Extensible software for hierarchical modeling: using the NIMBLE platform to explore models and algorithms

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http://r-nimble.org

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Background and Goals

- Software for fitting hierarchical models has opened their use to a wide variety of communities
- Most software for fitting such models is either model-specific or algorithm-specific
- Software is often a black box and hard to extend
- Our goal is to divorce model specification from algorithm, while
  - Retaining BUGS compatibility
  - Providing a variety of standard algorithms
  - **Allowing developers to add new algorithms (including modular combination of algorithms)**
  - Allowing users to operate within R
  - Providing speed via compilation to C++, with R wrappers

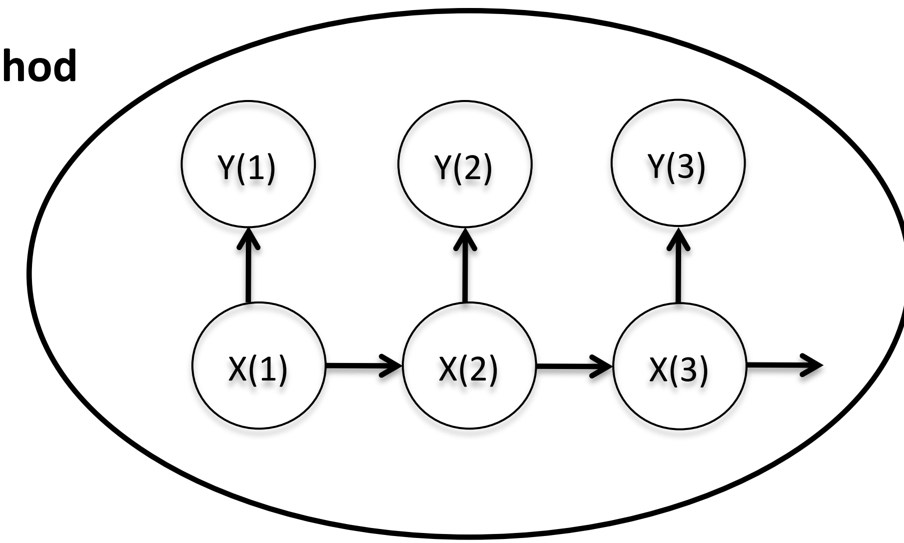
Divorcing Model Specification from Algorithm

MCMC Flavor 1

Your new method

MCMC Flavor 2

Data cloning



Particle Filter

MCEM

Quadrature

Importance Sampler

Unscented KF

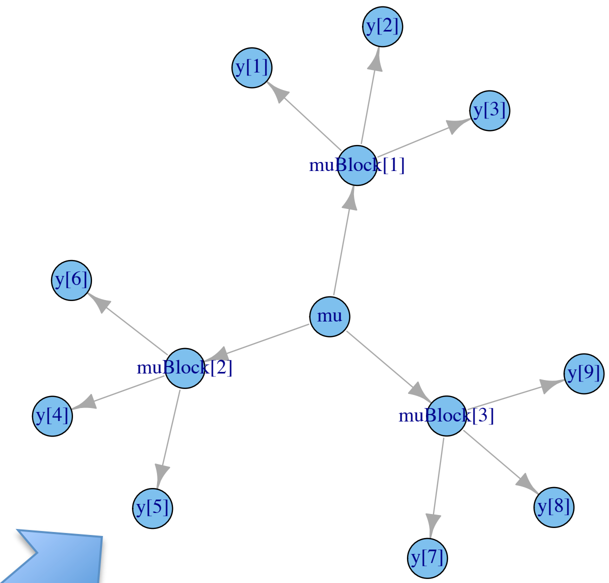
NIMBLE Design

- High-level processing in R (as much as possible)
  - Process BUGS language for declaring models (with some extensions)
  - Process model structure (node dependencies, conjugate relationships, etc.)
  - Generate and customize algorithm specifications
  - Generate model-specific C++ code to be compiled on the fly
  - Provide matching implementation in R for prototyping / debugging / testing
  - Some high-level algorithm control possible in R (adapting tuning parameters, monitoring convergence, high levels of iteration)

