Beyond the black box: Flexible programming of hierarchical modeling algorithms for BUGS-compatible models using NIMBLE

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http://r-nimble.org

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What do we want to do with hierarchical models?

1. Core algorithms

- MCMC
- Sequential Monte Carlo
- Laplace approximation
- Importance sampling

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2. Different flavors of algorithms

- Many flavors of MCMC
- Gaussian quadrature
- Monte Carlo expectation maximization (MCEM)
- Kalman Filter
- Auxiliary particle filter
- Posterior predictive simulation
- Posterior re-weighting
- Data cloning
- Bridge sampling (normalizing constants)
- YOUR FAVORITE HERE
- YOUR NEW IDEA HERE

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3. Idea combinations
- Particle MCMC
- Particle Filter with replenishment
- MCMC/Laplace approximation
- Dozens of ideas in recent JRSSB/JCGS issues

What can a practitioner do with hierarchical models?

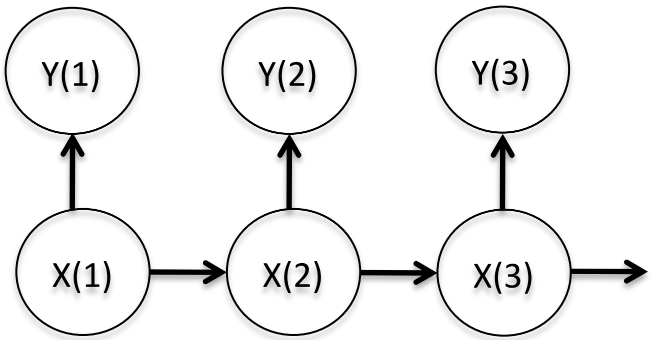
Two basic software designs:

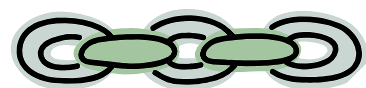
1. Typical R package = Model family + 1 or more algorithms
   - GLMMs: lme4, MCMCglmm
   - GAMMs: mgcv
   - spatial models: spBayes, INLA

