleFunction run code. Together Sections **??** and **??** describe what is allowed within the NIMBLE language, the language used for run code.

Chapter 9

Writing simple nimbleFunctions using the NIMBLE language

9.1 Introduction to simple nimbleFunctions

nimbleFunctions are the heart of programming in NIMBLE. In this part of the manual, you'll learn about the various ways to use nimbleFunctions. Here we'll start with simple nimbleFunctions that only contain the code to be compiled and executed, which we call the *run* code. nimbleFunctions are created with the `nimbleFunction` function.

Basic nimbleFunctions behave like R functions: `nimbleFunction` simply returns a function that can be executed and compiled. This is useful for doing math or the other kinds of processing available in NIMBLE when no model or modelValues is needed. The real benefits come from compiling the nimbleFunction; in other words, nimbleFunctions allow you to compile parts of R.

run code is written in the NIMBLE language. This is similar to a narrow subset of R, but it is important to remember that it is different – defined by what can be compiled – and much more limited. In addition, some information on variable types must be provided for input arguments, the return object, and in some circumstances for local variables.

Here's a basic example.

```
nimExp <- nimbleFunction(
      # run-time code for our computation
      run = function(x = double(1)) {
          returnType(double(1))
          n <- length(x)
          # some functions, like numeric, mimic R
          # but also may have additional/different features
          out <- numeric(n, init = FALSE)
          # core computation
          for( i in 1:n)
                out[i] <- exp(x[i])
          return(out)
```

```
        }
)

x <- rnorm(5)
exp(x)

## [1] 1.0193411 1.2934827 0.5225628 0.8876580 1.9428106

nimExp(x)

## [1] 1.0193411 1.2934827 0.5225628 0.8876580 1.9428106
```

9.2 Using and compiling simple nimbleFunctions

Here's a slightly more involved nimbleFunction that illustrates the use of linear algebra.

To a large extent, NIMBLE functions can be executed in R (uncompiled) as seen in the previous section or can be compiled as discussed next. Using them in R will be slow and is intended for testing and debugging algorithm logic (see Section **??**).

After we create the nimbleFunction, we can compile a fast version of the nimbleFunction using `compileNimble`.

```
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,] 0.20009897
## [2,] 0.01304248
## [3,] 0.09538966
## [4,] 0.06529313

CsolveLeastSquares <- compileNimble(solveLeastSquares)

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

```
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_51_33.dll > dynamicRegistrations_03_08_15_51_33.log'
had status 1
## Error:  Failed to create the shared library

CsolveLeastSquares(X, y)

## Error in eval(expr, envir, enclos):  could not find function "CsolveLeastSquares"
```

This example shows the textbook calculation of a least squares solution for regression of 100 data points on four explanatory variables, all generated randomly[1]. Such functions can be called from other nimbleFunctions or used in BUGS code.[2]

9.3 The NIMBLE language

9.3.1 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.
- Like R, NIMBLE uses 1-based indexing. For example, the first element of a vector `x` is `x[1]`, not `x[0]`.
- As in R, function calls in NIMBLE can provide arguments by name or in a default order.
- NIMBLE is the opposite of R for argument passing. R nearly always uses pass-by-value (formally call-by-value). NIMBLE nearly always uses pass-by-reference (or pointer). That means that in compiled execution only, changing the value of a variable that was a function input will change the value in the calling function. Thus it is possible to write a nimbleFunction that returns information by modifying an argument. Yes, that's a big difference in behavior!

  Although compiled nimbleFunctions can modify arguments, the R interface to a compiled 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 from R, 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.) perhaps this should be its own subsection with a single sentence as a bullet here?

---

[1]Of course in general, explicitly calculating the inverse is not the recommended numerical recipe for least squares.

[2]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.

- Variables in the NIMBLE language are typed, and types must be declared for arguments and return values.
- BUGS model nodes are implemented as nimbleFunctions with member functions for `calculate`, `calculateDiff`, `simulate`, `getLogProb`, `getParam`, and `getBound`.
- nimbleFunctions cannot generally be copied safely. Instead rerun `nimbleFunction` and record the result in a new object. useful to say here? Is there a case in which one would want to copy an RC function?

9.3.2 How numeric types work in NIMBLE

Variables in the NIMBLE language are typed – a given variable can only represent a specific kinds of value, such as a real number, integer, or character string, and the dimension (scalar, vector, matrix, etc.) cannot change once it is set.

Numeric types in NIMBLE are much less flexible than in R, a reflection of the fact that NIMBLE code can be compiled into C++[3]. In NIMBLE, the *type* of a numeric object refers to the number of dimensions and the numeric type of the elements. In Version 0.6-4, objects from 0 (scalar) to 4 dimensions are supported, and the numeric types *integer* and *double* are supported, as is a *logical* type. While the number of dimensions cannot change during run-time, numeric objects can be resized using `setSize` or by full (non-indexed) assignment.

Arguments and return values for functions must have their types and dimensions declared by the programmer.

Types and dimensions for variables declared within run code are handled differently. When possible, NIMBLE will determine the type of a local variable that is defined in run code for you. In particular, 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. In contrast, if the first uses of a variable involves indexing, the type must be declared explicitly and the size set as discussed in Section **??**. In addition, its size must be set before assigning into it.

Treatment of vectors of length 1 presents special challenges because they could be treated as scalars or vectors. Currently they are treated as scalars. I think we should say more here - we do allow length-one vectors and passing in a scalar from R into a double(1) (e.g.) will work. Perry, can you frame this more comprehensively here or somewhere else appropriate - I'm wondering if this should be its own subsection and also have a bullet on it in the previous subsection

`nimbleList`s provide containers for numeric, logical, and character type variables in NIMBLE. More information on using `nimbleList`s in `nimbleFunction`s can be found in Section **??**.

9.3.3 Declaring argument types and the return type

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

---

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

As illustrated in the example in Section **??**, the syntax for a type declaration is: `type(nDim, sizes)`.

`type` can be any of `double`, `integer`, `logical` or `character` (for scalars or vectors only). In a `returnType` statement, a type of `void()` is valid, and 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` (e.g. `double(2, c(4, 5))` declares a 4-×-5 matrix). If sizes are omitted, they will either be set when the entire object is assigned to, or an explicit call to `setSize` is needed.

In the case of scalar arguments only, a default value can be provided. For example, to provide 1.2 as a default:

```
myfun <- nimbleFunction(
    run = function(x = double(0, default = 1.2)) {
})
```

If one would like to use a `nimbleList` as an argument or the return value, one needs to specify the type as a `nimbleList` definition (see Section **??**).

9.3.4   Creating non-scalar variables: `numeric`, `integer`, `logical`, `matrix`, `array`, and `nimbleList`

When local variables in run code are created by assignment, their types will be automatically inferred. For example, `x <- A %*% B` will create `x` as a matrix. However, if a variable is to be filled by indexed assignment, then it must be explicitly created or re-sized first. For example, in the following code `x` must be created before being filled by indexed assignment:

```
## NOTE: must create x as a matrix here, first

for(i in 1:10)
    for(j in 1:5)
        x[i, j] <- foo(y[i, j])
```

Scalar variables never need to be created in advance.

NIMBLE provides several functions for creating non-scalar variables. These functions are similar to those of R, but they take additional arguments to set an initialization value, indicate floating-point or integer elements, and/or indicate no initialization is needed[4]. `numeric`, `integer`, and `logical` create floating-point, integer, and logical vectors (1-dimensional objects), respectively. `matrix` creates 2-dimensional objects, and `array` creates objects of 1, 2 or more dimensions. The latter two functions can be used for floating-point, integer, or logical objects.

After a variable has been created, its size may be changed either by non-indexed assignment or by `setSize`, as illustrated below. Note that `setSize` cannot change the number of dimensions of a variable, and it does *not* necessarily preserve the contents of the variable.

---

[4]Skipping initialization is more efficient, but this will typically be noticeable only for functions called many, many times.

numeric, integer, and logical

`numeric`, `integer`, or `logical` will create a 1-dimensional vector of floating-point, integer, or logical values, respectively. The `length` argument specifies the vector length (default 0), and the `value` argument specifies the initial scalar value for all vector elements (default 0). The `init` argument specifies whether or not to initialize the elements (default `TRUE`). If first use of the variable does not rely on initial values, you can use `init = FALSE`.

```
## Example of creating and resizing a floating-point vector
## myNumericVector will be of length 10, with all elements initialized to 2
myNumericVector <- numeric(10, value = 2)

## resize this numeric vector to be length 20
## both calls are equivalent
setSize(myNumericVector, 20)
setSize(myNumericVector, c(20))
```

```
## Example of creating a length-100 integer vector and filling it with the values 1, 2
n <- 100
myIntegerVector <- integer(n)
for(i in 1:n)
    myIntegerVector[i] <- i
```

```
## Example of creating a length-100 locical vector and filling it with TRUE
x <- 100
myIntegerVector <- logical(n, value = TRUE)
```

matrix and identityMatrix

`matrix` creates a 2-dimensional matrix object of either floating-point (if `type = 'double'`, the default), integer (if `type = 'integer'`), or logical (if `type = 'logical'`) values. The `nrow` and `ncol` arguments specify the number of rows and columns, respectively. The `value` and `init` argument are used in the same way as for `numeric()` and `integer()`.

```
## Example of creating a 10-by-1 column matrix of 1's and resizing it
onesMatrix <- matrix(1, nrow = 10, ncol = 1)

## resize this matrix to be a 10-by-10 matrix
## note that contents are not necessarily preserved
## both calls are equivalent
setSize(onesMatrix, 10, 10)
setSize(onesMatrix, c(10, 10))
```

NIMBLE provides the `identityMatrix` function for quickly creating instances of an identity matrix (all 0's with 1's on the main diagnol). This function takes a single argument, specifying the number of rows and colums in the resulting matrix.

```
I5 <- identityMatrix(5)
```

The resulting matrix may have its elements modified, or be used in arbitrary matematical expressions, as any variable in the DSL.

array

`array` creates a vector or higher-dimensional object, depending on the `dim` argument, which takes a vector of sizes for each dimension. The `type`, `value` and `init` argument behave the same as for `matrix`.

