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

Christopher Paciorek   UC Berkeley Statistics

Joint work with:

Perry de Valpine (PI)   UC Berkeley Environmental Science, Policy and Managem't
Daniel Turek   UC Berkeley Statistics and ESPM
Cliff Anderson-Bergman   Lawrence Livermore Lab (alumnus)
Duncan Temple Lang   UC Davis Statistics

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

What do we want to do with hierarchical models?

1. Core algorithms
- MCMC
- Sequential Monte Carlo
- Laplace approximation
- Importance sampling

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

2. Different flavors of algorithms
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- Monte Carlo expectation maximization (MCEM)
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- YOUR NEW IDEA HERE

What can a practitioner do with hierarchical models?

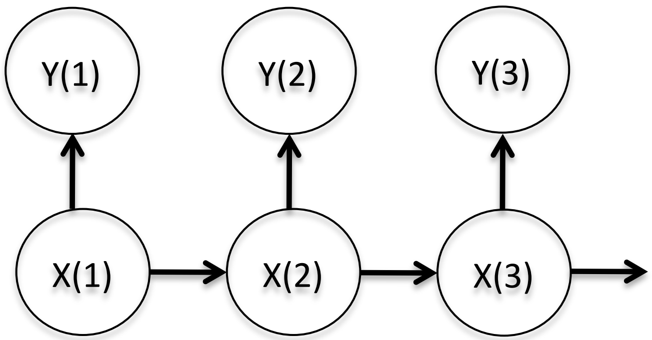
Two basic software designs:

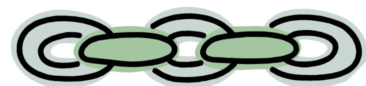
1. Typical R package = Model family + 1 or more algorithms
   - GLMMs: lme4, MCMCglmm
   - GAMMs: mgcv
   - spatial models: spBayes, INLA

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

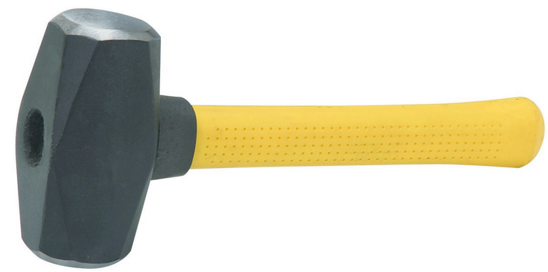
Existing software

Model





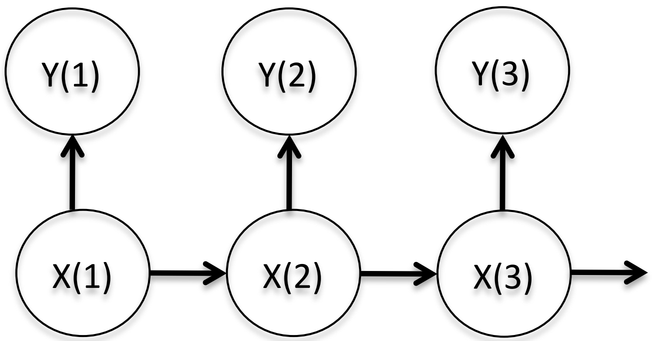
Algorithm



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

NIMBLE: The Goal

Model



+

Algorithm language

=

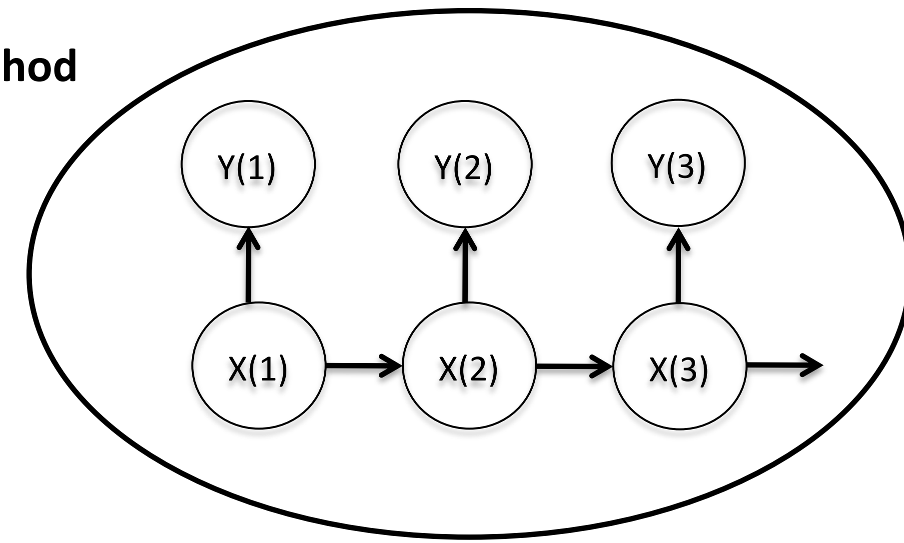
Divorcing Model Specification from Algorithm