2. Flexible model + black box algorithm
   - BUGS: WinBUGS, OpenBUGS, JAGS
   - PyMC
   - INLA
   - Stan

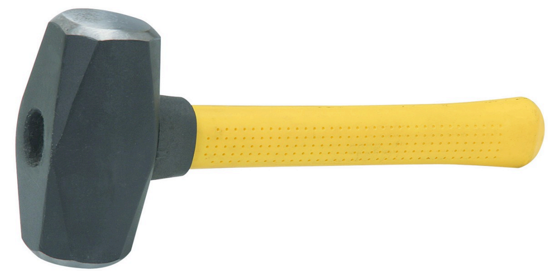
Existing software

Model





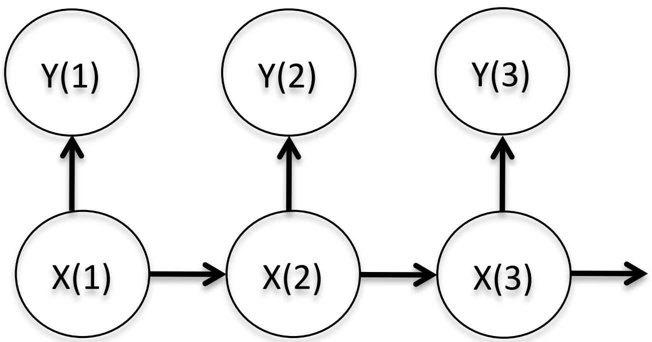
Algorithm



e.g., BUGS (WinBUGS, OpenBUGS, JAGS), INLA, Stan, various R packages

NIMBLE: The Goal

Model



+

Algorithm language

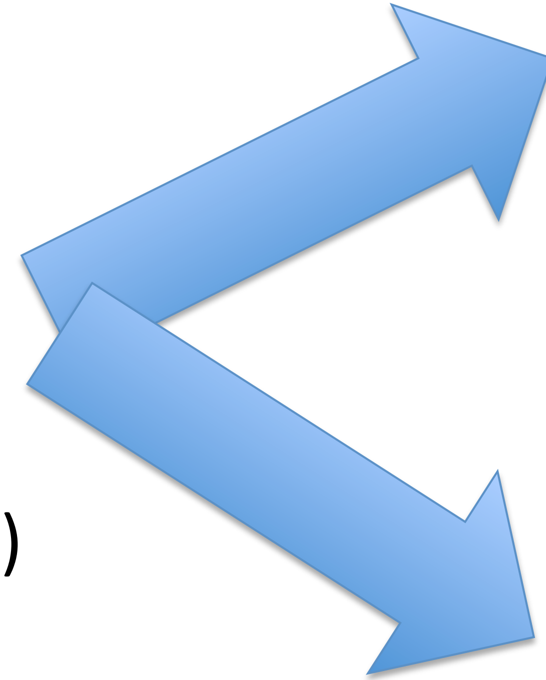
=

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

NIMBLE System Summary

statistical model
(BUGS code)
+
algorithm
(nimbleFunction)



R objects + R under the hood

R objects + C++ under the hood

✧ We generate C++ code,
✧ compile and load it,
✧ provide interface object.

NIMBLE

1. Model specification

   BUGS language → R/C++ model object

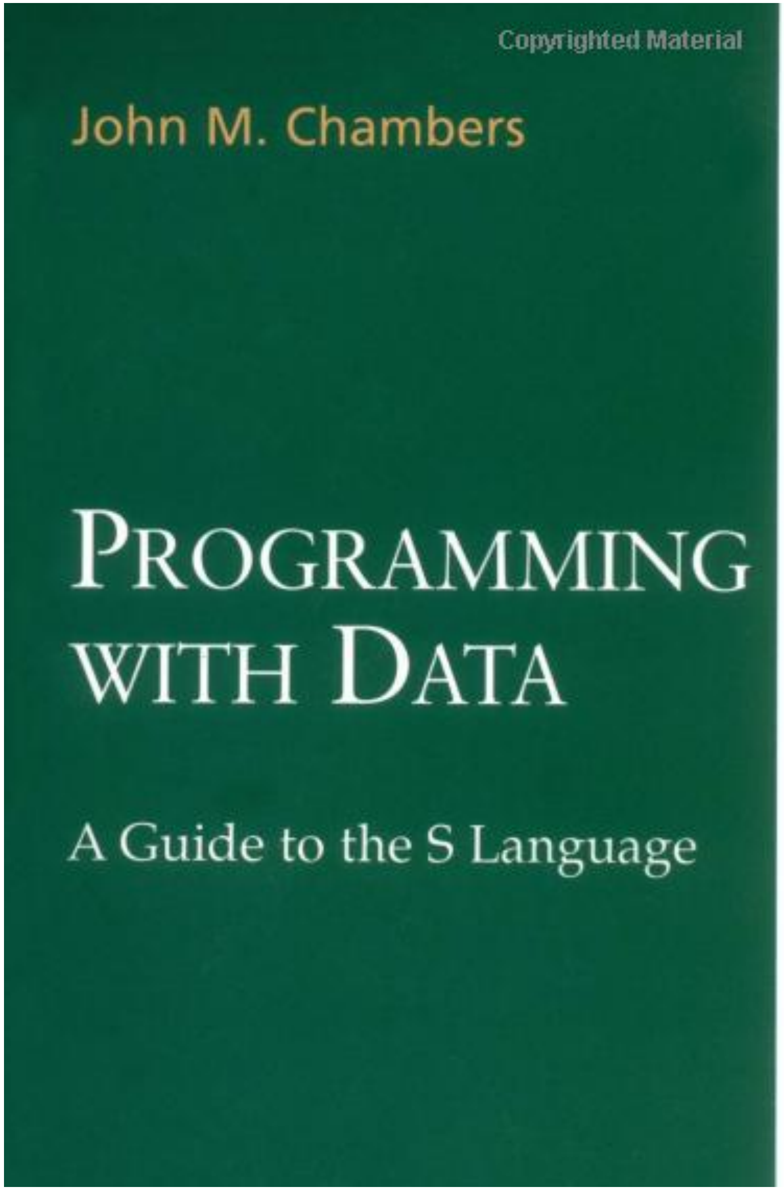
2. Algorithm specification

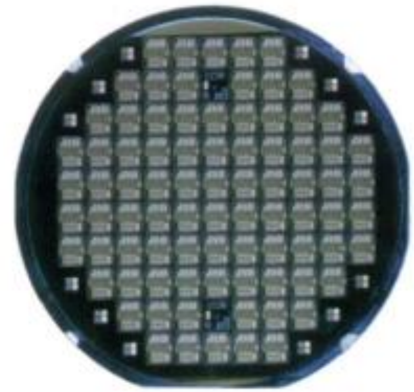
   NIMBLE programming language within R → R/C++ algorithm object

3. Algorithm library

   MCMC, Particle Filter/Sequential MC, etc.