- Low-level processing in C++
  - Model and algorithm computations
  - "Run-time" parameters allow some modification of behavior without recompiling

User Experience: Creating a Model from BUGS

```
littersModelCode <- quote({
  for(j in 1:G) {
    for(I in 1:N) {
          r[i, j] ~ dbin(p[i, j], n[i, j]);
          p[i, j] ~ dbeta(a[j], b[j]);
     }
     mu[j] <- a[j]/(a[j] + b[j]);
     theta[j] <- 1.0/(a[j] + b[j]);
     a[j] ~ dgamma(1, 0.001);
     b[j] ~ dgamma(1, 0.001);
 })
```



1

Parse and process BUGS code.
Collect information in model object.

2

Use igraph plot method.

```
> littersModel <- nimbleModel(littersModelCode, constants = list(N = 16, G = 2), data = list(r = input$r))
> littersModel_cpp <- compileNimble(littersModel)
```

3

Provides variables and functions (calculate, simulate) for algorithms to use.

User Experience: Specializing an Algorithm to a Model

```
littersModelCode <- modelCode({
  for(j in 1:G) {
    for(I in 1:N) {
        r[i, j] ~ dbin(p[i, j], n[i, j]);
        p[i, j] ~ dbeta(a[j], b[j]);
    }
    mu[j] <- a[j]/(a[j] + b[j]);
    theta[j] <- 1.0/(a[j] + b[j]);
    a[j] ~ dgamma(1, 0.001);
    b[j] ~ dgamma(1, 0.001);
})
```

```
sampler_slice <- nimbleFunction(
   setup = function((model, mvSaved, control) {
       calcNodes <- model$getDependencies(control$targetNode)
       discrete <- model$getNodeInfo()[[control$targetNode]]$isDiscrete()
[…snip…]
  run = function() {
      u <- getLogProb(model, calcNodes) - rexp(1, 1)
      x0 <- model[[targetNode]]
      L <- x0 - runif(1, 0, 1) * width
 […snip….]
…
```

```
> littersMCMCspec <- MCMCspec(littersModel)
> getUpdaters(littersMCMCspec)
[…snip…]
[3] RW sampler;   targetNode: b[1],  adaptive: TRUE,  adaptInterval: 200,  scale: 1
[4] RW sampler;   targetNode: b[2],  adaptive: TRUE,  adaptInterval: 200,  scale: 1
[5] conjugate_beta sampler;   targetNode: p[1, 1],  dependents_dbin: r[1, 1]
[6] conjugate_beta sampler;   targetNode: p[1, 2],  dependents_dbin: r[1, 2]
 [...snip...]
> littersMCMCspec$addSampler('slice', list(targetNodes = c('a[1]', 'a[2]'), adaptInterval = 100))
> littersMCMCspec$addMonitor('theta')
> littersMCMC <- buildMCMC(littersMCMCspec)
> littersMCMC_Cpp <- compileNimble(littersMCMC, project = littersModel)

> littersMCMC_Cpp (20000)
```

User Experience: Specializing an Algorithm to a Model (2)

```
littersModelCode <- quote({
 for(j in 1:G) {
  for(I in 1:N) {
      r[i, j] ~ dbin(p[i, j], n[i, j]);
      p[i, j] ~ dbeta(a[j], b[j]);
   }
   mu[j] <- a[j]/(a[j] + b[j]);
   theta[j] <- 1.0/(a[j] + b[j]);
   a[j] ~ dgamma(1, 0.001);
   b[j] ~ dgamma(1, 0.001);
 })
```

```
buildMCEM <- nimbleFunction(
 while(runtime(converged == 0)) {
 ....
   calculate(model, paramDepDetermNodes)
   mcmcFun(mcmc.its, initialize = FALSE)
   currentParamVals[1:nParamNodes] <- getValues(model,paramNodes)
   op <- optim(currentParamVals, objFun, maximum = TRUE)
   newParamVals <- op$maximum
.....
```

```
> littersMCEM <- buildMCEM(littersModel, latentNodes = 'p', mcmcControl = list(adaptInterval =
50), boxConstaints = list( list('a', 'b'), limits = c(0, Inf))), buffer = 1e-6)
> set.seed(0)
> littersMCEM(maxit = 50, m1 = 500, m2 = 5000)
```

Modularity (UNDER CONSTRUCTION):

One can plug any MCMC sampler into the MCEM, with user control of the sampling strategy, in place of the default MCMC.