MCMC Flavor 1

Your new method

MCMC Flavor 2

Data cloning



Particle Filter

MCEM

Quadrature

Importance Sampler

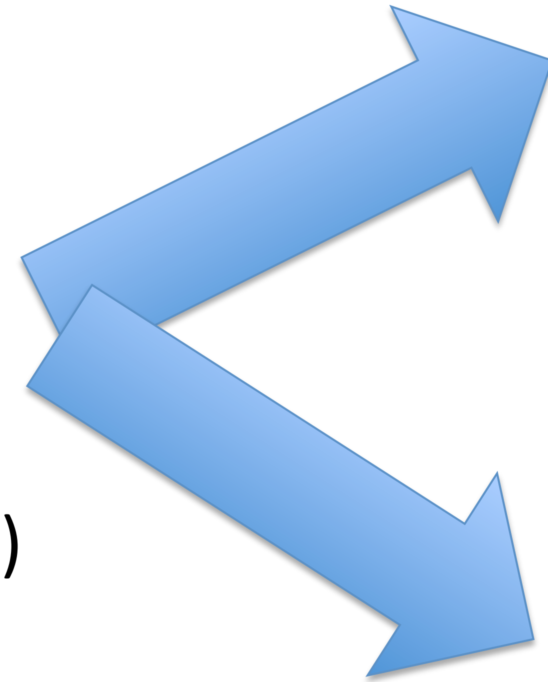
Maximum likelihood

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

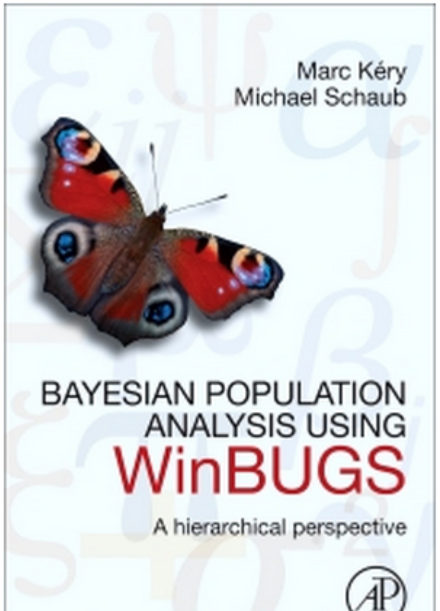
    BUGS language → R/C++ model object

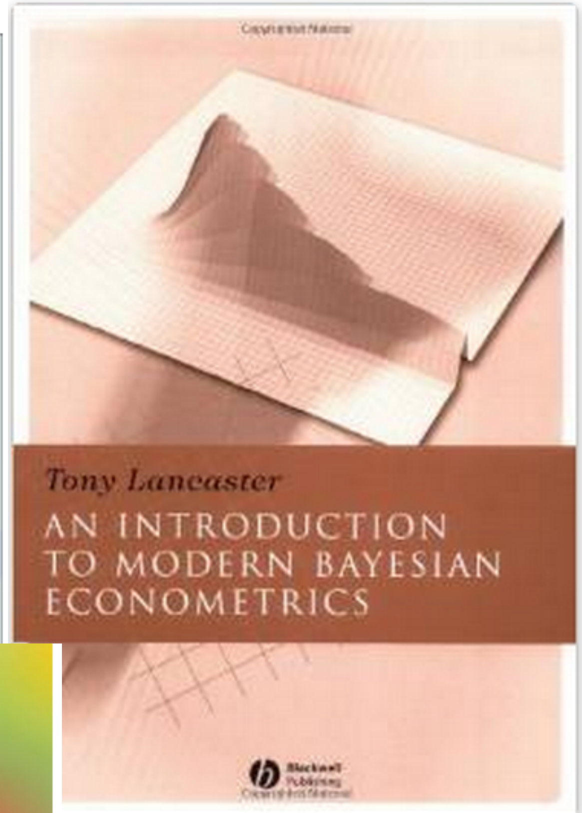
2. Algorithm specification

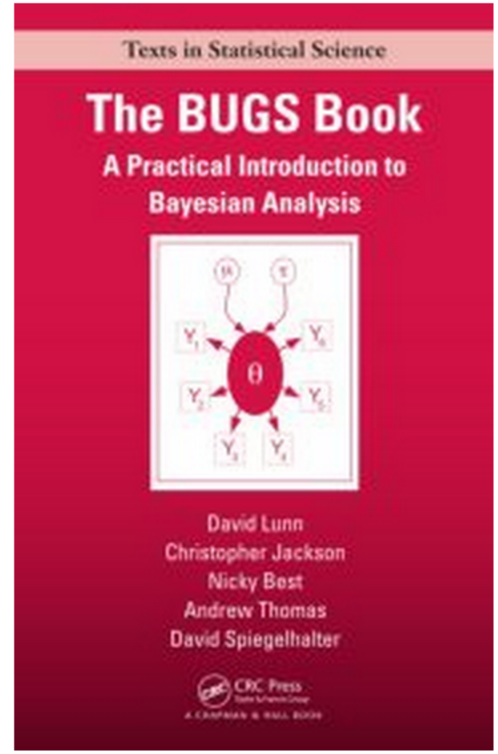
    NIMBLE programming language within R → R/C++ algorithm object

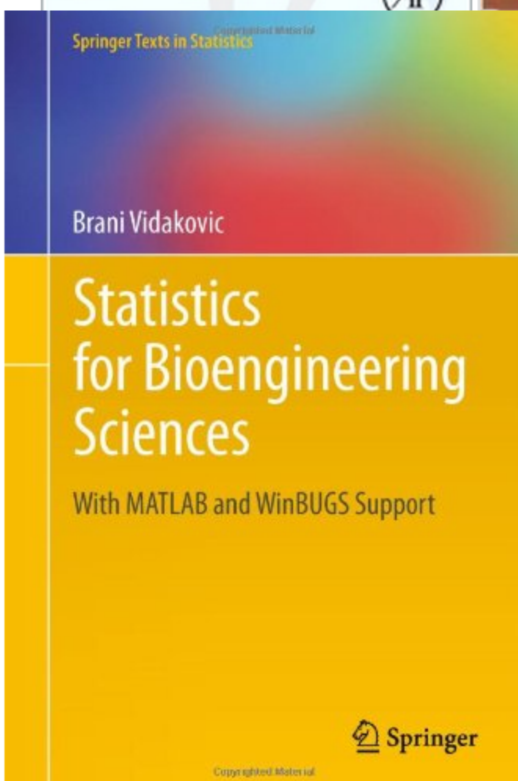
3. Algorithm library

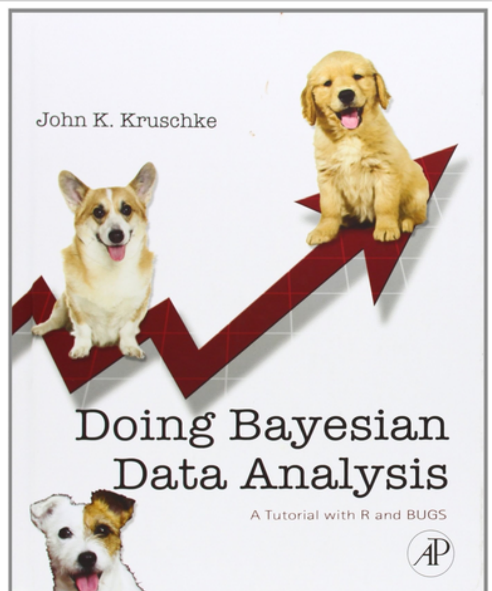
    MCMC, Particle Filter/Sequential MC, etc.