The Success of R





Programming with Models

You give NIMBLE:

```
> littersCode <- nimbleCode( {
  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);   } )
> littersModel <- nimbleModel(littersCode, constants = list(N = 16, G = 2),
        data = list(r = input$r))
> littersModel_cpp <- compileNimble(littersModel) # C++ version of model
```

You get this:

```
> littersModel$a[1] <- 5
> simulate(littersModel, 'p')
> p_deps <- littersModel$getDependencies('p')
> littersModel$calculate(p_deps)
> littersModel$getLogProb('r')
```

NIMBLE also extends BUGS: multiple parameterizations, named parameters, and user-defined distributions and functions.

User Experience: Specializing an Algorithm to a Model

```
littersCode <- 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….]
…
```

```
> littersMCMCconf <- configureMCMC(littersModel)
> littersMCMCconf$getSamplers()
[…snip…]
[3] RW sampler;   targetNode: b[1],  adaptive: TRUE,  adaptInterval: 200,  scale: 1
[4] RW sampler;   targetNode: b[2],  adaptive: TRUE,  adaptInterval: 200,  scale: 1
[5] conjugate_beta sampler;   targetNode: p[1, 1],  dependents_dbin: r[1, 1]
[6] conjugate_beta sampler;   targetNode: p[1, 2],  dependents_dbin: r[1, 2]
 [...snip...]
> littersMCMCconf$addSampler('a[1]', 'slice', list(adaptInterval = 100))
> littersMCMCconf$addSampler('a[2]', 'slice', list(adaptInterval = 100))
> littersMCMCconf$addMonitors('theta')
> littersMCMC <- buildMCMC(littersMCMCconf)
> littersMCMC_Cpp <- compileNimble(littersMCMC, project = littersModel)
> littersMCMC_Cpp$run(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), boxConstraints = list( list('a', 'b'), limits = c(0, Inf))), buffer = 1e-6)
> set.seed(0)
> littersMCEM(maxit = 50, m1 = 500, m2 = 5000)
```

Modularity:

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

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NIMBLE: Programming With Models

We want:

- High-level processing (model structure) in R
- Low-level processing in C++

NIMBLE: Programming With Models

```
objectiveFunction <- nimbleFunction (

 setup = function(model, nodes) {
  calcNodes <- model$getDependencies(nodes)
 },

 run = function(vals = double(1)) {
  values(model, nodes) <<- vals
  sumLogProb <- calculate(model, calcNodes)
  return(sumLogProb)
  returnType(double())
 })
```

2 kinds of functions

NIMBLE: Programming With Models

```
objectiveFunction <- nimbleFunction (

 setup = function(model, nodes) {
   calcNodes <- model$getDependencies(nodes)
 },

 run = function(vals = double(1)) {
   values(model, nodes) <<- vals
   sumLogProb <- calculate(model, calcNodes)
   return(sumLogProb)
   returnType(double())
 })
```

query model structure ONCE.

NIMBLE: Programming With Models

```
objectiveFunction <- nimbleFunction (

 setup = function(model, nodes) {
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 },

 run = function(vals = double(1)) {
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  sumLogProb <- calculate(model, calcNodes)
  return(sumLogProb)
  returnType(double())
 })
```