```
## the following three lines are equivalent
## each creates a length-10 vector, with elements equal to y
a <- numeric(10, value = y)
a <- array(y, dim = 10)
a <- array(y, dim = c(10))

## the following three lines are equivalent
## each creates an integer vector of length z[5], with elements equal to x+y
b <- integer(z[5], value = x + y)
b <- array(x+y, dim = z[5], type = 'integer')
b <- array(x+y, dim = c(z[5]), type = 'integer')

## the following two lines are equivalent
## each one creates a matrix of 0's of the same size as matrix x
c <- matrix(0, nrow = dim(x)[1], ncol = dim(x)[2])
c <- array(0, dim = c(dim(x)[1], dim(x)[2]))

## the following creates a 3-dimensional array of 0's
d <- array(0, dim = c(x, y, z))

## now resize this 3-dimensional array to be (x+1) by (y+1) by (z+1)
## both calls are equivalent
setSize(d, x+1, y+1, z+1)
setSize(d, c(x+1, y+1, z+1))
```

nimbleLists

`nimbleLists` can be created from a `nimbleList` definition as discussed in Section **??**.

Deprecated method of creating non-scalar objects using `declare`

Previous versions of NIMBLE provided a function `declare` for declaring variables. The more R-like functions `numeric`, `integer`, `matrix` and `array` are intended to replace `declare`, but `declare` is still supported for backward compatibility. In a future version of NIMBLE, `declare` may be removed.

9.3.5 Querying 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.
- `dim`, which has synonym `nimDim`, 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. Using `dim` vs. `nimDim` is a personal choice, but if you use `dim`, you should keep in mind that it behaves differently from R's `dim`.
  - A quirky limitation in Version 0.6-4: It not currently possible to assign the results from `nimDim` to another object using vector assignment. So the only practical way to use `nimDim` is to extract elements immediately, such as `nimDim(X)[1]`, `nimDim(X)[2]`, etc.

9.3.6 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.

We plan to include more flexible `for`-loops in the future, but for now we've included just one additional useful feature: `for(i in seq_along(NFL))` will work as in R, where `NFL` is a `nimbleFunctionList`. This is described below.

9.3.7 Using functions

You can call another nimbleFunction from within your nimbleFunction. Simply define the two functions and call one within the other. Similarly, you can define and use a nimbleFunction within another nimbleFunction.

please confirm these statements are true for RC functions

9.3.8 Basic math and linear algebra

Available mathematical operations

Numeric scalar and matrix mathematical operations are listed in tables **??** and **??**.

Perry please scan through these tables for accuracy. In particular, do we now allow vector inputs to distribution functions?

Table 9.1: 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	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; vector x and scalar y ok	✓	✓
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	$log(x+1)$	✓	✓
qDIST(x, PARAMS)	"q" distribution functions	canonical parameterization	✓	
pDIST(x, PARAMS)	"p" distribution functions	canonical parameterization	✓	
rDIST(1, PARAMS)	"r" distribution functions	canonical parameterization	✓	
dDIST(x, PARAMS)	"d" distribution functions	canonical parameterization	✓	
sort(x)				
rank(x, s)				
ranked(x, s)				
order(x)				

Table 9.2: Functions operating on 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	✓
`t(x)`	matrix transpose	$x^\top$	✓
`x%*%y`	matrix multiply	xy; x, y conformant	✓
`inprod(x, y)`	dot product	$x^\top y$; x and y vectors	✓
`solve(x, y)`	solve system of equations	$x^{-1}y$; y matrix or vector	✓
`forwardsolve(x, y)`	solve lower-triangular system of equations	$x^{-1}y$; x lower-triangular	✓
`backsolve(x, y)`	solve upper-triangular system of equations	$x^{-1}y$; x upper-triangular	✓
`logdet(x)`	log matrix determinant	$\log|x|$	✓
`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		
`eigen(x)`	matrix eigendecomposition	x symmetric, returns a nimbleList	✓
`svd(x)`	matrix singular value decomposition	returns a nimbleList	✓

More information on the `nimbleList`s returned by the `eigen()` and `svd()` functions in NIMBLE can be found in Section **??**.

NIMBLE uses the *Eigen* library in C++ to accomplish linear algebra. In Version 0.6-4, we use a lot of Eigen's capabilities, but not all of them.

No vectorized operations other than assignment are supported for more than two dimensions in v0.6-4. That means `A = B + C` will work only if B and C have dimensions $\leq$ 2.

Managing dimensions, sizes and indices

do we want to say anything else here about indexing? Vague memory that Perry had a vision for something more here (or perhaps somewhere else where we talk about indexing!)

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. If you want the inner product as a scalar, use `inprod(v1, 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. If you do not want this behavior, use `drop=FALSE` just as in R. For example, `M1[1,,drop=FALSE]` is a matrix.
- 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$x` will not work – and could crash your R session with a segmentation fault – if Y is not already at least 10x30 in size. This can be done by `setSize(Y, c(10, 30))`. See Section **??** for more details. Note that non-indexed assignment to `Y`, such as `Y <- model$x`, will automatically set `Y` to the necessary 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 Version 0.6-4, 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 Version 0.6-4 we limit ourselves to trying to provide useful information.

9.3.9 Distribution functions

Distribution "d", "r", "p", and "q" functions can all be used from nimbleFunctions (and in BUGS model code), but the care is needed in the syntax.

- We support only the canonical NIMBLE parameterization, as listed below (with a small number of exceptions, also listed).
- The names of the distributions are the names used under the hood in NIMBLE and differ from the standard BUGS distribution names.
- Currently "r" functions only return one random draw at a time, and the first argument must always be 1.
- For the multivariate normal and Wishart distributions the `prec_param` or `scale_param` argument must be provided, indicating when a covariance or precision matrix has been given.

Arguments are matched by order or by name (if given). If omitted, default argument values based on the standard R distribution functions will be used. Standard arguments to distribution functions in R (`log`, `log.p`, `lower.tail`) can be used and take the usual default values as in R. User-defined distributions can also be used from nimbleFunctions and are handled analogously with regard to matching by position and use of defaults (when provided via the nimbleFunction run function arguments) (Chapter **??**).

Supported distributions include:

- `dbinom(size, prob)`
- `dcat(prob)`
- `dmulti(size, prob)`
- `dnbinom(size, prob)`
- `dpois(lambda)`
- `dbeta(shape1, shape2)`
- `dchisq(df)`
- `dexp(rate)`
- `dexp_nimble(rate)`
- `dexp_nimble(scale)`
- `dgamma(shape, rate)`
- `dgamma(shape, scale)`
- `dlnorm(meanlog, sdlog)`
- `dlogis(location, scale)`
- `dnorm(mean, sd)`
- `dt_nonstandard(df, mu, sigma)`
- `dt(df)`
- `dunif(min, max)`
- `dweibull(shape, scale)`
- `ddirch(alpha)`
- `dmnorm_chol(mean, cholesky, prec_param)`
- `dwish_chol(cholesky, df, scale_param)`

In the last two, `cholesky` stands for Cholesky decomposition of the relevant matrix; `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.

In a future release, we will also extend the alternative parameterizations given in Section **??** to `nimbleFunctions`.

9.3.10 `print` and `stop`

As demonstrated above, the NIMBLE function `print`, or equivalently `nimPrint`, prints an arbitrary set of outputs in order and adds a newline character at the end. `cat` or `nimCat` is identical, except without a newline at the end. The NIMBLE function `stop`, or equivalently `nimStop`, throws control to R's error-handling system and can take one string (character) argument.

9.3.11 Checking for user interrupts

When you write algorithms that will run for a long time in C++, you may want to explicitly check whether a user has tried to interrupt the execution (e.g. by pressing Control-C). Simply include `checkInterrupt()` in `run` code to do so. If there has been an interrupt, the process will stop and return control to R.

9.3.12 Alternative keywords for some functions

NIMBLE uses some keywords, such as `dim` and `print`, in ways similar but not identical to 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

- `c` → `nimC`
- `copy` → `nimCopy`
- `dim` → `nimDim`
- `print` → `nimPrint`
- `cat` → `nimCat`
- `step` → `nimStep`
- `equals` → `nimEquals`
- `rep` → `nimRep`
- `round` → `nimRound`
- `seq` → `nimSeq`
- `stop` → `nimStop`
- `switch` → `nimSwitch`
- `numeric, integer, logical` → `nimNumeric, nimInteger, nimLogical`
- `matrix, array` → `nimMatrix, nimArray`

This system gives 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.

Chapter 10

Creating user-defined BUGS distributions and functions

NIMBLE allows you to define your own functions and distributions as *nimbleFunction*s for use in BUGS code. As a result, NIMBLE frees you from being constrained to the functions and distributions just discussed. For example, instead of setting up a Dirichlet prior with multinomial data and needing to use MCMC, one could recognize that this results in a Dirichlet-multinomial distribution for the data and provide that as a user-defined distribution instead.

Further, while NIMBLE at the moment does not allow the use of random indices, such as is common in clustering contexts, you may be able to analytically integrate over the random indices, resulting in a mixture distribution that you could implement as a user-defined distribution. For example, one could implement the *dnormmix* distribution provided in JAGS as a user-defined distribution in NIMBLE.

10.1   User-defined functions

To provide a new function for use in BUGS code, simply create a nimbleFunction that has no *setup* code as discussed in Chapter **??**. Then use it in your BUGS code. That's it.

Writing nimbleFunctions requires that you declare the dimensionality of arguments and the returned object (Section **??**). Make sure that the dimensionality specified in your nimble-Function matches how you use it in BUGS code. For example, if you define scalar parameters in your BUGS code you will want to define nimbleFunctions that take scalar arguments. Here is an example that returns twice its input argument:

```
timesTwo <- nimbleFunction(
    run = function(x = double(0)) {
        returnType(double(0))
        return(2*x)
    })

code <- nimbleCode({
```

```
    for(i in 1:3) {
        mu[i] ~ dnorm(0, 1)
        mu_times_two[i] <- timesTwo(mu[i])
    }
})
```

The `x = double(0)` argument and `returnType(double(0))` establish that the input and output will both be 0-dimensional (scalar) numbers.

You can define nimbleFunctions that take inputs and outputs with more dimensions. Here is an example that takes a vector (1-dimensional) as input and returns a vector with twice the input values:

```
vectorTimesTwo  <- nimbleFunction(
    run = function(x = double(1)) {
        returnType(double(1))
        return(2*x)
    }
    )
code <- nimbleCode({
    for(i in 1:3) {
        mu[i] ~ dnorm(0, 1)
    }
    mu_times_two[1:3] <- vectorTimesTwo(mu[1:3])
})
```

There is a subtle difference between the `mu_times_two` variables in the two examples. In the first example, there are individual nodes for each `mu_times_two[i]`. In the second example, there is a single multivariate node, `mu_times_two[1:3]`. Each implementation could be more efficient for different needs. For example, suppose an algorithm modifies the value of `mu[2]` and then updates nodes that depend on it. In the first example, `mu_times_two[2]` would be updated. In the second example `mu_times_two[1:3]` would be updated because it is a single, vector node.

At present you cannot provide a scalar argument where a nimbleFunction expects a vector; unlike in R, scalars are not simply vectors of length 1. this comment could be confusing - one can pass an R 'scalar' into a double(1). And the example here relates to passing scalars vs vector nodes which involves notions of node dimensionality. Thoughts on how to reword?

10.2   User-defined distributions

To provide a user-defined distribution, you need to define density ("d") and simulation ("r") `nimbleFunctions`, without setup code, for your distribution. In some cases you can then simply use your distribution in BUGS code as you would any distribution already provided

by NIMBLE, while in others you need to explicitly register your distribution as described in Section ??.

You can optionally provide distribution ("p") and quantile ("q") functions, which will allow truncation to be applied to a user-defined distribution. You can also provide a list of alternative parameterizations, but only if you explicitly register the distribution.

Here is an extended example of providing a univariate exponential distribution (although this is already provided by NIMBLE) and a multivariate Dirichlet-multinomial distribution.

```
dmyexp <- nimbleFunction(
    run = function(x = double(0), rate = double(0, default = 1),
        log = integer(0, default = 0)) {
        returnType(double(0))
        logProb <- log(rate) - x*rate
        if(log) return(logProb)
        else return(exp(logProb))
    })

rmyexp <- nimbleFunction(
    run = function(n = integer(0), rate = double(0, default = 1)) {
        returnType(double(0))
        if(n != 1) print("rmyexp only allows n = 1; using n = 1.")
        dev <- runif(1, 0, 1)
        return(-log(1-dev) / rate)
    })

pmyexp <- nimbleFunction(
    run = function(q = double(0), rate = double(0, default = 1),
        lower.tail = integer(0, default = 1),
        log.p = integer(0, default = 0)) {
        returnType(double(0))
        if(!lower.tail) {
            logp <- -rate * q
            if(log.p) return(logp)
            else return(exp(logp))
        } else {
            p <- 1 - exp(-rate * q)
            if(!log.p) return(p)
            else return(log(p))
        }
    })

qmyexp <- nimbleFunction(
    run = function(p = double(0), rate = double(0, default = 1),
        lower.tail = integer(0, default = 1),
        log.p = integer(0, default = 0)) {
```

```
        returnType(double(0))
        if(log.p) p <- exp(p)
        if(!lower.tail) p <- 1 - p
        return(-log(1 - p) / rate)
    })

ddirchmulti <- nimbleFunction(
    run = function(x = double(1), alpha = double(1), size = double(0),
        log = integer(0, default = 0)) {
        returnType(double(0))
        logProb <- lgamma(size) - sum(lgamma(x)) + lgamma(sum(alpha)) -
            sum(lgamma(alpha)) + sum(lgamma(alpha + x)) - lgamma(sum(alpha) +
                                                                        size)
        if(log) return(logProb)
        else return(exp(logProb))
    })

rdirchmulti <- nimbleFunction(
    run = function(n = integer(0), alpha = double(1), size = double(0)) {
        returnType(double(1))
        if(n != 1) print("rdirchmulti only allows n = 1; using n = 1.")
        p <- rdirch(1, alpha)
        return(rmulti(1, size = size, prob = p))
    })

code <- nimbleCode({
    y[1:K] ~ ddirchmulti(alpha[1:K], n)
    for(i in 1:K) {
        alpha[i] ~ dmyexp(1/3)
    }
})

model <- nimbleModel(code, constants = list(K = 5, n = 10))

## defining model...

## Registering the following user-provided distributions: ddirchmulti .
## NIMBLE has registered ddirchmulti as a distribution based on its use in BUGS code. No
## Registering the following user-provided distributions: dmyexp .
## NIMBLE has registered dmyexp as a distribution based on its use in BUGS code. Note th

## building model...
## running calculate on model (any error reports that follow may simply reflect
## missing values in model variables) ...
##
```

```
## checking model sizes and dimensions...
##  note that missing values (NAs) or non-finite values were found in model
variables:  y, alpha.  This is not an error, but some or all variables may need
to be initialized for certain algorithms to operate properly.
##
## model building finished.
```

The distribution-related functions should take as input the parameters for a single parameterization, which will be the canonical parameterization that NIMBLE will use.

Here are more details on the requirements for distribution-related `nimbleFunctions`, which follow R's conventions:

- Your distribution-related functions must have names that begin with "d", "r", "p" and "q". The name of the distribution must not be identical to any of the NIMBLE-provided distributions.

- All simulation ("r") functions must take `n` as their first argument. Note that you may simply have your function only handle `n=1` and return an warning for other values of `n`.

- NIMBLE uses doubles for numerical calculations, so we suggest simply using doubles in general, even for integer-valued parameters or values of random variables.

- All density functions must have as their last argument `log` and implement return of the log probability density. NIMBLE algorithms typically use only `log = 1`, but we recommend you implement the `log = 0` case for completeness.

- All distribution and quantile functions must have their last two arguments be (in order) `lower.tail` and `log.p`. These functions must work for `lower.tail = 1` (i.e., TRUE) and `log.p = 0` (i.e., FALSE), as these are the inputs we use when working with truncated distributions. It is your choice whether you implement the necessary calculations for other combinations of these inputs, but again we recommend doing so for completeness.

- Define the `nimbleFunctions` in R's global environment. Don't expect R's standard scoping to work[1].

10.2.1 Using `registerDistributions` for alternative parameterizations and providing other information

Behind the scenes, NIMBLE uses a function called `registerDistributions` to set up new distributions for use in BUGS code. In some circumstances, you will need to call `registerDistributions` directly to provide information that NIMBLE can't obtain automatically from the `nimbleFunctions` you write.

The cases in which you'll need to explicitly call `registerDistributions` are when you want to do any of the following:

- provide alternative parameterizations,

---

[1]NIMBLE can't use R's standard scoping because it doesn't work for R reference classes, and nimbleFunctions are implemented as custom-generated reference classes.

- indicate a distribution is discrete, and
- provide the range of possible values for a distribution.

If you would like to allow for multiple parameterizations, you can do this via the `Rdist` element of the list provided to `registerDistributions` as illustrated. If you provide CDF ("p") and inverse CDF (quantile, i.e. "q") functions, be sure to specify `pqAvail = TRUE` when you call `registerDistributions`. Here's an example of using `registerDistributions` to provide an alternative parameterization and to provide the range for the user-defined exponential distribution. We can then use the alternative parameterization in our BUGS code.

```r
registerDistributions(list(
    dmyexp = list(
        BUGSdist = "dmyexp(rate, scale)",
        Rdist = "dmyexp(rate = 1/scale)",
        altParams = c("scale = 1/rate", "mean = 1/rate"),
        pqAvail = TRUE,
        range = c(0, Inf)
        )
    ))

## Registering the following user-provided distributions: dmyexp .
## Overwriting the following user-supplied distributions: dmyexp .

code <- nimbleCode({
    y[1:K] ~ ddirchmulti(alpha[1:K], n)
    for(i in 1:K) {
        alpha[i] ~ T(dmyexp(scale = 3), 0, 100)
    }
})

model <- nimbleModel(code, constants = list(K = 5, n = 10),
                    inits = list(alpha = rep(1, 5)))

## defining model...
## building model...
## setting data and initial values...
## running calculate on model (any error reports that follow may simply reflect
missing values in model variables) ...
##
## checking model sizes and dimensions...
##  note that missing values (NAs) or non-finite values were found in model
variables:  y.  This is not an error, but some or all variables may need to
be initialized for certain algorithms to operate properly.
##
## model building finished.
```

There are a few rules for how you specify the information about a distribution that you provide to `registerDistributions`:

- The function name in the `BUGSdist` entry in the list provided to `registerDistributions` will be the name you can use in BUGS code.
- The names of your nimbleFunctions must match the function name in the `Rdist` entry. If missing, the `Rdist` entry defaults to be the same as the `BUGSdist` entry.
- Your distribution-related functions must take as arguments the parameters in default order, starting as the second argument and in the order used in the parameterizations in the `Rdist` argument to `registerDistributions` or the `BUGSdist` argument if there are no alternative parameterizations.
- You must specify a `types` entry in the list provided to `registerDistributions` if the distribution is multivariate or if any parameter is non-scalar.

Further details on using `registerDistributions` can be found via `help(registerDistributions)`. NIMBLE uses the same list format as `registerDistributions` to define its distributions. This list can be found in the `R/distributions_inputList.R` file in the package source code directory.

Chapter 11

Working with NIMBLE models

Here we describe how one can get information about NIMBLE models and carry out operations on a model. While all of this functionality can be used from R, its primary use occurs when writing nimbleFunctions (see Chapter **??**). Information about node types, distributions, and dimensions can be used to determine algorithm behavior in *setup* code of nimbleFunctions. Information about node or variable values or the parameter and bound values of a node would generally be used for algorithm calculations in *run* code of nimbleFunctions. Similarly, carrying out numerical operations on a model, including setting node or variable values, would generally be done in run code.

11.1 The variables and nodes in a NIMBLE model

Section **??** defines what we mean by variables and nodes in a NIMBLE model and discusses how to determine and access the nodes in a model and their dependency relationships. Here we'll review and go into more detail on the topics of determining the nodes and node dependencies in a model.

11.1.1 Determining the nodes in a model

the content on getNodeNames (but not expandNodeNames) repeats stuff from Chap. 6; thoughts? one idea is to just have getNodeNames in its most basic usage shown in Chap 6 and more extended usage here

One can determine the variables in a model using `getVarNames` and the nodes in a model using `getNodeNames`, with optional arguments allowing you to select only certain types of nodes. We illustrate here with the pump model from Chapter **??**.