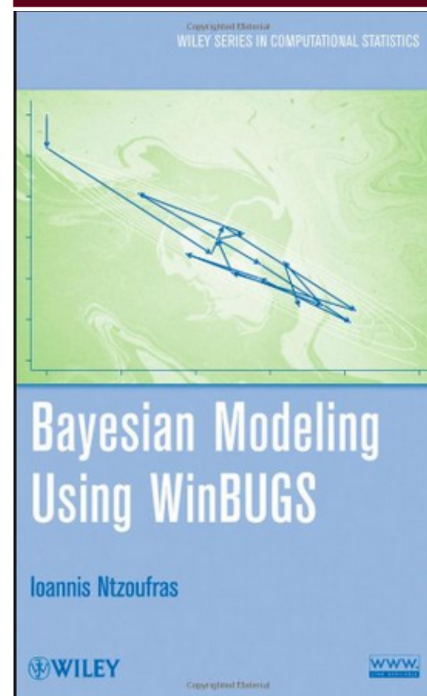

Marc Kéry
Michael Schaub
BAYESIAN POPULATION ANALYSIS USING
WinBUGS
A hierarchical perspective


Tony Lancaster
AN INTRODUCTION TO MODERN BAYESIAN ECONOMETRICS


Texts in Statistical Science
The BUGS Book
A Practical Introduction to Bayesian Analysis
David Lunn
Christopher Jackson
Nicky Best
Andrew Thomas
David Spiegelhalter
CRC Press

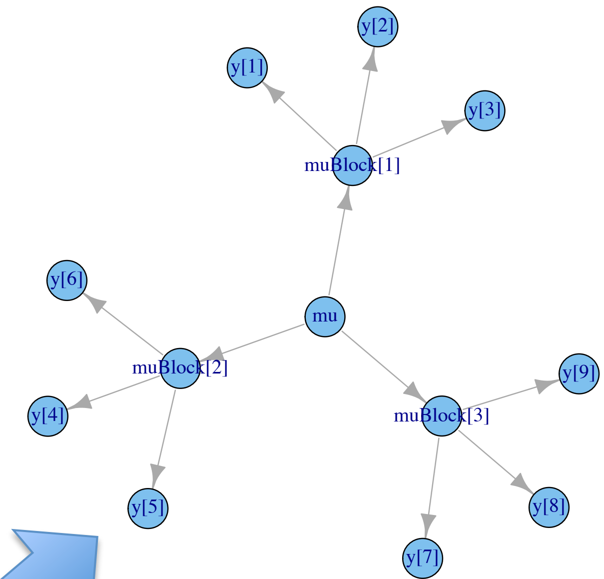

Springer Texts in Statistics
Brani Vidakovic
Statistics for Bioengineering Sciences
With MATLAB and WinBUGS Support
Springer


John K. Kruschke
Doing Bayesian Data Analysis
A Tutorial with R and BUGS


WILEY SERIES IN COMPUTATIONAL STATISTICS
Bayesian Modeling Using WinBUGS
Ioannis Ntzoufras
WILEY

User Experience: Creating a Model from BUGS

```
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);
})
```



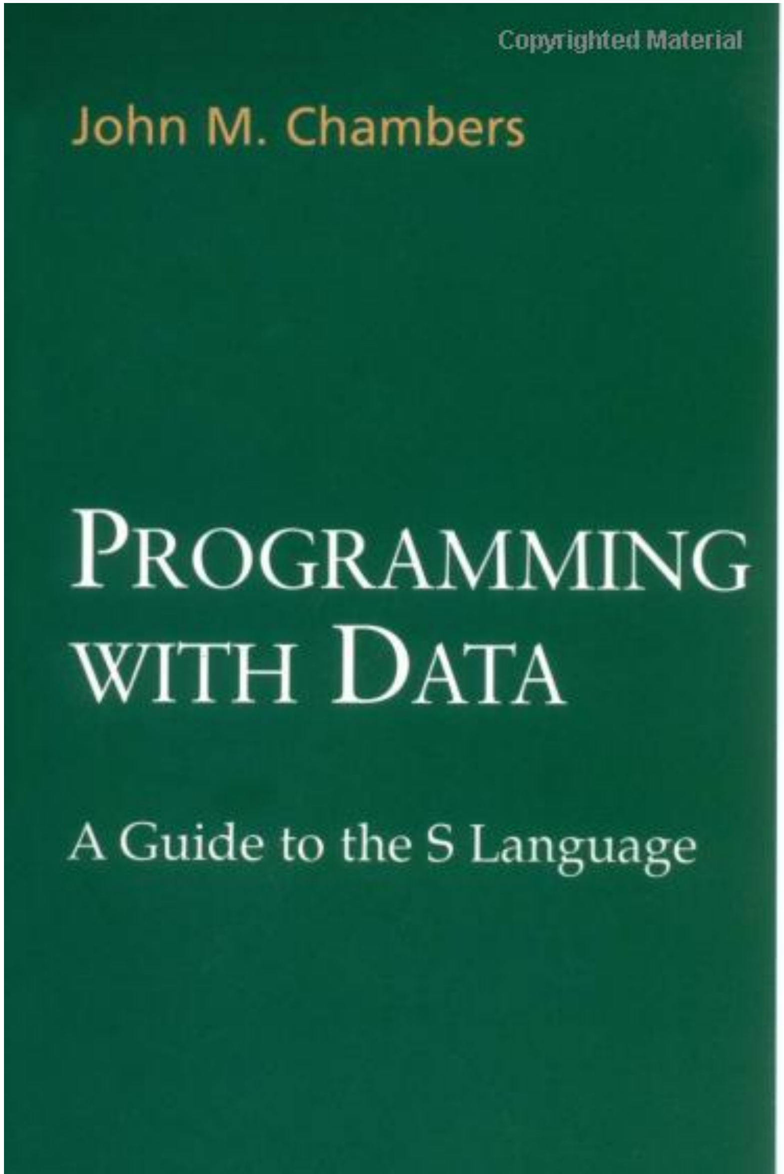
1 — Parse and process BUGS code.
Collect information in model object.