Programmer Experience: NIMBLE Algorithm DSL

- Analogy: BUGS is a Domain-Specific Language (DSL) for models
- NIMBLE provides a DSL for algorithms
    - The DSL is a modified subset of R.
- We provide
    - Basic types (double, logical)
    - Basic (vectorized) math and distribution/probability calculations
    - Basic data storage classes ("modelValues")
    - Control structures – for loops and if-then-else
    - Ability to define functions
    - Linear algebra (via the Eigen package)
    - Specific functions for a model: *calculate*, *simulate*
- Function definitions in the DSL include code for two steps:
    - A generic run-time function is written in the DSL for any model structure
    - When a model is provided, a set of one-time setup processing is executed in R based on the model structure to "specialize" algorithm to model
    - Run-time code can use information determined from the setup processing

Programmer Experience: Creating an Algorithm

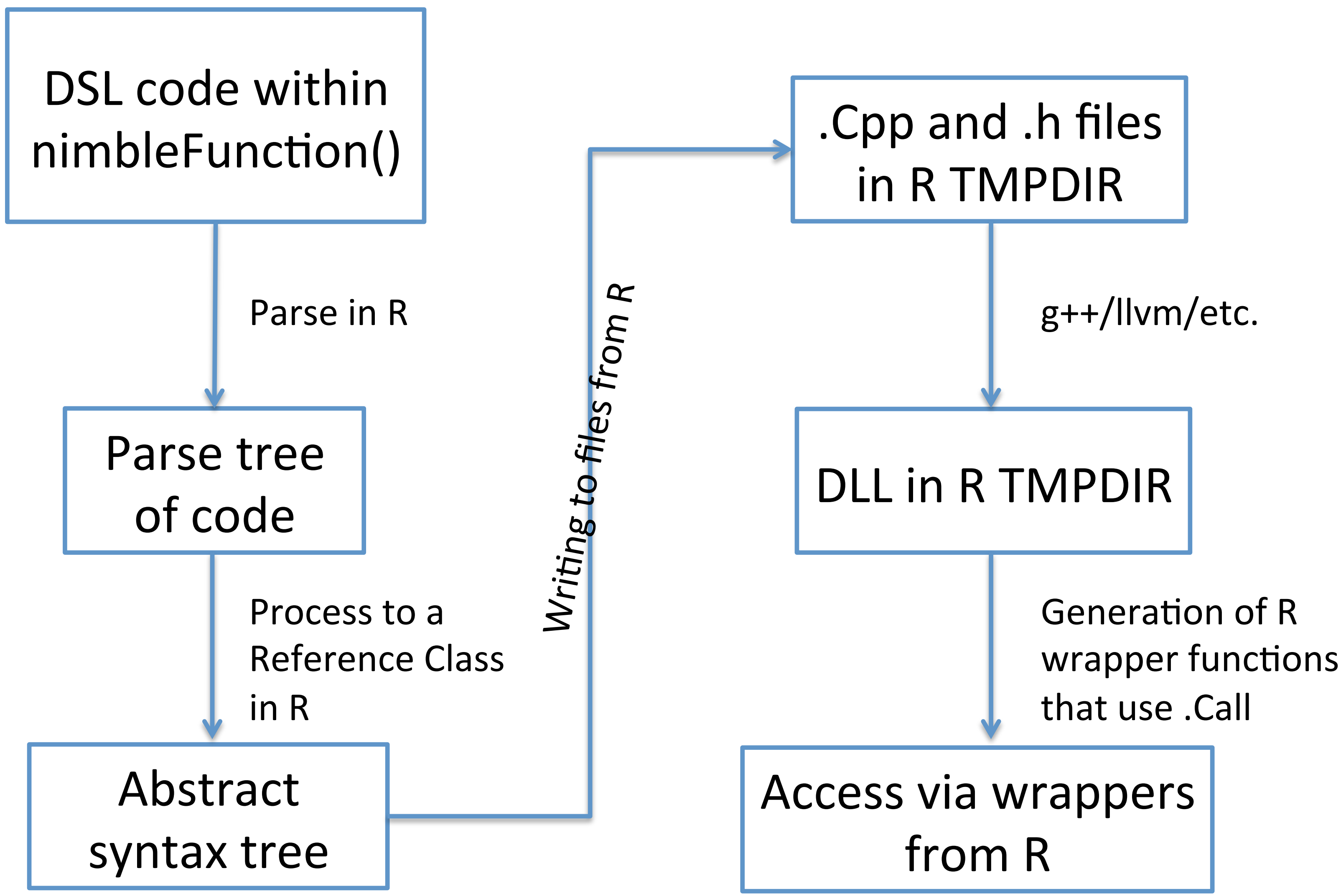
```
myAlgorithmGenerator <- nimbleFunction (

 setup = function(model, <otherSetupArguments>) {

  # code that does the specialization of algorithm to model
  # e.g., determine nodes to sample,
  # initialize storage

 },

 run = function(<runtimeArguments>) {

  # code that carries out the generic algorithm
  # for example, iterations of an algorithm
  # simulate into nodes, calculate log probability values
  returnType(double())
  return(x)
 })
```