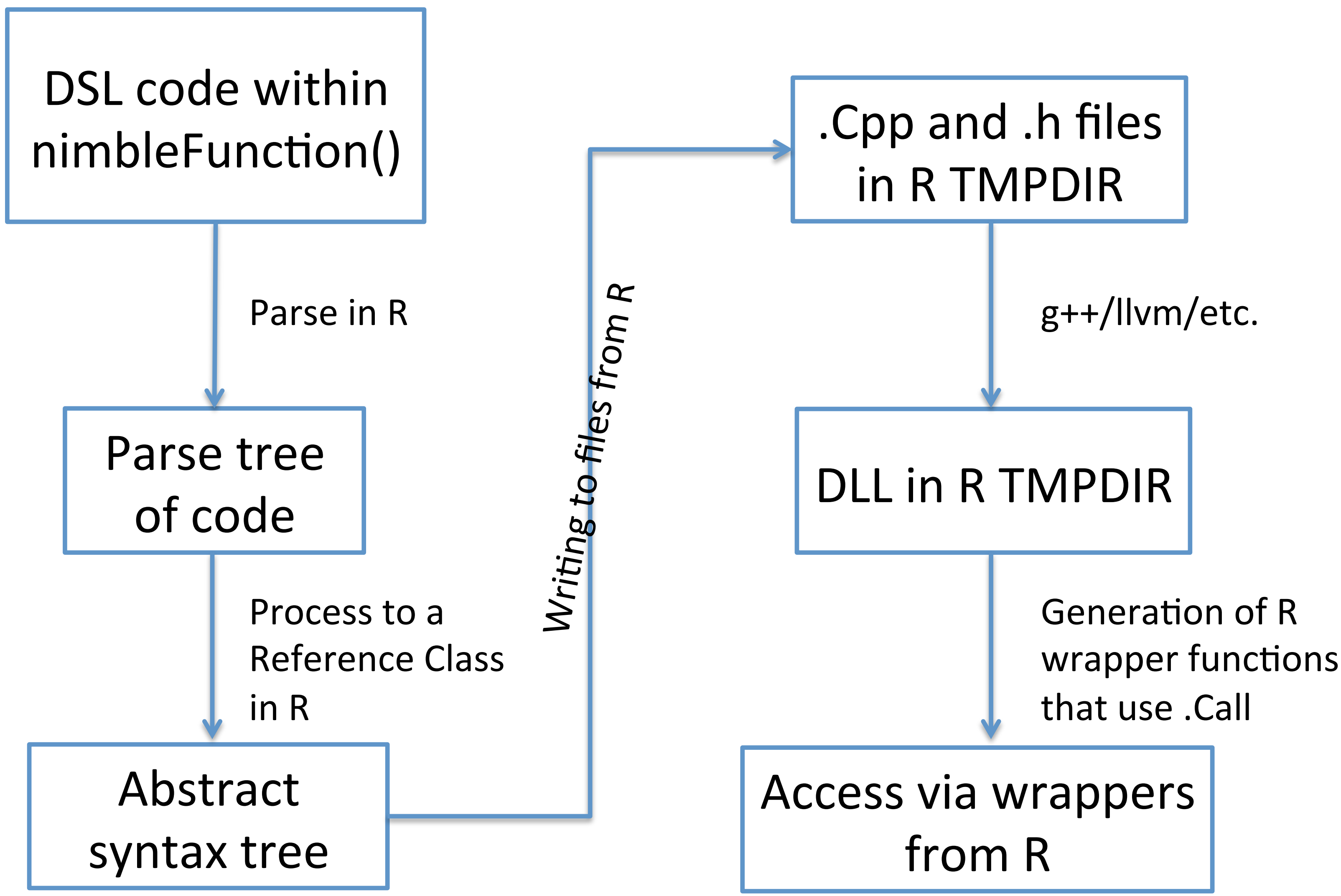
the actual algorithm

The NIMBLE compiler

<u>Feature summary:</u>

- R-like matrix algebra (using Eigen library)
- R-like indexing (e.g. X[1:5,])
- Use of model variables and nodes
- Model calculate (logProb) and simulate functions
- Sequential integer iteration
- if-then-else, do-while
- Declare input & output types only
- Access to much of Rmath.h (e.g. distributions)
- Automatic R interface / wrapper
- Many improvements / extensions planned