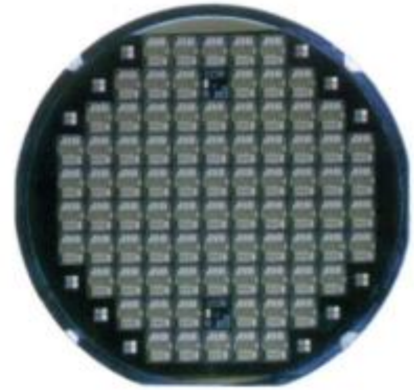
2 — Use igraph plot method (we also use this to determine dependencies).

```
> littersModel <- nimbleModel(littersCode, 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.

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);   } )
```

You get this:

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

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

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 <- configureMCMC(littersModel)
> littersMCMCspec$getSamplers()
[…snip…]
[3] RW sampler;   targetNode: b[1],  adaptive: TRUE,  adaptInterval: 200,  scale: 1
[4] RW sampler;   targetNode: b[2],  adaptive: TRUE,  adaptInterval: 200,  scale: 1
[5] conjugate_beta sampler;   targetNode: p[1, 1],  dependents_dbin: r[1, 1]
[6] conjugate_beta sampler;   targetNode: p[1, 2],  dependents_dbin: r[1, 2]
 [...snip...]
> littersMCMCspec$addSampler('a[1]', 'slice', list(adaptInterval = 100))
> littersMCMCspec$addSampler('a[2]', 'slice', list(adaptInterval = 100))
> littersMCMCspec$addMonitors('theta')
> littersMCMC <- buildMCMC(littersMCMCspec)
> 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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   MCMC, Particle Filter/Sequential MC, etc.

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

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

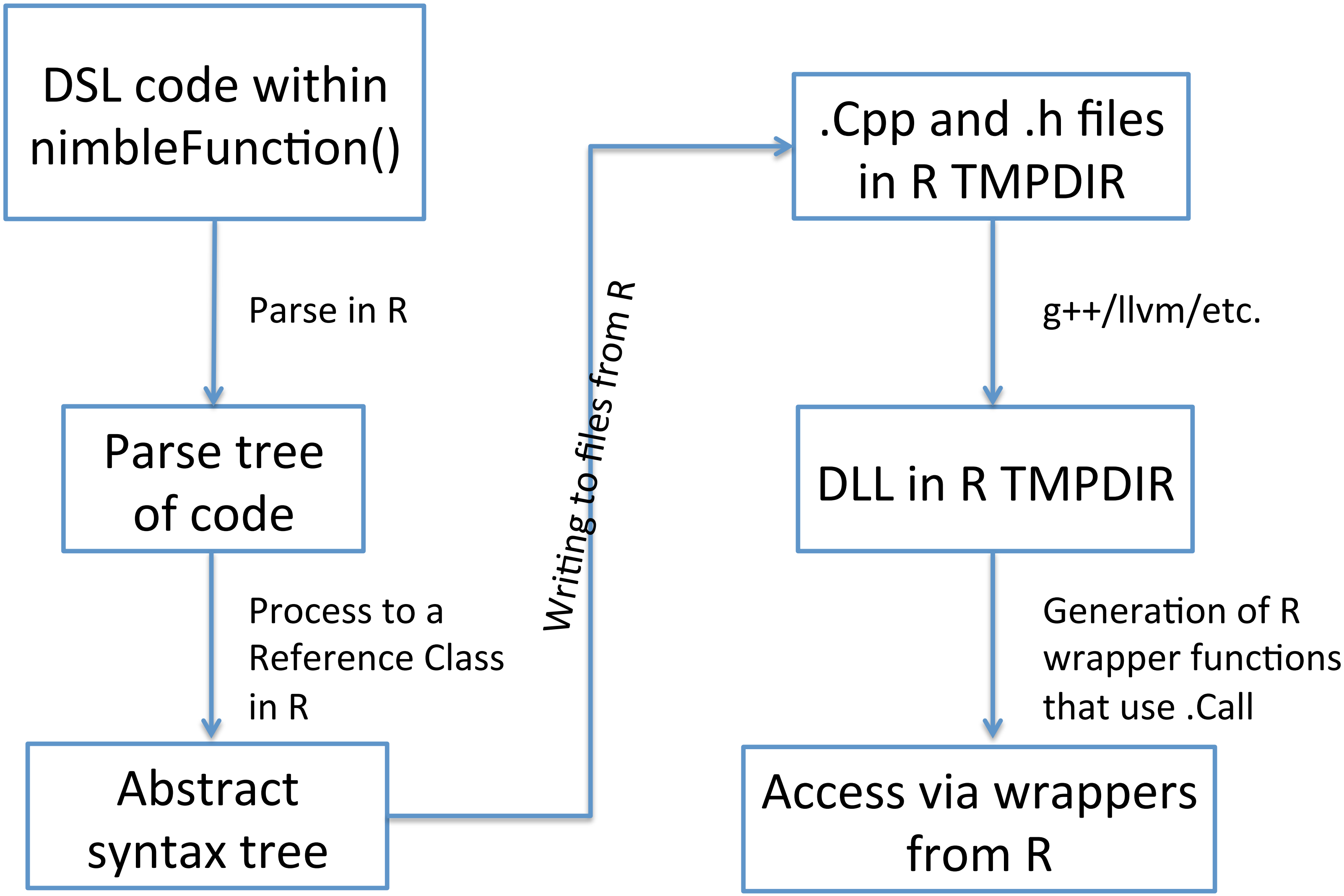
the actual algorithm

The NIMBLE compiler

Feature summary:

- 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)
   })
```

NIMBLE

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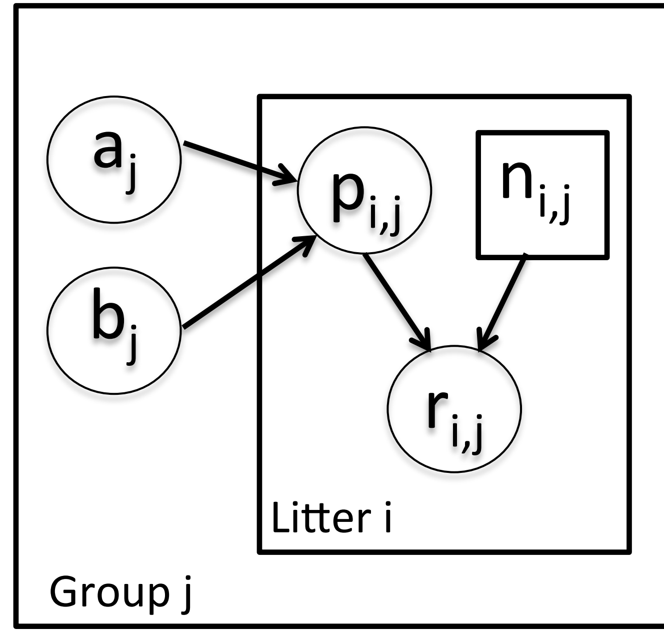
   MCMC, Particle Filter/Sequential MC, MCEM, etc.

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);
 })
```

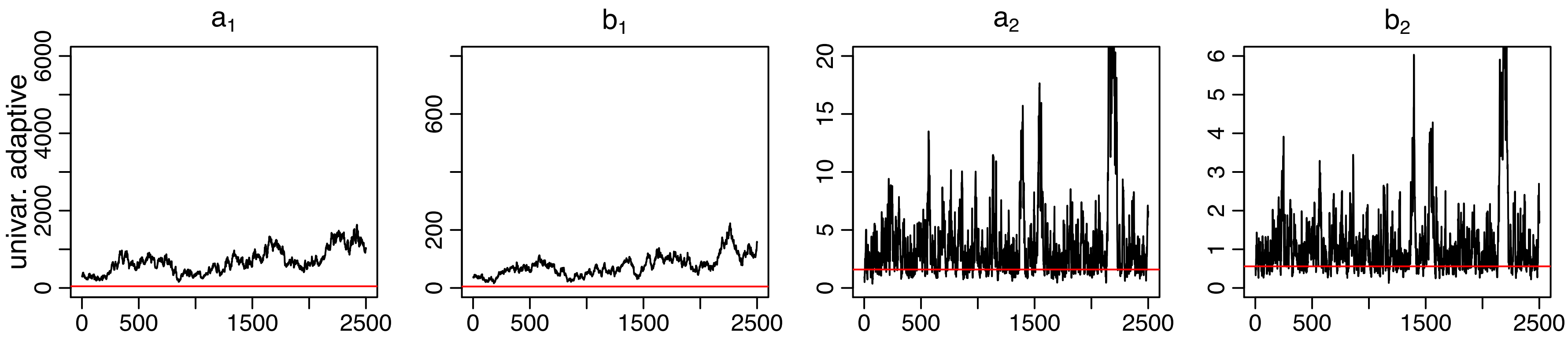


Challenges of the toy example:

- 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

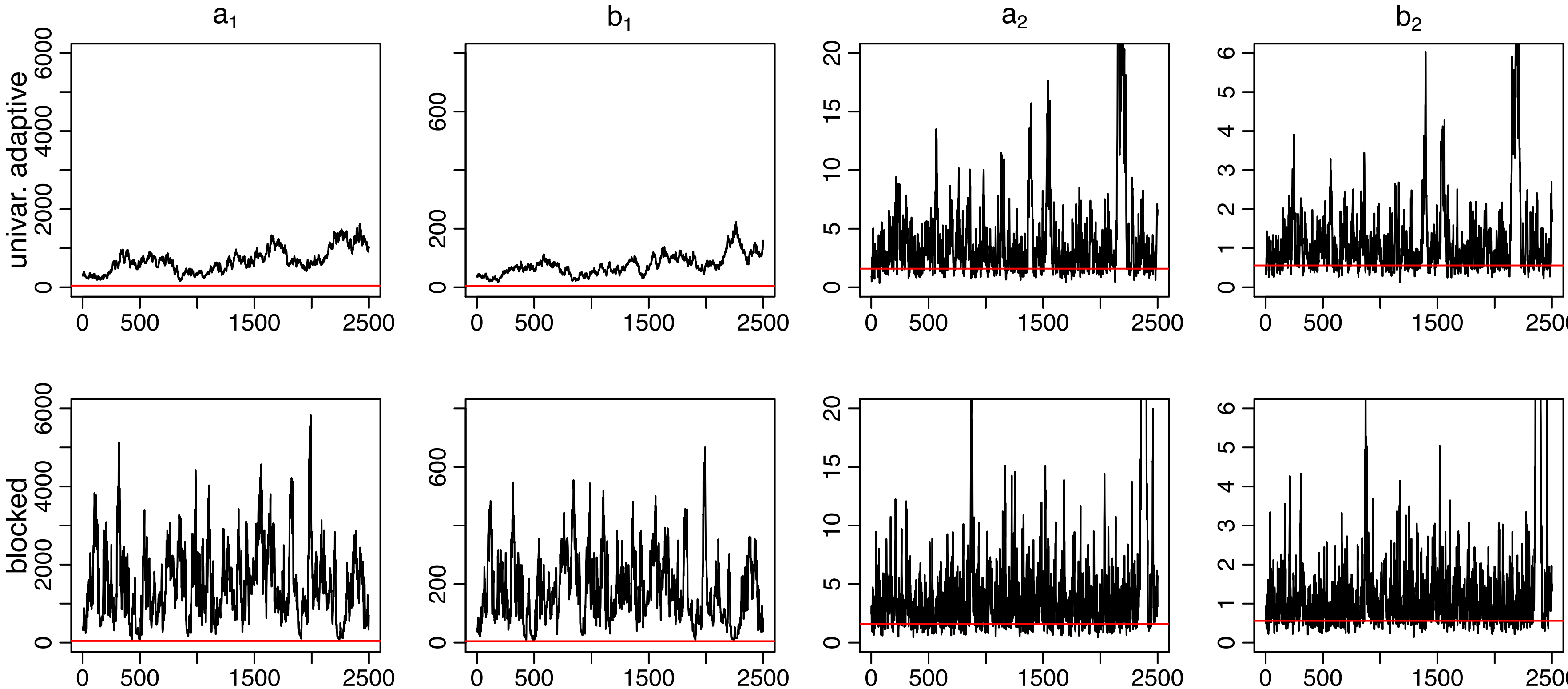
```
> littersMCMCspec <- configureMCMC(littersModel, list(adaptInterval = 100))
> littersMCMC <- buildMCMC(littersMCMCspec)
> littersMCMC_cpp <- compileNIMBLE(littersModel, project = littersModel)
> littersMCMC_cpp$run(10000)
```