Two sections to a NIMBLE function.

Usage:

```
specializedAlgo <- myAlgorithmGenerator(myModel, <setupArgs>)
specializedAlgo(<runtimeArguments>)
```

How an Algorithm is Processed in NIMBLE



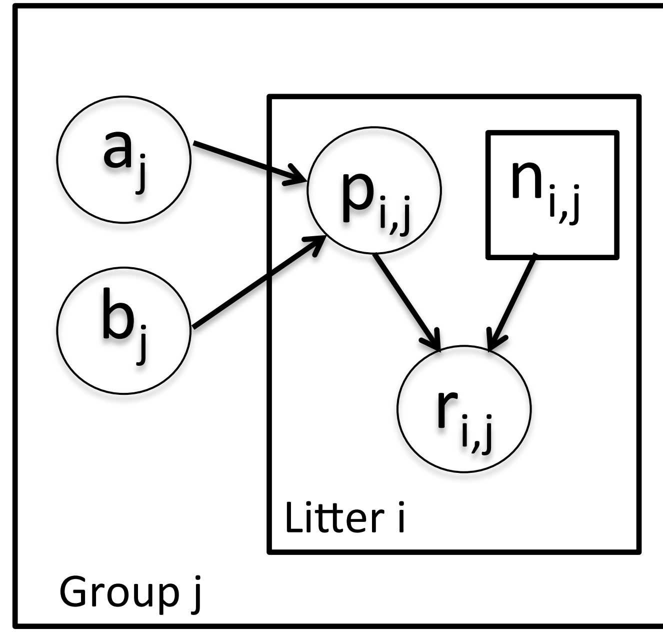
Programmer experience: Random walk updater

```
sampler_myRW <- nimbleFunction(contains = sampler_BASE,

setup = function(model, mvSaved, targetNode, scale) {
   calcNodes <- model$getDependencies(targetNode)
},

run = function() {
   model_lp_initial <- getLogProb(model, calcNodes)
   proposal <- rnorm(1, model[[targetNode]], scale)
   model[[targetNode]] <<- proposal
   model_lp_proposed <- calculate(model, calcNodes)
   log_MH_ratio <- model_lp_proposed - model_lp_initial

    if(decide(log_MH_ratio)) jump <- TRUE
       else                 jump <- FALSE

    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)
   })
```