```
pump$getVarNames()

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

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]"
```

You can see one lifted node (see next section), **lifted_d1_over_beta**, involved in a reparameterization to NIMBLE's canonical parameterization of the gamma distribution for the **theta** nodes.

We can determine the set of nodes contained in one or more nodes or variables using **expandNodeNames**, illustrated here for an example with multivariate nodes. The **returnScalarComponents**

argument also allows us to return all of the scalar components of multivariate nodes.

```
multiVarCode2 <- nimbleCode({
    X[1, 1:5] ~ dmnorm(mu[], cov[,])
    X[6:10, 3] ~ dmnorm(mu[], cov[,])
    for(i in 1:4)
        Y[i] ~ dnorm(mn, 1)
})

multiVarModel2 <- nimbleModel(multiVarCode2, dimensions = list(mu = 5, cov = c(5,5)),
                              calculate = FALSE)


multiVarModel2$expandNodeNames('Y')

## [1] "Y[1]" "Y[2]" "Y[3]" "Y[4]"

multiVarModel2$expandNodeNames(c('X', 'Y'), returnScalarComponents = TRUE)

##  [1] "X[1, 1]"  "X[1, 2]"  "X[1, 3]"  "X[6, 3]"  "X[7, 3]"
##  [6] "X[8, 3]"  "X[9, 3]"  "X[10, 3]" "X[1, 4]"  "X[1, 5]"
## [11] "Y[1]"     "Y[2]"     "Y[3]"     "Y[4]"
```

As discussed in Section **??**, you can determine whether a node is flagged as data using `isData`.

11.1.2   Understanding lifted 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 Section **??** the use of link functions causes new nodes to be introduced. This requires care if you need to initialize values in stochastic declarations with link functions.

- Use of alternative parameterizations of distributions, described in Section **??**. 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.

11.1.3   Determining dependencies in a model

this repeats stuff from Chap. 6; thoughts?

   Next we'll see how to determine the node dependencies (or "descendants") in a model. There are a variety of arguments to `getDependencies` 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 emanating from the node(s) specified as input. 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]"
```

11.2 Accessing information about nodes and variables

11.2.1 Getting distributional information about a node

We briefly demonstrate some of the functionality for information about a node here, but refer readers to the R help on `modelBaseClass` for full details.

Here is an example model, with use of various functions to determine information about nodes or variables.

```
code <- nimbleCode({
    for(i in 1:4)
        y[i] ~ dnorm(mu, sd = sigma)
    mu ~ T(dnorm(0, 5), -20, 20)
    sigma ~ dunif(0, 10)
    })
m <- nimbleModel(code, data = list(y = rnorm(4)),
                       inits = list(mu = 0, sigma = 1))
m$isEndNode('y')

## y[1] y[2] y[3] y[4]
## TRUE TRUE TRUE TRUE

m$getDistribution('sigma')

##   sigma
## "dunif"

m$isDiscrete(c('y', 'mu', 'sigma'))

##  y[1]  y[2]  y[3]  y[4]     mu sigma
## FALSE FALSE FALSE FALSE FALSE FALSE
```

```
m$isDeterm('mu')

##   mu
## FALSE

m$getDimension('mu')

## value
##     0

m$getDimension('mu', includeParams = TRUE)

## value  mean    sd   tau   var
##     0     0     0     0     0
```

Note that any variables provided to these functions are expanded into their constituent node names, so the length of results may not be the same length as the input vector of node and variable names. However the order of the results should be preserved relative to the order of the inputs, once the expansion is accounted for.

11.2.2 Getting information about a distribution

One can also get generic information about a distribution based on the name of the distribution. In particular, one can determine whether a distribution was provided by the user (`isUserDefined`), whether a distribution provides CDF and quantile functions (`pqDefined`), whether a distribution is a discrete distribution (`isDiscrete`), the parameter names (include alternative parameterizations) for a distribution (`getParamNames`), and the dimension of the distribution and its parameters (`getDimension`). For more extensive information, please see the R help for `getDistributionInfo`.

11.2.3 Getting distribution parameter values for a node

The function `getParam` provides access to values of the parameters of a node's distribution. Like the above functions, `getParam` can be used as global function taking a model as the first argument, or it can be used as a model member function. The next two arguments must be the name of one (stochastic) node and the name of a parameter for the distribution followed by that node. The parameter does not have to be one of the parameters used when the node was declared. Alternative parameterization values can also be obtained. See section(**??**) for available parameterizations. (These can also be seen via `distributionsInputList`.)

Here is an example:

```
gammaModel <- nimbleModel(
    nimbleCode({
        a ~ dlnorm(0, 1)
        x ~ dgamma(shape = 2, scale = a)
```

```
    }), data = list(x = 2.4), inits = list(a = 1.2))
getParam(gammaModel, 'x', 'scale')

## [1] 1.2

getParam(gammaModel, 'x', 'rate')

## [1] 0.8333333

gammaModel$getParam('x','rate')

## [1] 0.8333333
```

getParam is part of the NIMBLE language, so it can be used in run code of nimbleFunctions.

11.2.4   Getting distribution bounds for a node

The function getBound provides access to the lower and upper bounds of the distribution for a node. In most cases these bounds will be fixed based on the distribution, but for the uniform distribution the bounds are the parameters of the distribution, and when truncation (see Section **??**) is used, the bounds will be determined by the truncation. Like the functions described in the previous section, getBound can be used as global function taking a model as the first argument, or it can be used as a model member function. The next two arguments must be the name of one (stochastic) node and either 'lower' or 'upper' indicating whether the lower or upper bound is desired. For multivariate nodes the bound is a scalar that is the bound for all elements of the node, as we do not handle truncation for multivariate nodes.

Here is an example:

```
exampleModel <- nimbleModel(
    nimbleCode({
        y ~ T(dnorm(mu, sd = sig), a, Inf)
        a ~ dunif(-1, b)
        b ~ dgamma(1, 1)
    }), inits = list(a = -0.5, mu = 1, sig = 1, b = 4),
        data = list(y = 4))
getBound(exampleModel, 'y', 'lower')

## [1] -0.5

getBound(exampleModel, 'y', 'upper')

## [1] Inf

exampleModel$b <- 3
exampleModel$calculate(exampleModel$getDependencies('b'))
```

```
## [1] -4.386294

getBound(exampleModel, 'a', 'upper')

## [1] 3

exampleModel$getBound('b','lower')

## [1] 0
```

getBound is part of the NIMBLE language, so it can be used in run code of nimbleFunctions. In fact, we anticipate that most use of getBound will be for algorithms, such as for the reflection version of the random walk MCMC sampler.

11.3   Carrying out model calculations

11.3.1   Core model operations: calculation and simulation

The four basic ways to operate a model are to calculate nodes, simulate into nodes, get the log probabilities (or probability densities) that have already been calculated, and compare the log probability of a new value to that of an old value. In more detail:

calculate For a stochastic node, calculate determines the log probability value, stores it in the appropriate logProb variable, 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.

calculateDiff calculateDiff is identical to calculate, but it returns the new log probability value minus the one that was previously stored. This is useful when one wants to change the value or values of node(s) in the model (e.g., by setting a value or simulate) and then determine the change in the log probability, such as needed for a Metropolis-Hastings acceptance probability.

Each of these functions is accessed as a member function of a model object, taking a vector of node names as an argument[1]. If there is more than one node name, calculate and getLogProb return the sum of the log probabilities from each node, while calculateDiff returns the sum of the new values minus the old values. Next we show an example using simulate.

---

[1]Standard usage is model$calculate(nodes) but calculat(model, nodes) is synonymous.

Example: simulating arbitrary collections of nodes

```
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)
    }
    y.squared[1:5] <- y[1:5]^2
})

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

```
## defining model...
## building model...
## setting data and initial values...
## running calculate on model (any error reports that follow may simply reflect
missing values in model variables) ...
##
## checking model sizes and dimensions...
##  note that missing values (NAs) or non-finite values were found in model
variables:  a, y, y.squared.  This is not an error, but some or all variables
may need to be initialized for certain algorithms to operate properly.
##
## model building finished.
```

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

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

```
model[['a']]
```

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

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

```
## [1]          NA  0.2876671 -1.5054011  1.5192970          NA
```

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

```
## [1]  0.3674094  0.2876671 -1.5054011  1.5192970  1.6998624
```

```
model$z[1,]

## [1] -0.7621735 -0.6030044  0.8061233

model$y

## [1]  0.3674094  0.2876671 -1.5054011  1.5192970  1.6998624

model$simulate('y[1:3]')
## model£simulate('y[1:3]') does the same thing
model$y

## [1]  7.0371297 -0.3372955  7.0480365  1.5192970  1.6998624

model$simulate('y')
model$y

## [1] 6.419212 8.245452 8.399380 6.449302 6.997253

model$z

##              [,1]        [,2]        [,3]
## [1,] -0.7621735 -0.6030044  0.8061233
## [2,] -0.2917486 -1.0939347 -1.7398351
## [3,] -0.5751885  0.7147062 -0.4013203
## [4,] -0.4439419 -0.1088123 -0.2875825
## [5,] -0.3125704 -1.4437979 -0.9384074

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

## [1]  3.1644041 10.0096554 -0.5782355  6.4493023  6.9972527

model$z

##              [,1]        [,2]        [,3]
## [1,] -0.7621735 -0.6030044  0.8061233
## [2,] -0.2917486 -1.0939347 -1.7398351
## [3,] -0.5751885  0.7147062 -0.4013203
## [4,] -0.4439419 -0.1088123 -0.2875825
## [5,] -0.3125704 -1.4437979 -0.9384074

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

```
##             [,1]        [,2]        [,3]
## [1,]   2.9763419   3.0352322   3.2553711
## [2,]   9.8988799   9.9712430  10.0179289
## [3,]  -0.6266237  -0.7867096  -0.4614768
## [4,]   6.4416197   6.5023444   6.4497931
## [5,]   6.9442296   7.0074729   7.0787987


## ## @knitr calcSimGLPdirect


## y2lp <- model£nodes[['y[2]']]£calculate()
## y2lp
## model£nodes[['y[2]']]£getLogProb()
```

Note the following.