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)
   })
```

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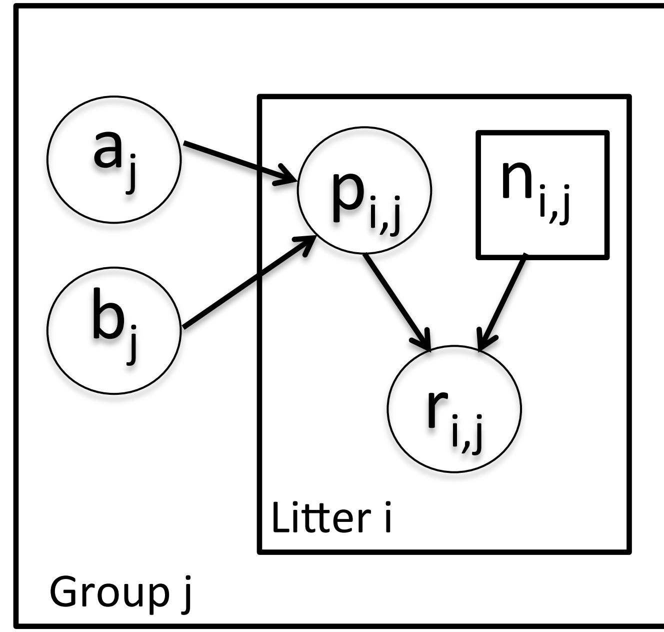
NIMBLE in Action: the Litters Example

Beta-binomial GLMM for clustered binary response data
Survival in two sets of 16 litters of pigs