NIMBLE in Action: the Litters Example

Beta-binomial for clustered binary response data

```
littersModelCode <- quote({
 for(j in 1:G) {
  for(I in 1:N) {
        r[i, j] ~ dbin(p[i, j], n[i, j]);
        p[i, j] ~ dbeta(a[j], b[j]);
   }
   mu[j] <- a[j]/(a[j] + b[j]);
   theta[j] <- 1.0/(a[j] + b[j]);
   a[j] ~ dgamma(1, 0.001);
   b[j] ~ dgamma(1, 0.001);
})
```

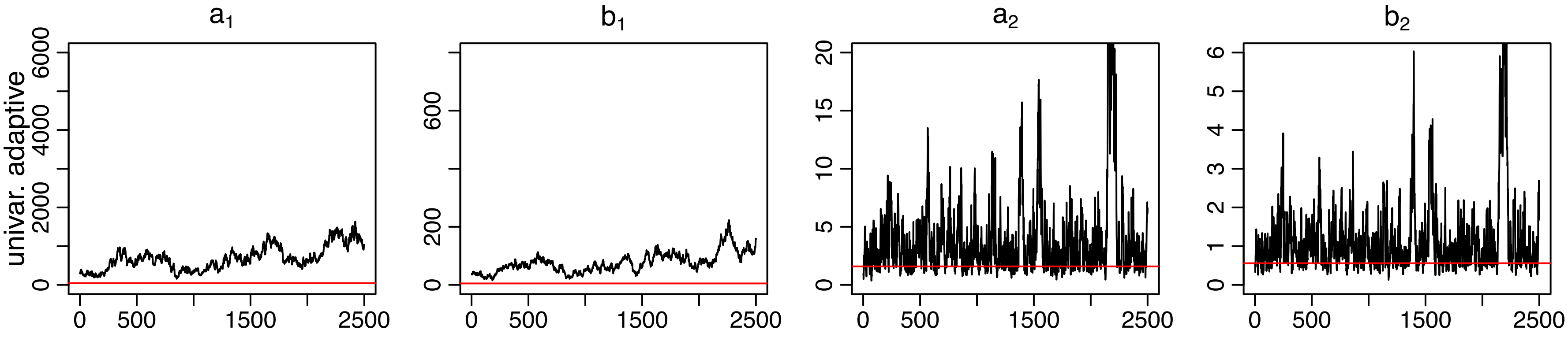


Challenges of the toy example:

- BUGS manual: "The estimates, particularly a_1, a_2 suffer from extremely poor convergence, limited agreement with m.l.e.'s and considerable prior sensitivity. This appears to be due primarily to the parameterisation in terms of the highly related a_j and b_j, whereas direct sampling of mu_j and $theta_j$ would be strongly preferable."
- But that's not all that's going on. Consider the dependence between the p's and their a_j, b_j hyperparameters.
- And perhaps we want to do something other than MCMC.