1. `simulate(model, nodes)` is equivalent to `model$simulate(nodes)`. You can use either, but the latter is encouraged and the former may be deprecated inthe future.
2. 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`.
3. An arbitrary number of nodes can be provided as a character vector.
4. Simulations will be done in the order provided, so in practice the nodes should 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.
5. The data nodes `z` were not simulated into until `includeData = TRUE` was used.

Use of `calculate`, `calculateDiff` and `getLogProb` are similar to `simulate`, except that they return a value (described above) and they have no `includeData` argument.

11.3.2   simNodes, calcNodes, and getLogProbs

under discussion: how to clarify the point of these and where to put this text

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 will be topologically sorted to simulate in the correct order. For `calcNodes` and `getLogProb`, the nodes will be sorted and dependent nodes will be 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, check = FALSE)

## defining model...
## building model...
## running calculate on model (any error reports that follow may simply reflect
missing values in model variables) ...
##
## checking model sizes and dimensions...
##  note that missing values (NAs) or non-finite values were found in model
variables:  x, y, z.  This is not an error, but some or all variables may need
to be initialized for certain algorithms to operate properly.
##
## model building finished.

cSimpleModel <- compileNimble(simpleModel)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_51_45.dll > dynamicRegistrations_03_08_15_51_45.log'
had status 1
## Error:  Failed to create the shared library

#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)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_51_48.dll > dynamicRegistrations_03_08_15_51_48.log'
had status 1
## Error:  Failed to create the shared library
```

```
cCalcXDep <- compileNimble(rCalcXDep, project = simpleModel)
```

compiling... this may take a minute. Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
Warning: running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_51_52.dll > dynamicRegistrations_03_08_15_51_52.log'
had status 1
Error: Failed to create the shared library

```
cGetLogProbXDep <- compileNimble(rGetLogProbXDep,
                       project = simpleModel)
```

compiling... this may take a minute. Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
Warning: running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_51_54.dll > dynamicRegistrations_03_08_15_51_54.log'
had status 1
Error: Failed to create the shared library

```
cSimpleModel$x
```

Error in eval(expr, envir, enclos): object 'cSimpleModel' not found

```
cSimpleModel$y
```

Error in eval(expr, envir, enclos): object 'cSimpleModel' not found

#simulating x and y
```
cSimXY$run()
```

Error in eval(expr, envir, enclos): object 'cSimXY' not found

```
cSimpleModel$x
```

Error in eval(expr, envir, enclos): object 'cSimpleModel' not found

```
cSimpleModel$y
```

Error in eval(expr, envir, enclos): object 'cSimpleModel' not found

```
cCalcXDep$run()
```

Error in eval(expr, envir, enclos): object 'cCalcXDep' not found

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

Error in eval(expr, envir, enclos): object 'cGetLogProbXDep' not found

```
cSimXY$run()
```

```
## Error in eval(expr, envir, enclos):  object 'cSimXY' not found

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

## Error in eval(expr, envir, enclos):  object 'cGetLogProbXDep' not found

cCalcXDep$run()

## Error in eval(expr, envir, enclos):  object 'cCalcXDep' not found
```

11.3.3   Accessing log probabilities via logProb variables

I'm somewhat inclined to remove this - this feels like access to private member data in OOP - we provide getLogProb as the public accessor, so is there a need to even tell users about this? Or if not remove, we might mention when we talk about getLogProb that what it does is return the relevant current value(s) in logProb_variableName.

For each variable that contains at least one stochastic node, NIMBLE generates a model variable with the prefix "logProb_". When the stochastic node is scalar, the `logProb` variable will have the same size. For example:

```
model$logProb_y

## [1] NA NA NA NA NA

model$calculate('y')

## [1] -13.63477

model$logProb_y

## [1] -2.238702 -3.325063 -3.626067 -2.175255 -2.269682
```

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`.

Chapter 12

Data structures in NIMBLE

NIMBLE provides several data structures useful for programming.

We'll first describe `modelValues`, which are containers designed for storing values for models. Then in Section **??** we'll describe `nimbleLists`, which have a similar purpose to lists in `R`, allowing you to store heterogeneous information in a single object.

`modelValues` can be created in either `R` or in `nimbleFunction` setup code. `nimbleLists` can be created in `R` code, in `nimbleFunction` setup code, and in `nimbleFunction` run code, from a nimbleList definition created in R or setup code. Once created, `modelValues` and `nimbleLists` can then be used either in `R` or in `nimbleFunction` setup or run code. If used in run code, they will be compiled along with the `nimbleFunction`.

12.1   The *modelValues* data structure

`modelValues` are containers designed for storing values for models. They may be used for model outputs or model inputs. A modelValues object will contain *rows* of variables. Each row contains one object of each variable, which may be multivariate. 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. Although they were motivated by models, one is free to set up a `modelValues` with any variables one wants.

As with the material in the rest of this chapter, modelValues objects will generally be used in nimbleFunctions that interact with models (see Chapter **??**, so one may want to read this section after an inital reading of that chapter. modelValues objects can be defined either in setup code or separately in R (and then passed as an argument to setup code). The modelValues object can then used in run code of nimbleFunctions.

12.1.1   Creating modelValues objects

Here is a simple example of creating a modelValues object:

```
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`, and we set `pumpModelValues` to have `m = 2` rows. As you can see, the rows are stored as elements of a list.

Alternatively, one can define a modelValues object manually by first defining a model-Values configuration via the `modelValuesConf` function, and then creating an instance from that configuration, like this:

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

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

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

The arguments to `modelValuesConf` are matching lists of variable names, types, and sizes. See `help(modelValuesConf)` for more details. 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 nimble-Function 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)

## compiling...   this may take a minute.   Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_51_58.dll > dynamicRegistrations_03_08_15_51_58.log'
had status 1
## Error:  Failed to create the shared library

cCustomMV <- cResize$mv

## Error in eval(expr, envir, enclos):  object 'cResize' not found

# 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.

12.1.2   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]`.

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 useful to convert a modelValues object to a matrix for use in R. For example, we may want to convert MCMC output into a matrix for use with the `coda` package for processing MCMC samples. This can be done with the `as.matrix` method for modelValues objects. This will generate column names from every scalar element of variables (e.g. "x[1, 1]" ,"x[2, 1]", etc.). 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]
## [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 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 its contents via 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
```

As with most NIMBLE objects, modelValues are passed by reference, not by value. That means any modifications of modelValues objects in either R functions or `nimbleFunction`s will persist outside of the function. This allows for more efficient computation, as stored values are immediately shared among `nimbleFunction`s.

```
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.

Automating calculation and simulation using modelValues

as with calcNodes, I'd like to discuss when a user would be expected to use this and figure out if this is where to talk about it in light of that

The nimbleFunctions `simNodesMV`, `calcNodesMV`, and `getLogProbsMV` can be used to operate on a model based on rows in 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)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_02.dll > dynamicRegistrations_03_08_15_52_02.log'
had status 1
## Error:  Failed to create the shared library

cCalcManyXDeps <- compileNimble(rCalcManyXDeps, project = simpleModel)

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

```
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_05.dll > dynamicRegistrations_03_08_15_52_05.log'
had status 1
## Error:  Failed to create the shared library

cGetLogProbMany <- compileNimble(rGetLogProbMany, project = simpleModel)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_08.dll > dynamicRegistrations_03_08_15_52_08.log'
had status 1
## Error:  Failed to create the shared library

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

## Error in eval(expr, envir, enclos):  object 'cSimManyXY' not found

cCalcManyXDeps$run(saveLP = TRUE) # calculating

## Error in eval(expr, envir, enclos):  object 'cCalcManyXDeps' not found

cGetLogProbMany$run() #

## Error in eval(expr, envir, enclos):  object 'cGetLogProbMany' not found
```

12.2   The *nimbleList* data structure

`nimbleList`s provide a container for storing different types of objects in `nimble`, similar to the `list` data structure in R. Before a `nimbleList` can be created and used, a definition for that `nimbleList` must be created that provides the names, types, and dimensions of the elements in the `nimbleList`. nimbleList definitions must be created in R, but the nimbleList instances can be created in run code, provided the definition is created or passed into setup code.

Nick, please check last sentence

Unlike `list`s in R, `nimbleList`s must have the names and types of all list elements provided by a definition before the list can be used. A `nimbleList` definition can be made by using the `nimbleList` function in one of two manners. The first manner is to provide the `nimbleList` function with a series of expressions of the type

- `name = type(nDim)`

similar to the specification of runtime arguments to `nimbleFunction`s. The types allowed for a `nimbleList` are the same as those allowed as runtime arguments to a `nimbleFunction`, described in Section **??**. For example, the following line of code creates a `nimbleList` definition with two elements: `x`, which is a scalar integer, and `Y`, which is a matrix of doubles.

```
exampleNimListDef <- nimbleList(x = integer(0),
                                Y = double(2))
```

The second method of creating a `nimbleList` definition is by providing an `R list` of `nimbleType` objects to the `nimbleList()` function. A `nimbleType` object can be created using the `nimbleType()` function, which must be provided with three arguments: the `name` of the object being created, the `type` of the object being created, and the `dim` of the object being created. For example, the following code creates a list with two `nimbleType` objects, and uses these objects to create a `nimbleList` definition.

```
nimbleListTypes <- list(nimbleType(name = 'x',
                                   type = 'integer', dim = 0),
                        nimbleType(name = 'Y',
                                   type = 'double', dim = 2))

## this nimbleList definition is identical to the one created above
exampleNimListDef <- nimbleList(nimbleListTypes)
```

Creating definitions using a `list` of `nimbleType`s can be useful, as it allows for programmatic generation of `nimbleList` elements.