```
littersModelCode <- nimbleCode({
  for(j in 1:2) {
    for(I in 1:16) {
          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);
})
```

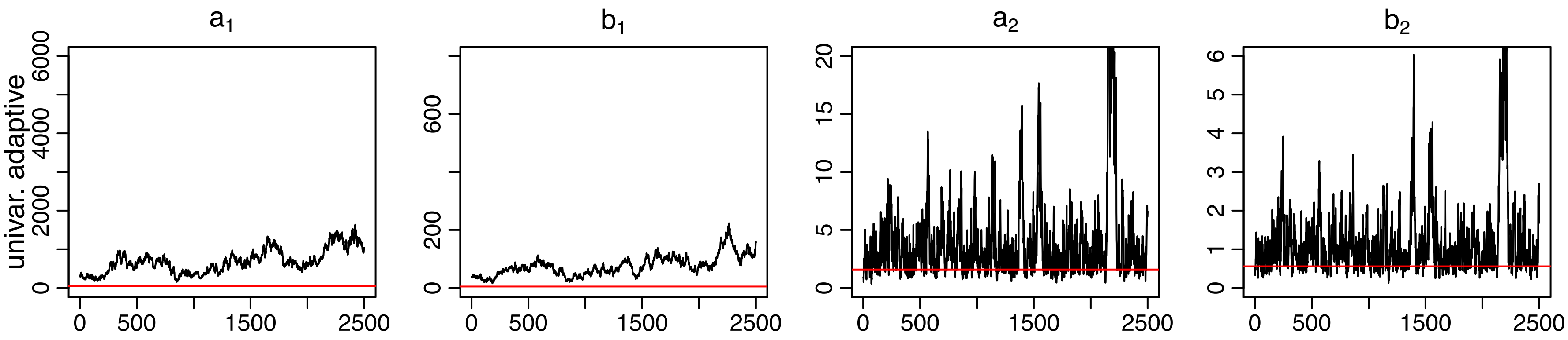


Challenges of the toy example:

- 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

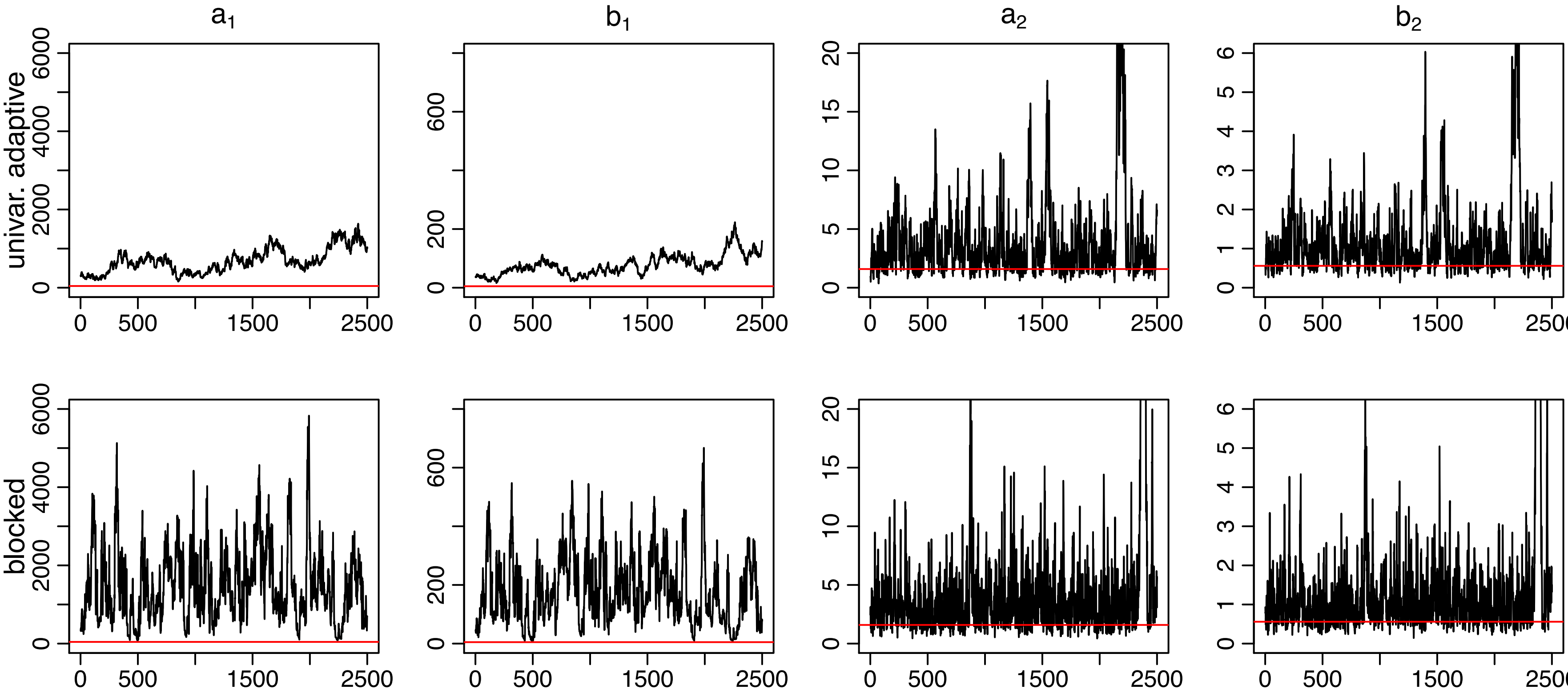
```
> littersMCMCconf <- configureMCMC(littersModel, list(adaptInterval = 100))
> littersMCMC <- buildMCMC(littersMCMCconf)
> littersMCMC_cpp <- compileNIMBLE(littersModel, project = littersModel)
> littersMCMC_cpp$run(10000)
```



Red line is MLE

Blocked MCMC: Gibbs + Blocked Metropolis

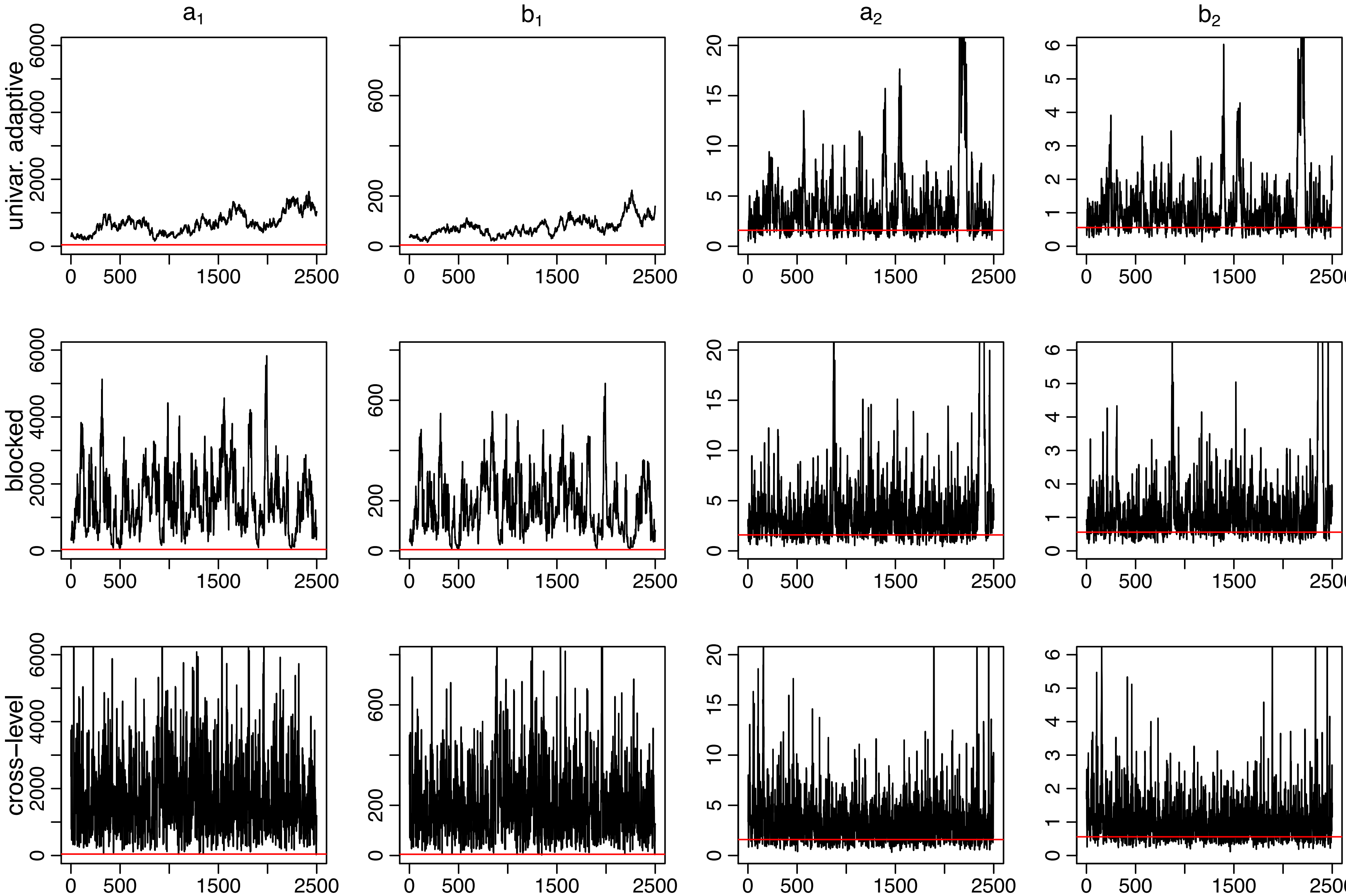
```
> littersMCMCconf2 <- configureMCMC(littersModel, list(adaptInterval = 100))
> littersMCMCconf2$addSampler(c('a[1]', 'b[1]'), 'RW_block', list(adaptInterval = 100)
> littersMCMCconf2$addSampler(c('a[2]', 'b[2]'), 'RW_block', list(adaptInterval = 100)
> littersMCMC2 <- buildMCMC(littersMCMCconf2)
> littersMCMC2_cpp <- compileNIMBLE(littersMCMC2, project = littersModel)
> littersMCMC2_cpp$run(10000)
```


a1
b1
a2
b2
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.
  - Blocked Metropolis random walk on a set of hyperparameters with conditional Gibbs updates on dependent nodes (provided they are in a conjugate relationship).
  - Equivalent to (analytically) integrating the dependent (latent) nodes out of the model.