Red line is MLE

Blocked MCMC: Gibbs + Blocked Metropolis

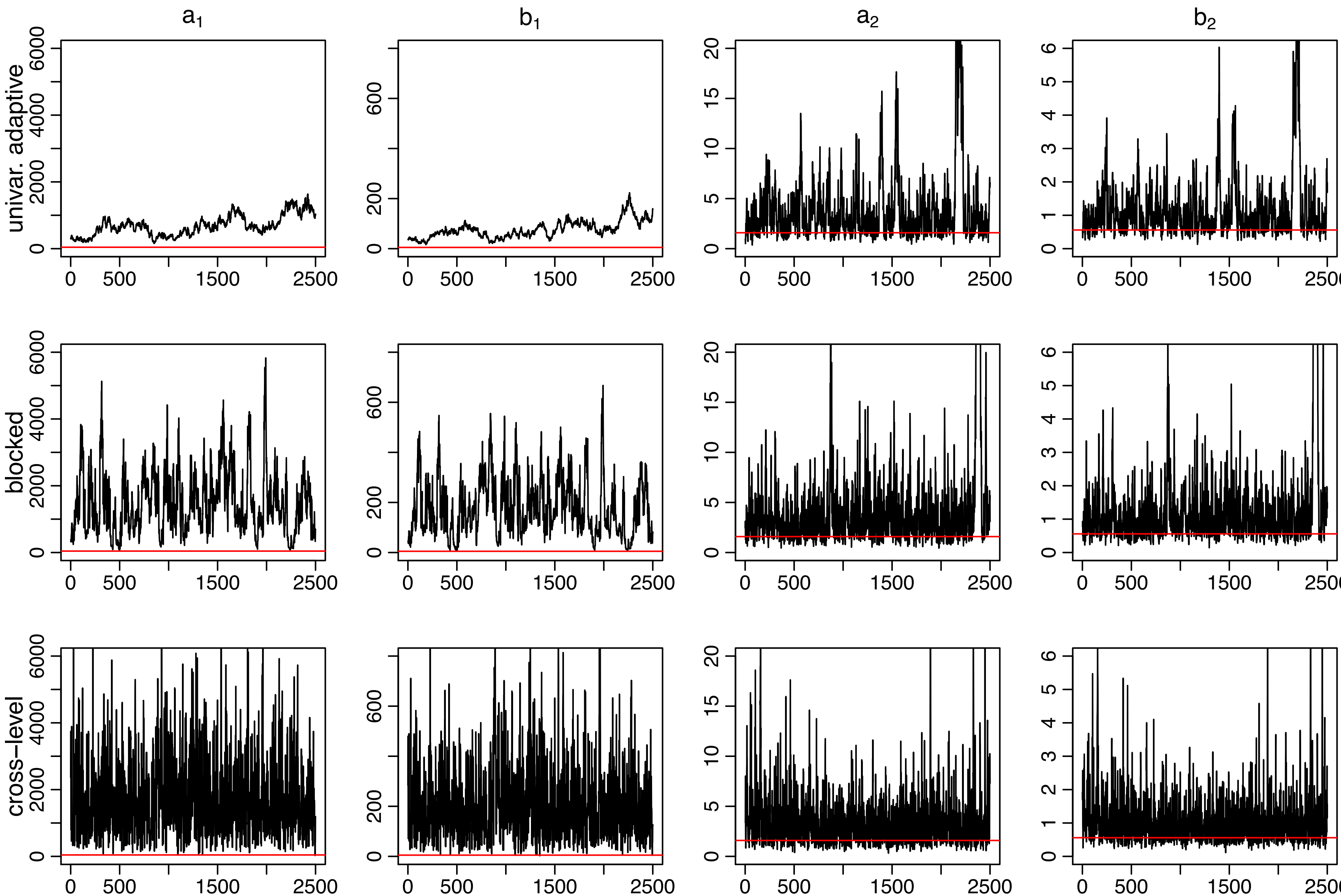
```
> littersMCMCspec2 <- configureMCMC(littersModel, list(adaptInterval = 100))
> littersMCMCspec2$addSampler(c('a[1]', 'b[1]'), 'RW_block', list(adaptInterval = 100)
> littersMCMCspec2$addSampler(c('a[2]', 'b[2]'), 'RW_block', list(adaptInterval = 100)
> littersMCMC2 <- buildMCMC(littersMCMCspec2)
> 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.

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



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

Litters MCMC: BUGS and JAGS

- Customized sampling possible in NIMBLE greatly improves performance.
- 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), though not always.
  - 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

---

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 with regular releases since. 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?
  - 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

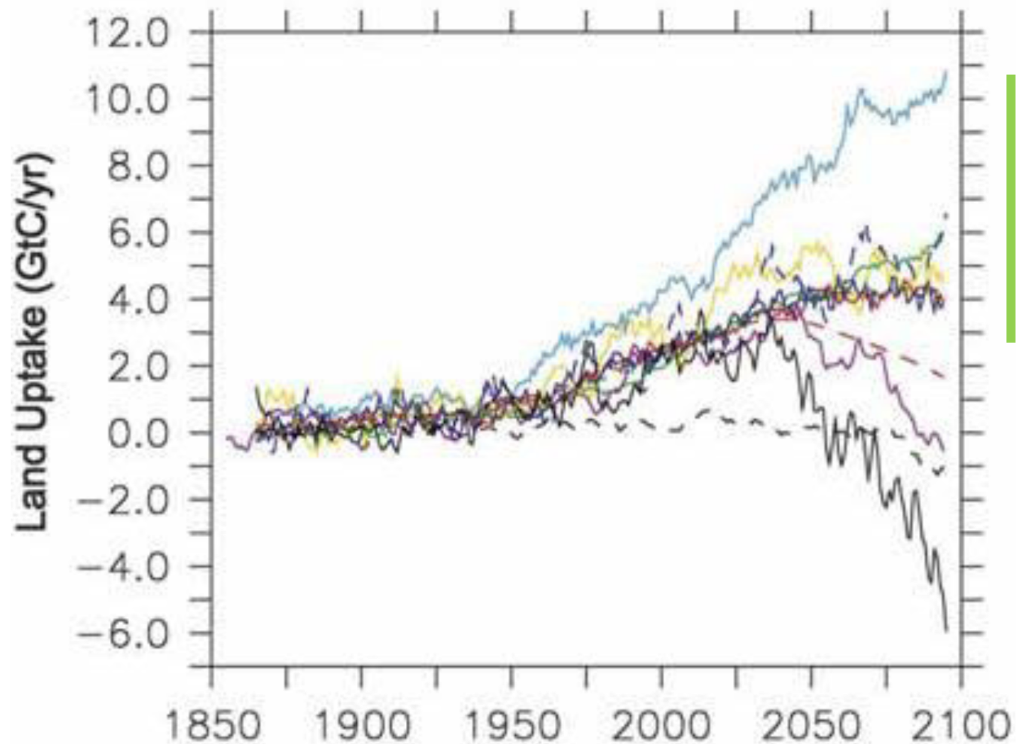
PalEON Project

www3.nd.edu/~paleolab/paleonproject

Goal: Improve the predictive capacity of terrestrial ecosystem models