Once a `nimbleList` definition has been created, new instances of `nimbleList`s can be made from that definition using the `new()` member function. The `new()` function can optionally take initial values for the list elements as arguments. Below, we create a new `nimbleList` from our `exampleNimListDef` and specify values for the two elements of our list:

```
exampleNimList <- exampleNimListDef$new(x = 1,
                                        Y = diag(2))
```

Once created, `nimbleList` elements can be accessed using the `$` operator, just as with `list`s in R. For example, the value of the `x` element of our `exampleNimbleList` can be set to `11` using

```
exampleNimList$x <- 11
```

`nimbleList` definitions can be created either in R's global environment, or in `setup` code of a `nimbleFunction`. Once a `nimbleList` definition has been made, new instances of `nimbleList`s can be created using the `new()` function in R's global environment, in `setup` code, or in `run` code of a `nimbleFunction`.

`nimbleList`s can also be passed as arguments to run code of `nimbleFunction`s, and returned from `nimbleFunction`s. To use a `nimbleList` as a run code argument, the name of the `nimbleList` definition should be provided as the argument type, with a set of parentheses following. To return a `nimbleList` from the run code of a `nimbleFunction`, the `returnType` of that function should be the name of the `nimbleList` definition, again using a following set of parentheses.

Below, we demonstrate a function that takes the `exampleNimList` as an argument, modifies its Y element, and returns the `nimbleList`. We note that `nimbleFunctions` that take `nimbleLists` as run arguments must have setup code. For functions that need no setup code, setting `setup = TRUE` will allow these functions to work correctly.

```
nimListFunctionGenerator <- nimbleFunction(
  setup = TRUE,
  run = function(argumentList = exampleNimListDef()){
    onesMatrix <- matrix(value = 1, nrow = 2, ncol = 2)
    argumentList$Y  <- onesMatrix
    returnType(exampleNimListDef())
    return(argumentList)
  })

## Warning in nf_checkDSLcode(code):  Detected possible use of R functions in
nimbleFunction run code.  For this nimbleFunction to compile, these objects must
defined as nimbleFunctions, nimbleLists, or nimbleFunction methods:  exampleNimListDef.

nimListFunction <- nimListFunctionGenerator()

## pass exampleNimList as argument to run function
nimListFunction$run(exampleNimList)

## nimbleList object of type nfRefClass_95
## Field "x":
## [1] 11
## Field "Y":
##      [,1] [,2]
## [1,]    1    1
## [2,]    1    1
```

`nimbleList` arguments to run functions are passed by reference – this means that if an element of a `nimbleList` argument is modified within a function, that element will remain modified when the function has finished running. To see this, we can inspect the value of the Y element of the `exampleNimList` object:

```
exampleNimList$Y

##      [,1] [,2]
## [1,]    1    1
## [2,]    1    1
```

Note that Y was assigned a new value (a matrix of all 1's) within the function, and this new value persists outside of the function.

In addition to storing basic data types, `nimbleLists` can also store other `nimbleLists`. To achieve this, we must create a `nimbleList` definition that declares the types of nested

nimbleLists a nimbleList will store. Below, we create two types of nimbleLists: the first, named innerNimList, will be stored inside the second, named outerNimList:

```
## first, create definitions for both inner and outer nimbleLists
innerNimListDef <- nimbleList(someText = character(0))
outerNimListDef <- nimbleList(innerNimList = innerNimListDef(),
                              z = double(0))

## then, create outer nimbleList
outerNimList <- outerNimListDef$new(z = 3.14)

## access element of inner nimbleList
outerNimList$innerNimList$someText <- "hello, world"
```

Note that definitions for inner, or nested, nimbleLists must be created before the definition for an outer nimbleList.

12.2.1 Using eigen() and svd() in nimbleFunctions

nimble has two linear algebra functions that return nimbleLists. The eigen() function takes a symmetric matrix X as an argument, and returns a list with two elements: values, a vector with the eigenvalues of X, and vectors, a square matrix with the same dimension as X whose columns are the eigenvectors of X. The eigen() function has an optional argument named only.values, which defaults to FALSE. If only.values = TRUE, the eigen() function will not calculate the eigenvectors of X, leaving the vectors nimbleList element empty. This can reduce calculation time if only the eigenvalues of X are needed.

The svd() function takes an n-by-p matrix Y as an argument, and returns a list with three elements: d, a vector with the singular values of Y, u a matrix with the left singular vectors of Y, and v, a matrix with the right singular vectors of Y. The svd() function has an optional argument vectors which defaults to a value of "full". The vectors argument can be used to specify the number of singular vectors that are returned. If vectors = "full", v will be an n-by-n matrix and u will be an p-by-p matrix. If vectors = "thin", v will be an n-by-m matrix, where m = min(n,p), and u will be an m-by-p matrix. If vectors = "none", the u and v elements of the returned nimbleList will not be populated. nimbleLists created by either eigen() or svd() can be returned from a nimbleFunction, using returnType(eigen()) or returnType(svd()) respectively. nimbleLists created by eigen() and svd() can also be used as nested lists within other nimbleLists by specifyng the nimbleList element types as eigen() and svd(). The below example demonstrates the use of eigen() and svd() within a nimbleFunction.

```
eigenListFunctionGenerator <- nimbleFunction(
  setup = function(){
    demoMatrix <- diag(4) + 2
    eigenAndSvdListDef <- nimbleList(eigenList = eigen(), svdList = svd())
    eigenAndSvdList <- eigenAndSvdListDef$new()
```

```
  },
  run = function(){
    ## we will take the eigendecomposition and svd of a symmetric matrix
    eigenAndSvdList$eigenList <<- eigen(demoMatrix, only.values = TRUE)
    eigenAndSvdList$svdList <<- svd(demoMatrix, vectors = 'none')
    returnType(eigenAndSvdListDef())
    return(eigenAndSvdList)
  })

## Warning in nf_checkDSLcode(code):  For this nimbleFunction to compile, these
objects must be defined as nimbleFunctions, nimbleLists, or nimbleFunction methods:
eigenAndSvdListDef.

eigenListFunction <- eigenListFunctionGenerator()

outputList <-  eigenListFunction$run()

## Error in nimEigen(demoMatrix, only.values = TRUE): PACKAGE argument must be
a single character string

outputList$eigenList$values

## Error in eval(expr, envir, enclos):  object 'outputList' not found

outputList$svdList$d

## Error in eval(expr, envir, enclos):  object 'outputList' not found
```

The eigenvalues and singular values returned from the above function are the same since the matrix being decomposed was symmetric. However, note that both eigendecompositions and singular value decompositions are numerical procedures, and computed solutions may have slight differences even for a symmetric input matrix.

Chapter 13

Writing *nimbleFunctions* that interact with models

13.1 Overview

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 similar, but 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. Typically the inputs to *setup* code are objects like a model, a vector of nodes, a modelValues object or a modelValues configuration, 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 – defined by what can be compiled – 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.

Here is a small example to fix ideas:

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

---

[1]Normally this is the value of the last evaluated code, or the argument to return().
[2]This can be omitted if you don't need it.

```
        dependentNodes <- model$getDependencies(node)
        valueToAdd <- 1
    },
    run = function(P = double(0)) {
        model[[node]] <<- P + valueToAdd
        return(model$calculate(dependentNodes))
        returnType(double(0))
    })


code <- nimbleCode({
    a ~ dnorm(0, 1)
    b ~ dnorm(a, 1)
})
testModel <- nimbleModel(code, check = FALSE)

## defining model...
## building model...
## running calculate on model (any error reports that follow may simply reflect
missing values in model variables) ...
##
## checking model sizes and dimensions...
##  note that missing values (NAs) or non-finite values were found in model
variables:  a, b.  This is not an error, but some or all variables may need
to be initialized for certain algorithms to operate properly.
##
## model building finished.

logProbCalcPlusA <- logProbCalcPlus(testModel, 'a')
testModel$b <- 1.5
logProbCalcPlusA$run(0.25)

## [1] -2.650377

dnorm(1.25,0,1,TRUE)+dnorm(1.5,1.25,1,TRUE) ## direct validation

## [1] -2.650377

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

## [1] 1.25
```

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 Section

??) 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 an "instance" of `logProbCalcPlus` that is "specialized" or "bound" to `a` and `testModel`. Usually, the `setup` code will be where information about the model structure is determined, and then the `run` code can use that information without repeatedly, redundantly recomputing it. A nimbleFunction can be called repeatedly (one can think of it as a generator), 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.

13.2 Using and compiling nimbleFunctions

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

```
CnfDemo <- compileNimble(testModel, logProbCalcPlusA)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_14.dll > dynamicRegistrations_03_08_15_52_14.log'
had status 1
## Error:  Failed to create the shared library

CtestModel <- CnfDemo$testModel

## Error in eval(expr, envir, enclos):  object 'CnfDemo' not found

ClogProbCalcPlusA <- CnfDemo$logProbCalcPlusA

## Error in eval(expr, envir, enclos):  object 'CnfDemo' not found
```

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

## Error in eval(expr, envir, enclos):  object 'CtestModel' not found
```

---

[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.