```
> littersMCMCconf3 <- configureMCMC(littersModel, adaptInterval = 100)
> topNodes1 <- c('a[1]', 'b[1]')
> littersMCMCconf3$addSampler(topNodes1, 'crossLevel', list(adaptInterval = 100)
> topNodes2 <- c('a[2]', 'b[2]')
> littersMCMCconf3$addSampler(topNodes2, 'crossLevel', list(adaptInterval = 100)
> littersMCMC3 <- buildMCMC(littersMCMCconf3)
> littersMCMC3_cpp <- compileNIMBLE(littersMCMC3, project = littersModel)
> littersMCMC3_cpp$run(10000)
```


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

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; version 0.5 in process of being released on CRAN.
- Lots to do:
  - Sequential MC methods in next release (particle filter, ensemble Kalman filter, particle MCMC)
  - Improve the user interface and speed up compilation
  - Allow indices of vectors to be random (e.g., mixture models)
  - Refinement/extension of the DSL for algorithms
  - Additional algorithms written in NIMBLE DSL (e.g., normalizing constant calculation, Laplace approximations)
  - Advanced features (e.g., auto. differentiation, paralleliz'n)
- Interested?
  - Upcoming SBSS webinar, April 19 at 3 pm EDT: www.amstat.org/education/weblectures/index.cfm#DD
  - 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