"This large variation among carbon-cycle models … has been called 'uncertainty'. I prefer to call it 'ignorance'."
- Prentice (2013) Grantham Institute

Friedlingstein et al. 2006 J. Climate

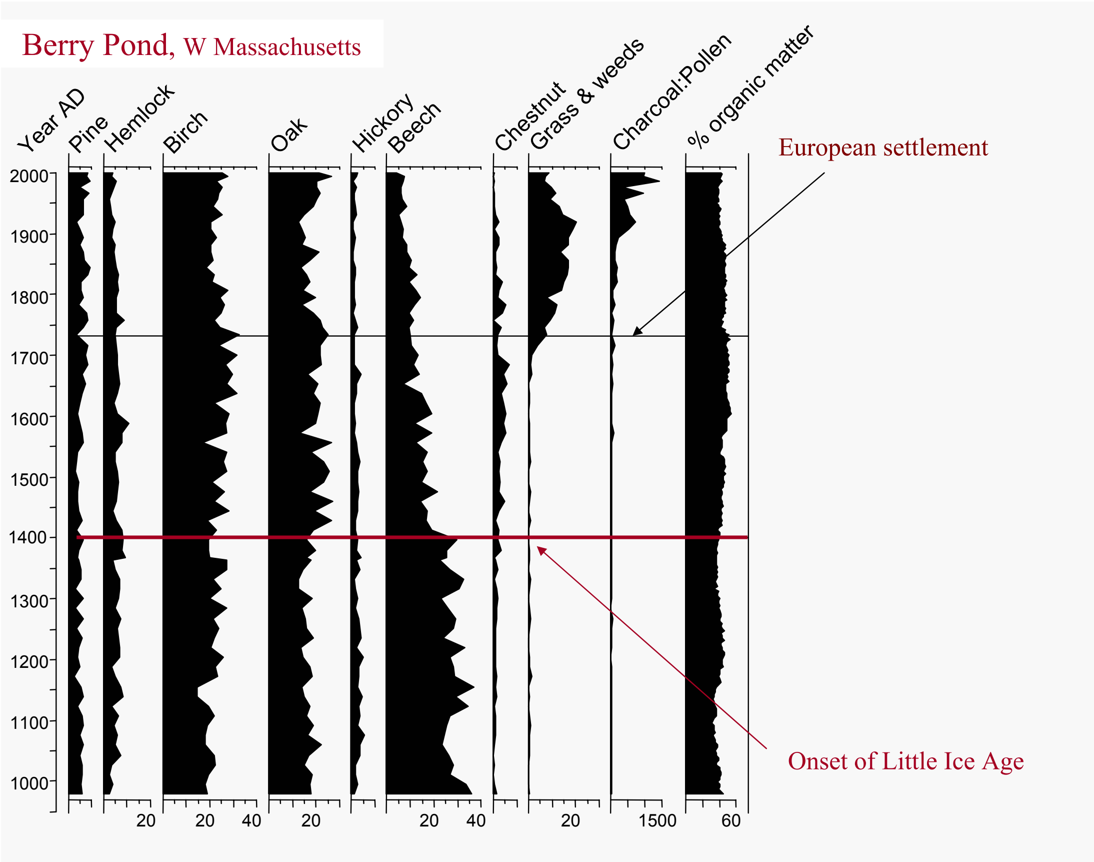


Critical issue: model parameterization and representation of decadal- to centennial-scale processes are poorly constrained by data
Approach: use historical and fossil data to estimate past vegetation and climate and use this information for model initialization, assessment, and improvement

PalEON Statistical Applications

- Estimate spatially-varying composition and biomass of tree species from count and zero-inflated size data in year 1850
- Estimate temporal variations in temperature and precipitation over 2000 years from tree rings and lake/bog records
- Estimate tree composition spatially over 2000 years from fossil pollen in lake sediment cores
- Estimate biomass over time at a site from fossil pollen in lake sediment cores

Fossil Pollen Data



Inferring Biomass from Pollen

- Calibration with multiple spatial locations:
  - "Regress" multinomial counts on biomass
  - For each taxon, have proportion of the taxon be a smooth function of biomass using splines and Dirichlet parameters:
    - $\alpha_k = \exp(Z(b)\beta_k)$