Default MCMC: Gibbs + Metropolis

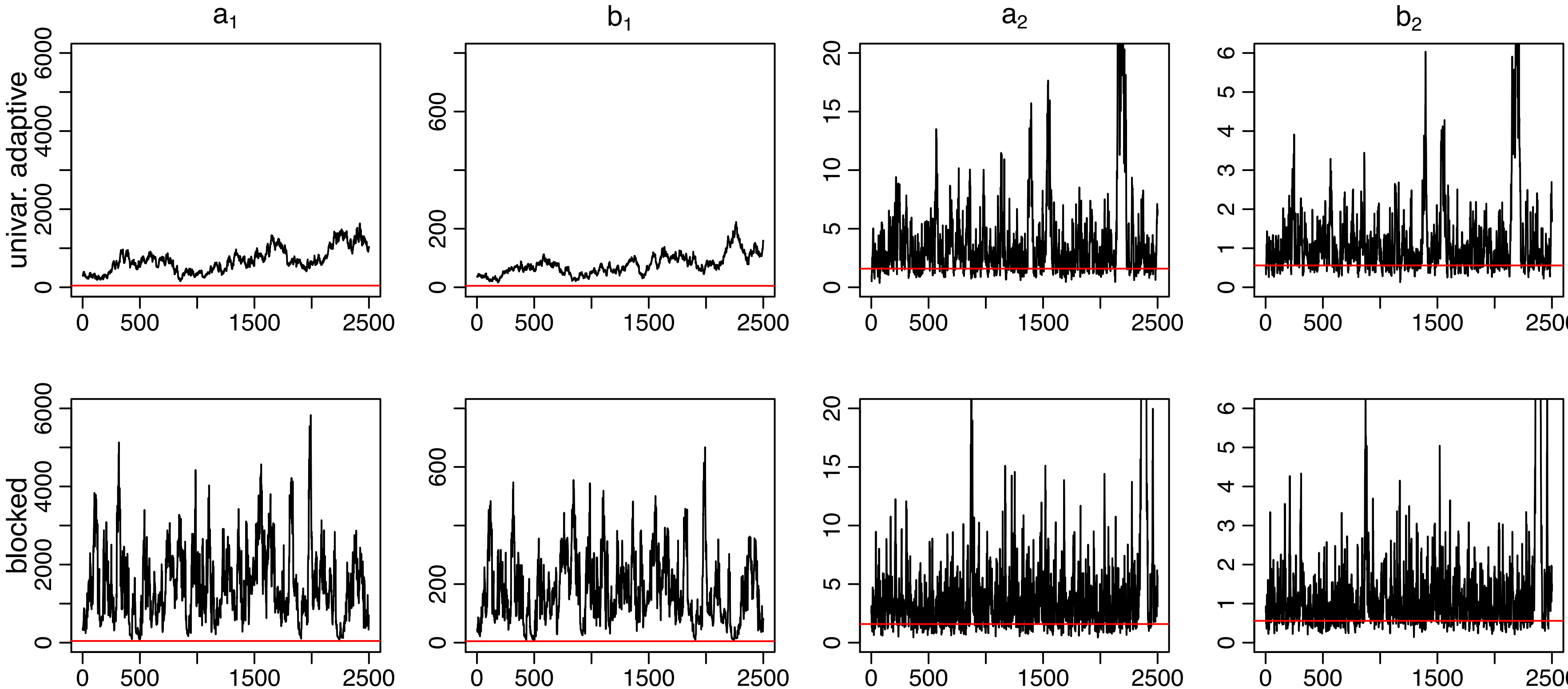
```
> littersMCMCspec <- MCMCspec(littersModel, list(adaptInterval = 100))
> littersMCMC <- buildMCMC(littersMCMCspec)
> littersMCMC_cpp <- compileNIMBLE(littersModel, project = littersModel)
> littersMCMC_cpp(10000)
```



Red line is MLE

Blocked MCMC: Gibbs + Blocked Metropolis

```
> littersMCMCspec2 <- MCMCspec(littersModel, list(adaptInterval = 100))
> littersMCMCspec2$addSampler('RW_block', list(targetNodes = c('a[1]', 'b[1]'),
      adaptInterval = 100)
> littersMCMCspec2$addSampler('RW_block', list(targetNodes = c('a[2]', 'b[2]'),
      adaptInterval = 100)
> littersMCMC2 <- buildMCMC(littersMCMCspec2)
> littersMCMC2_cpp <- compileNIMBLE(littersMCMC2, project = littersModel)
> littersMCMC2_cpp(10000)
```