```
CtestModel$b

## Error in eval(expr, envir, enclos):  object 'CtestModel' not found

lpA <- ClogProbCalcPlusA$run(1.5)

## Error in eval(expr, envir, enclos):  object 'ClogProbCalcPlusA' not found

lpA

## Error in eval(expr, envir, enclos):  object 'lpA' not found

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

## Error in dnorm(CtestModel$b, CtestModel$a, 1, log = TRUE): object 'CtestModel'
not found

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

## Error in eval(expr, envir, enclos):  object 'CtestModel' not found

testModel$a         ## the uncompiled model was not modified

## [1] 1.25
```

13.3   Writing setup code

13.3.1   Useful tools for `setup` functions

The setup function is typically used to determine information on nodes in a model, set up modelValues objects, set up (nested) nimbleFunctions or nimbleFunctionLists, and set up any persistent numeric objects. For example, the `setup` code of an MCMC nimbleFunction creates the nimbleFunctionList of sampler nimbleFunctions. The values of numeric objects created in `setup` can be modified by run code and will persist across calls.

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 **??**.

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 runtime code.

lists of other nimbleFunctions In addition to containing single other nimbleFunctions, a nimbleFunction can contain a list of other nimbleFunctions. These are discussed more below.

nimbleList definitions It can be useful to create `nimbleList` definitions in setup code. New instances of `nimbleLists` can then be created from this definition in either setup or run code. See Section **??** for more information.

Functionality for getting information about a model and the nodes in a model (see Sections **??**-**??**) are also often used in setup code.

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

13.3.2 Accessing and modifying numeric values from setup

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

```
logProbCalcPlusA$valueToAdd  ## in the uncompiled version

## [1] 1

logProbCalcPlusA$valueToAdd <- 2
ClogProbCalcPlusA$valueToAdd  ## or in the compiled version

## Error in eval(expr, envir, enclos):  object 'ClogProbCalcPlusA' not found

ClogProbCalcPlusA$valueToAdd <- 3

## Error in ClogProbCalcPlusA$valueToAdd <- 3:  object 'ClogProbCalcPlusA' not
found

ClogProbCalcPlusA$run(1.5)

## Error in eval(expr, envir, enclos):  object 'ClogProbCalcPlusA' not found

CtestModel$a     ## a == 1.5 + 3

## Error in eval(expr, envir, enclos):  object 'CtestModel' not found
```

13.3.3 Determining numeric types in nimbleFunctions

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 values created by the `setup` code. 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.

---

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

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 then use `setSize` in the run-time code.

13.3.4   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 or character 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, which provides a way of using nimbleFunctions as general data structures. To force NIMBLE to include variables around during compilation, for example `X` and `Y`, simply include

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

anywhere in the `setup` code.

13.4   Writing run code

In Section **??** we described the functionality of the NIMBLE language that could be used in run code in which models were not used. When writing nimbleFunctions that use models, one can use that functionality already described as well as the functionality discussed in this section.

13.4.1   Driving models: `calculate`, `calculateDiff`, `simulate`, `getLogProb`

These four functions are the primary ways to operate a model. Their syntax was explained in Section **??**. Except for `getLogProb`, it is usually important for the `nodes` object to be created in `setup` code such that they are sorted in topological order, and functions such as `getDependencies` and `expandNodeNames` will always do so.

It is possible to use an entire vector of node names, single elements indexed by a variable, or fixed ranges (indexed by constants) , but not ranges indexed by a variable. For example

```
myModel$calculate(nodes)
```

and

```
myModel$calculate(nodes[i])
```

and

```
myModel$calculate(nodes[1:3])
```

check on outcome of discussion on fixed ranges
will all compile correctly, but

```
myModel$calculate(nodes[1:i])
```

is not allowed.

13.4.2   Getting and setting variable and node values

Using indexing with nodes

Model variables and nodes can be accessed and set using [[ ]] in run code, but there are some limitations on what can be compiled relative to the syntax discussed in Section **??**.

Here is an example that illustrates getting and setting of nodes and subsets of nodes. Note the following:

- use of [[ ]] is restricted to use with a single node (potentially a non-scalar node), and
- one should use the <<- global assignment operator to assign into model nodes.

This deserves a careful pass from Perry or Daniel to check that I've gotten right what we allow and that I'm not omitting any important syntax that we do allow.

```
code <- nimbleCode({
    z ~ dnorm(0, sd = sigma)
    sigma ~ dunif(0, 10)
    y[1:n] ~ dmnorm(zeroes[1:n], cov = C[1:5, 1:5])
})
n <- 5
m <- nimbleModel(code, constants = list(n = n, zeroes = rep(0, n),
                                        C = diag(n)))

## Adding zeroes,C as data for building model.

cm <- compileNimble(m)

## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_24.dll > dynamicRegistrations_03_08_15_52_24.log'
had status 1
## Error:  Failed to create the shared library
```

```
nfGen <- nimbleFunction(
    setup = function(model, node1, node2) {
    },
    run = function(vals = double(1)) {
        tmp0 <- model[[node1]]      # tmp0 will be a scalar
        tmp1 <- model[['sigma']]    # allowed but not model-generic
        tmp2 <- model[[node2]]      # tmp2 will be a vector
        tmp3 <- model[[node2]][1]   # tmp3 will be a scalar
        model[[node1]] <<- runif(1) # node1 is scalar so can be assigned a scalar
        model[['sigma']] <<- runif(1) # allowed but not model-generic
        model[[node2]][1] <<- runif(1)
                          # only an element of node2 can be assigned a scalar
        model[[node2]][1:3] <<- vals[1:3]
        returnType(double(1))
        out <- model[[node2]]
        return(out)

    }
    )


Rnf <- nfGen(m, 'sigma', 'y[1:5]')
Cnf <- compileNimble(Rnf)

## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_27.dll > dynamicRegistrations_03_08_15_52_27.log'
had status 1
## Error:  Failed to create the shared library

Cnf$run(rnorm(10))

## Error in eval(expr, envir, enclos):  object 'Cnf' not found
```

Use of `[[ ]]` allows one to programmatically access a node based on a character variable that stores the name of the node; this character variable would generally be set in setup code. In contrast, use of `$` hard codes the variable name and would not generally be suitable for nimbleFunctions intended for use with arbitrary models. Furthermore one can only use `$` in very limited ways.

do we want to show any use of $?

Getting and setting more than one model node or variable at a time using `values`

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 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. This can be done using `values()`:

```
## get values from a set of model nodes into a vector
P <- values(model, nodes)
## or put values from a vector into a set of 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.

`values(model, nodes)` may be used as a vector in other expressions, e.g. `Y <- A %*% values(model, nodes) + b`.

One can also use indexing, but one can only have a single index, and not a range of indices:

```
## get values from a set of model nodes into a vector
i <- 2
P <- values(model, nodes[i])
## or put values from a vector into a set of model nodes
values(model, nodes[i]) <- P
# P <- values(model, nodes[1:2] # won't compile
```

Note that `values()` returns a 1-d vector and expects a 1-d vector when used on the left-hand side of an assignment. This means that one needs to do some extra work to use scalars with `values()`. For example:

```
tmp <- numeric(1)
tmp[1] <- rnorm(1)
values(model, nodes[1]) <- tmp
# values(model, nodes[1]) <- rnorm(1)  # won't compile

out <- values(model, nodes[1])
returnType(double(0))
return(out[1])
# return(out)  # won't compile unless one has returnType(double(1))
```

13.4.3   Getting parameter values and node bounds

Sections **??**-**??** describe how to get the parameter values for a node and the range (bounds) of possible values for the node using `getParam` and `getBound`. Both of these can be used in run code.

13.4.4   Using modelValues objects

The `modelValues` structure was introduced in Section **??**. Inside nimbleFunctions, modelValues are designed to easily save values from a model object during the running of a

nimbleFunction. A `modelValues` object used in `run` code must always exist in the setup code, either by passing it in as a setup argument or creating it 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
    savedWeightsConf <- modelValuesConf(vars = 'w',
                                        types = 'double',
                                        sizes = 1)
    savedWeights <- modelValues(conf = savedWeightsConf)
    ## 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 `copy`, which has the synonym `nimCopy`. See `help(nimCopy)` for argument details.

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 `run` code.

Here is a `run` 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 <- model$calculate()
        ## 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 $, 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, check = FALSE)

## defining model...
## building model...
## running calculate on model (any error reports that follow may simply reflect
missing values in model variables) ...
##
## checking model sizes and dimensions...
##   note that missing values (NAs) or non-finite values were found in model
variables:  x, y.  This is not an error, but some or all variables may need
to be initialized for certain algorithms to operate properly.
##
## model building finished.

propModel = nimbleModel(propModelCode, check = FALSE)

## defining model...
## building model...
## running calculate on model (any error reports that follow may simply reflect
missing values in model variables) ...
```

```
##
## checking model sizes and dimensions...
##  note that missing values (NAs) or non-finite values were found in model
variables:  x, y.  This is not an error, but some or all variables may need
to be initialized for certain algorithms to operate properly.
##
## model building finished.

cTargetModel = compileNimble(targetModel)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_33.dll > dynamicRegistrations_03_08_15_52_33.log'
had status 1
## Error:  Failed to create the shared library

cPropModel = compileNimble(propModel)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_37.dll > dynamicRegistrations_03_08_15_52_37.log'
had status 1
## Error:  Failed to create the shared library

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


sampleMV <- modelValues(sampleMVConf)

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

```
## 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)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_41.dll > dynamicRegistrations_03_08_15_52_41.log'
had status 1
## Error:  Failed to create the shared library

CImpWeights <- compileNimble(RImpWeights, project = targetModel)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_43.dll > dynamicRegistrations_03_08_15_52_43.log'
had status 1
## Error:  Failed to create the shared library

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

## Error in eval(expr, envir, enclos):  object 'CPropSamp' not found

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

## Error in eval(expr, envir, enclos):  object 'CImpWeights' not found

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

savedPropSamp_1 = CImpWeights$propModelValues

## Error in eval(expr, envir, enclos):  object 'CImpWeights' not found

savedPropSamp_2 = CPropSamp$mv
```

```
## Error in eval(expr, envir, enclos):  object 'CPropSamp' not found

# 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]

## Error in eval(expr, envir, enclos):  object 'savedPropSamp_1' not found

savedPropSamp_2['x',1]

## Error in eval(expr, envir, enclos):  object 'savedPropSamp_2' not found

savedPropSamp_1['x',1] <- 0 ## example of directly setting a value

## Error in savedPropSamp_1["x", 1] <- 0:  object 'savedPropSamp_1' not found

savedPropSamp_2['x',1]

## Error in eval(expr, envir, enclos):  object 'savedPropSamp_2' not found

## Viewing the saved importance weights
savedWeights <- CImpWeights$savedWeights

## Error in eval(expr, envir, enclos):  object 'CImpWeights' not found

unlist(savedWeights[['w']])

## Error in unlist(savedWeights[["w"]]):  object 'savedWeights' not found

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

## Error in as.matrix(savedPropSamp_1):  object 'savedPropSamp_1' not found
```

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.

13.4.5   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 models defined from BUGS code are never created as 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$z` or `model[['z']]`, NIMBLE will try to do the right thing by treating this as a scalar. In the event of problems[5], a more explicit way to access z is `model$z[1]` or `model[['z']][1]`.

13.4.6 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 default main method name. Any method can then call another method.

```
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())
        }))

## Warning in nf_checkDSLcode(code):  For this nimbleFunction to compile, these
## objects must be defined as nimbleFunctions, nimbleLists, or nimbleFunction methods:
## increment, times.

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

## sharedValues = 1
```

---

[5]please tell us!