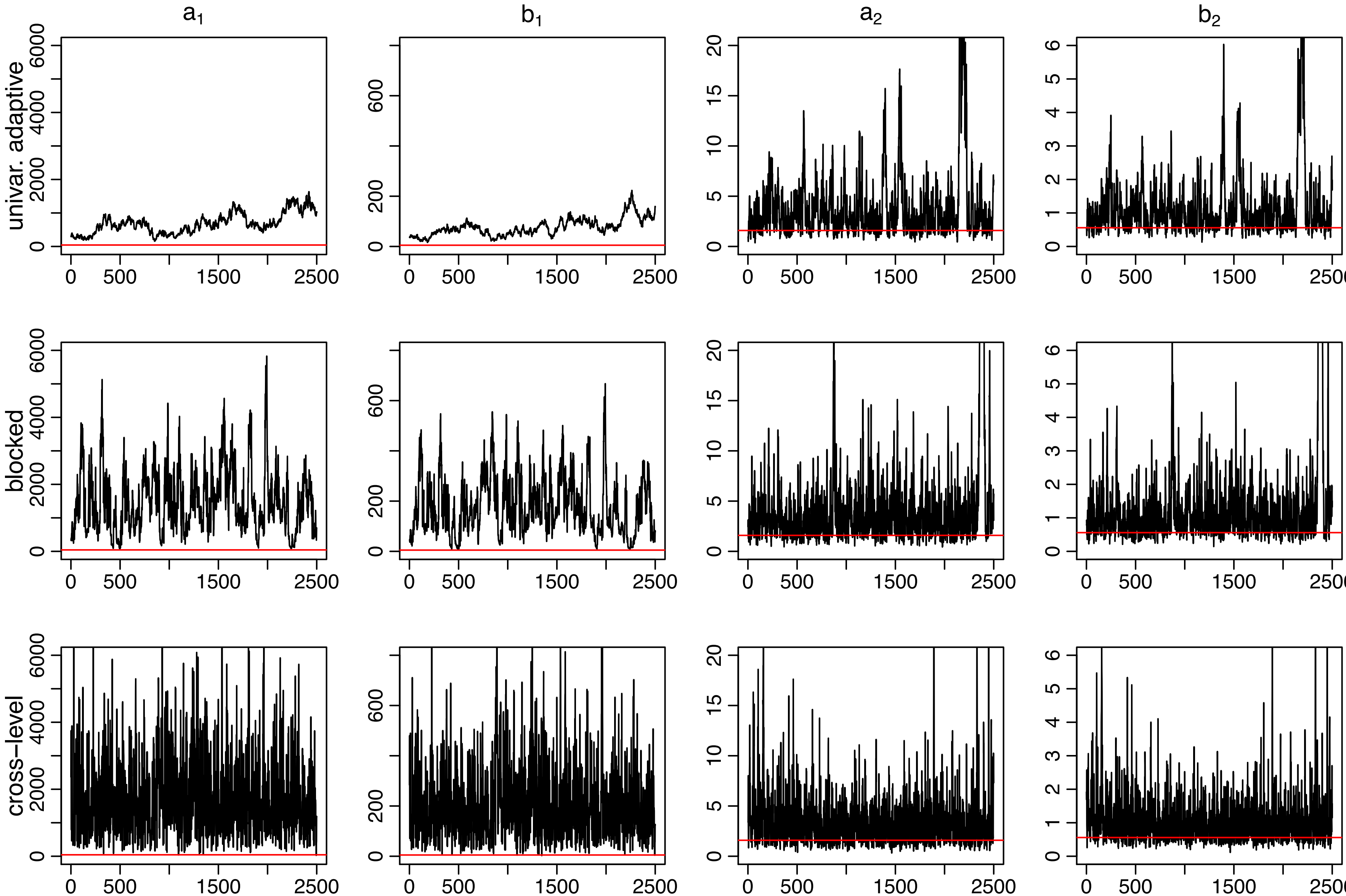


a_1
b_1
a_2
b_2
univar. adaptive
blocked
0
2000
4000
6000
200
600
5
10
15
20
1
2
3
4
5
6
500
1500
2500