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

methodsDemo1$sharedValue <- 1
CmethodsDemo1 <- compileNimble(methodsDemo1)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_47.dll > dynamicRegistrations_03_08_15_52_47.log'
had status 1
## Error:  Failed to create the shared library

CmethodsDemo1$run(1:10)

## Error in eval(expr, envir, enclos):  object 'CmethodsDemo1' not found
```

13.4.7   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$sharedValue <<- initialSharedValue
        print(myMethodsDemo$sharedValue)
        A <- myMethodsDemo$run(x[1:5])
        print(A)
        B <- myMethodsDemo$times(10)
        return(B)
        returnType(double())
    })

## Warning in nf_checkDSLcode(code):  For this nimbleFunction to compile, these
objects must be defined as nimbleFunctions, nimbleLists, or nimbleFunction methods:
times.

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

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


CusePreviousDemo1 <- compileNimble(usePreviousDemo1)


## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_50.dll > dynamicRegistrations_03_08_15_52_50.log'
had status 1
## Error:  Failed to create the shared library

CusePreviousDemo1$run(1:10)

## Error in eval(expr, envir, enclos):  object 'CusePreviousDemo1' not found
```

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 may not be shown here because this document is created with `knitr` and for some reason output printed from C++ does not make it into `knitr` output.

13.4.8   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 Version 0.6-4 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()
    },
    run = function(x = double(1)) {
        for(i in seq_along(nfl)) {
            print( nfl[[i]]$run(x) )
            print( nfl[[i]]$foo() )
        }
    }
    )
```

```
## Warning in nf_checkDSLcode(code):  For this nimbleFunction to compile, these
objects must be defined as nimbleFunctions, nimbleLists, or nimbleFunction methods:
```

```
foo.

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




CuseThem1 <- compileNimble(useThem1)

## compiling...  this may take a minute.  Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_54.dll > dynamicRegistrations_03_08_15_52_54.log'
had status 1
## Error:  Failed to create the shared library

set.seed(0)
CuseThem1$run(1:5)

## Error in eval(expr, envir, enclos):  object 'CuseThem1' not found
```

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.

13.4.9 Character objects

NIMBLE provides limited uses of character objects in `run` code. Character vectors created in `setup` code will be available in `run` code, but the only thing you can really do with them is include them in a `print` or `stop` statement.

Note that character vectors of model node and variable names are processed during compilation. For example, in `model[[node]]`, `node` may be a character object, and the NIMBLE compiler processes this differently than `print(''The node name was '', node)`. In the former, the NIMBLE compiler sets up a C++ pointer directly to the `node` in the `model`, so that the character content of `node` is never needed in C++. In the latter, `node` is used as a C++ string and therefore is needed in C++.

13.4.10 User-defined data structures

need to determine if/how obsolete this is given nimbleLists; if text is kept, make clear when one would use this instead of a nimbleList

NIMBLE does not explicitly 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$run(as.numeric(100), as.numeric(100:110),
                matrix(as.numeric(101:120), nrow = 2))
myDataNF$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
```

```
nimbleOptions(useMultiInterfaceForNestedNimbleFunctions = FALSE)
CmyUseDataNF <- compileNimble(myUseDataNF)

## compiling...   this may take a minute.   Use 'showCompilerOutput = TRUE' to
see C++ compiler details.
## Warning:  running command 'C:/PROGRA~1/R/R-33~1.2/bin/x64/R CMD SHLIB dynamicRegistra
-o dynamicRegistrations_03_08_15_52_58.dll > dynamicRegistrations_03_08_15_52_58.log'
had status 1
## Error:  Failed to create the shared library

CmyUseDataNF$run(-100, -(100:110), matrix(-(101:120), nrow = 2))

## Error in eval(expr, envir, enclos):  object 'CmyUseDataNF' not found

CmyDataNF <- CmyUseDataNF$myDataNF

## Error in eval(expr, envir, enclos):  object 'CmyUseDataNF' not found

CmyDataNF$X

## Error in eval(expr, envir, enclos):  object 'CmyDataNF' not found

CmyDataNF$Y

## Error in eval(expr, envir, enclos):  object 'CmyDataNF' not found

CmyDataNF$Z

## Error in eval(expr, envir, enclos):  object 'CmyDataNF' not found
```

You'll notice that:

- After execution of the compiled function, access to the X, Y, and Z is the same as for the uncompiled case. This occurs because `CmyUseDataNF` is an interface to the compiled version of `myUseDataNF`, and it provides access to member objects and functions. In this case, one member object is `myDataNF`, which is an interface to the compiled version of `myUseDataNF$myDataNF`, which in turn provides access to X, Y, and Z. To reduce memory use, NIMBLE defaults to *not* providing full interfaces to nested nimbleFunctions like `myUseDataNF$myDataNF`. In this example we made it provide full interfaces by setting the `buildInterfacesForCompiledNestedNimbleFunctions` option via `nimbleOptions` to TRUE. If we had left that option FALSE (its default value), we could still get to the values of interest using

```
valueInCompiledNimbleFunction(CmyDataNF, 'X')
```

- We need to take care that at the time of compilation, the X, Y and Z values contain 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.

13.5 Example: writing user-defined samplers to extend NIMBLE's MCMC engine

One important use of nimbleFunctions is to write additional samplers that can be used in NIMBLE's MCMC engine. This allows a user to write a custom sampler for one or more nodes in a model, as well as for programmers to provide general samplers for use in addition to the library of samplers provided with NIMBLE.

The following code illustrates how a NIMBLE developer would implement and use a Metropolis-Hastings random walk sampler with fixed proposal standard deviation.

```r
my_RW <- nimbleFunction(

    contains = sampler_BASE,

    setup = function(model, mvSaved, target, control) {
        scale <- control$scale    ## proposal standard deviation
        calcNodes <- model$getDependencies(target)
    },

    run = function() {
        model_lp_initial <- getLogProb(model, calcNodes) ## initial model logProb
        proposal <- rnorm(1, model[[target]], scale)     ## generate proposal
        model[[target]] <<- proposal                      ## store proposal into model
        model_lp_proposed <- calculate(model, calcNodes) ## proposal model logProb

        ## 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

        ## keep the model and mvSaved objects consistent
        if(jump) copy(from = model, to = mvSaved, row = 1,
                      nodes = calcNodes, logProb = TRUE)
        else     copy(from = mvSaved, to = model, row = 1,
                      nodes = calcNodes, logProb = TRUE)
    },

    methods = list(   reset = function () {}   )
)
```

The name of this sampler function, for the purposes of using it in an MCMC algorithm, is `my_RW`. Thus, this sampler can be added to an exisiting MCMC configuration object `conf` using:

```
mcmcConf$addSampler(target = 'x', type = 'my_RW',
                    control = list(scale = 0.1))
```

To be used within the MCMC engine, sampler functions definitions must adhere exactly to the following:

- Include the contains statement `contains = sampler_BASE`.
- The `setup` function must have the exact four arguments `model, mvSaved, target, control`, in that order.
- The `run` function must accept no arguments, and have no return value. Further, after execution it must leave the `mvSaved` modelValues object as an up-to-date copy of the values and logProb values in the model object.
- Have a member method called `reset`, which takes no arguments and has no return value.

The purpose of the `setup` function is generally two-fold. First, to extract control parameters from the `control` list; in the example, the proposal standard deviation `scale`. Second, to generate any sets of nodes needed in the `run` function. In many sampling algorithms, as here, `calcNodes` is used to represent the target node(s) and dependencies up to the first layer of stochastic nodes, as this is precisely what is required for calculating the Metropolis-Hastings acceptance probability. These probability calculations are done using `model$calculate(calcNodes)`.

In the `run` function, the `mvSaved` modelValues object is kept up-to-date with the current state of the model, depending on whether the proposed changed was accepted. This is done using the `copy` function, to copy values between the model and `mvSaved` objects.

13.6 Copying nimbleFunctions (and NIMBLE models)

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, the model member function `newModel` will create a new copy of the model from the same model definition (Section **??**). 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. For example, say you have a

nimbleFunction called `foo` and 1000 instances of `foo` are compiled as part of an algorithm related to a model called `model1`. If you then need to use `foo` in an algorithm for another model, `model2`, doing so may work without any problems. However, there are cases where the NIMBLE compiler will tell you during compilation that the second set of `foo` instances cannot be built from the previous compiled version. A solution is to re-define `foo` from the beginning – i.e. call `nimbleFunction` again – and then proceed with building and compiling the algorithm for `model2`.

13.7 Debugging nimbleFunctions

One of the main reasons that NIMBLE provides an R (uncompiled) version of each nimbleFunction is for debugging. One can call `debug` on nimbleFunction methods (in particular the main *run* method) and then step through the code in R using R's debugger. One can also insert `browser` calls into run code and then run the nimbleFunction from R.

In contrast, directly debugging a compiled nimbleFunction is difficult, although those familiar with running R through a debugger and accessing the underlying C code may be able to operate similarly with NIMBLE code.

TODO: basic info on inserting browser in nf run code and running in R as well as using debug(nf$run)

13.8 Some options for reducing memory usage

TODO: needs to be revised so only memory use is covered here and other material is moved as appropriate

NIMBLE can make a lot of objects in its processing, and some of them use R features like reference classes that are not light in memory usage. We have noticed that building large models can use lots of memory. To help alleviate this, we provide two options, which can be controlled via `nimbleOptions`.

As noted above, the option `buildInterfacesForCompiledNestedNimbleFunctions` defaults to FALSE, which means NIMBLE will not build full interfaces to compiled nimbleFunctions that ony appear within other nimbleFunctions. If you want access to all such nimbleFunctions, use the option `buildInterfacesForCompiledNestedNimbleFunctions = TRUE`.

The option `clearNimbleFunctionsAfterCompiling` is more drastic, and it is experimental, so "buyer beware". This will clear much of the contents of an uncompiled nimbleFunction object after it has been compiled in an effort to free some memory. We expect to be able to keep making NIMBLE more efficient – faster execution and lower memory use – in the future.

Bibliography