Blocked MCMC: Gibbs + Cross-level Updaters

- Cross-level dependence is a key barrier in this and many other models.
- We wrote a new "cross-level" updater function using the NIMBLE DSL.
  - The updater is a blocked Metropolis random walk on a set of hyperparameters with conditional Gibbs updates on dependent nodes (provided they are in a conjugate relationship).
  - This is equivalent to (analytically) integrating the dependent (latent) nodes out of the model.

```
> littersMCMCspec3 <- MCMCspec(littersModel, adaptInterval = 100)
> topNodes1 <- c('a[1]', 'b[1]')
> littersMCMCspec3$addSampler('crossLevel', list(topNodes = topNodes1, adaptInterval
     = 100)
> topNodes2 <- c('a[2]', 'b[2]')
> littersMCMCspec3$addSampler('crossLevel', list(topNodes = topNodes1, adaptInterval
     = 100)
> littersMCMC3 <- buildMCMC(littersMCMCspec3)
> littersMCMC3_cpp <- compileNIMBLE(littersMCMC3, project = littersModel)
> littersMCMC3_cpp (10000)
```



a1
b1
a2
b2
univar. adaptive
blocked
cross−level

Litters MCMC: BUGS and JAGS

- BUGS gives similar performance to the default NIMBLE MCMC
  - Be careful – values of $sim.list and $sims.matrix in R2WinBUGS output are randomly permuted
  - Mixing for a2 and b2 modestly better than default NIMBLE MCMC
- JAGS slice sampler gives similar performance as BUGS, but fails for some starting values with this (troublesome) parameterization
- NIMBLE provides user control and transparency.
  - NIMBLE is faster than JAGS on this example (if one ignores the compilation time).
  - Note: we're not out to build the best MCMC but rather a flexible framework for algorithms – we'd love to have someone else build a better default MCMC and distribute for use in our system.

Stepping outside the MCMC box: maximum likelihood/empirical Bayes via MCEM

```
> littersMCEM    <- buildMCEM(littersModel, latentNodes = 'p')
> littersMCEM(maxit = 500, m1 = 500, m2 = 5000)
```

- Gives estimates consistent with direct ML estimation (possible in this simple model with conjugacy for ‘p’) to 2-3 digits
- VERY slow to converge, analogous to MCMC mixing issues
- Current implementation is basic; more sophisticated treatments should help

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Many algorithms are of a modular nature/combine other algorithms, e.g.

- particle MCMC
- normalizing constant algorithms
- many, many others in the literature in the last 15 years

Status of NIMBLE and Next Steps

- First release was June 2014; lots to do, including:
  - Improve the user interface and speed up compilation
  - Refinement/extension of the DSL for algorithms
  - Enhance current algorithms provided (e.g., add multivariate conjugate updates for MCMC)
  - Additional algorithms written in NIMBLE DSL (e.g., particle MCMC)
  - Advanced features (e.g., auto. differentiation, paralleliz'n)
- Interested?
  - Announcements: nimble-announce Google site
  - User support/discussion: nimble-users Google site
  - Write an algorithm using NIMBLE!
  - Help with development of NIMBLE: email nimble.stats@gmail.com or see github.com/nimble-dev

Programmer Experience: Slice Sampler Example

```
sampler_slice <- nimbleFunction( contains = sampler_BASE,
    setup = function(model, mvSaved, control) {
        targetNode    <- control$targetNode
        adaptive      <- control$adaptive
         ....
        calcNodes <- model$getDependencies(targetNode)
         ....
        discrete      <- model$getNodeInfo()[[targetNode]]$isDiscrete()
    },
   run = function() {
        u <- getLogProb(model, calcNodes) - rexp(1, 1)
        x0 <- model[[targetNode]
        L <- x0 - runif(1, 0, 1) * width
        R <- L + width
        maxStepsL <- floor(runif(1, 0, 1) * maxSteps)
        maxStepsR <- maxSteps - 1 – maxStepsL
        lp <- setAndCalculateTarget(L)
        while(maxStepsL > 0 & !is.nan(lp) & lp >= u) {
            L <- L - width
            lp <- setAndCalculateTarget(L)
            maxStepsL <- maxStepsL - 1
        }  .....
```