  - Estimate spline coefficients for each taxon
- Predict biomass over time at one location:
  - State space model for biomass over time
  - Fixed spline coefficients from calibration
  - Inverse problem (just Bayesian inference)
    - $\alpha_k = \exp(Z(b_t)\beta_k)$

Relating biomass to composition

- Using multiple sites (i = 1,…,n) with measured pollen composition (y_i) for k=1,…,K taxa and known local biomass (b_i), we regress the counts on biomass:

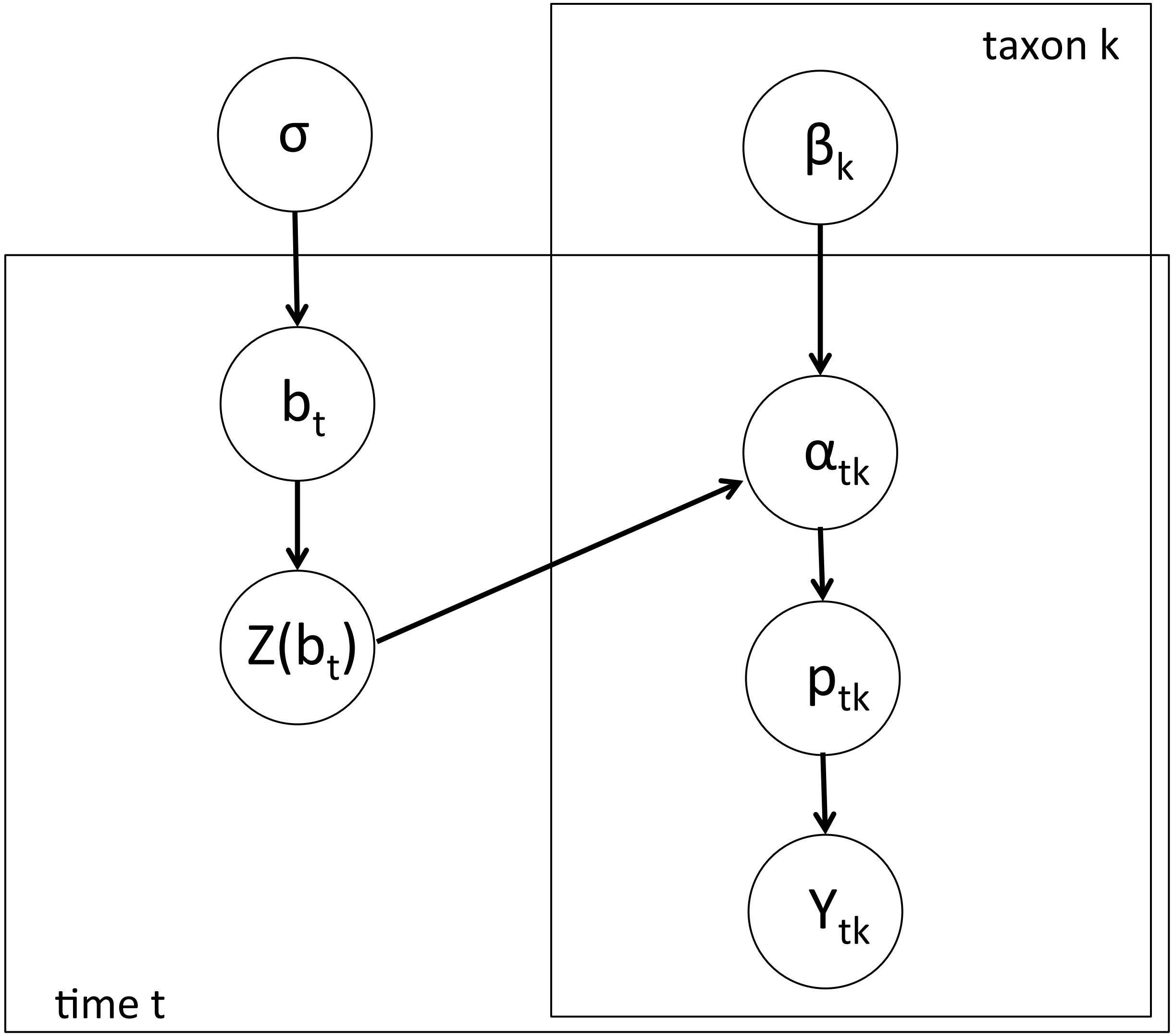
$$\alpha_{i,k} = \exp(Z(b_i)^\top \beta_k)$$

$$p_i \sim \text{Dirich}(\alpha_{i,\cdot})$$

$$y_i \sim \text{Multinom}(p_i)$$

- This uses b-splines to relate proportional abundance of a taxon to biomass.
- Estimate the β_k parameters (basis coefficients) for each taxon, k=1,…,K.

Prediction Model



Prediction Model

```
for(t in 1:nTimes)
     Y[t, 1:nTaxa] ~ ddirchmulti(alpha[t, 1:nTaxa], n[t])

for (k in 1:nTaxa)
   for(t in 1:nTimes)
     alpha[t, k] <- exp(Zb[t, 1:nKnots] %*% beta[1:nKnots, k])

for( t in 1:nTimes)
     Zb[t, 1:nKnots] <- bspline(b[t], knots[1:w])

for(t in 2:nTimes)
     b[t] ~ dlnorm(log(b[t-1]), sdlog = sigma)

sigma ~ dunif(0, 10) # Gelman (2006)
b[1] ~ dunif(0, 400)
```

pollen likelihood

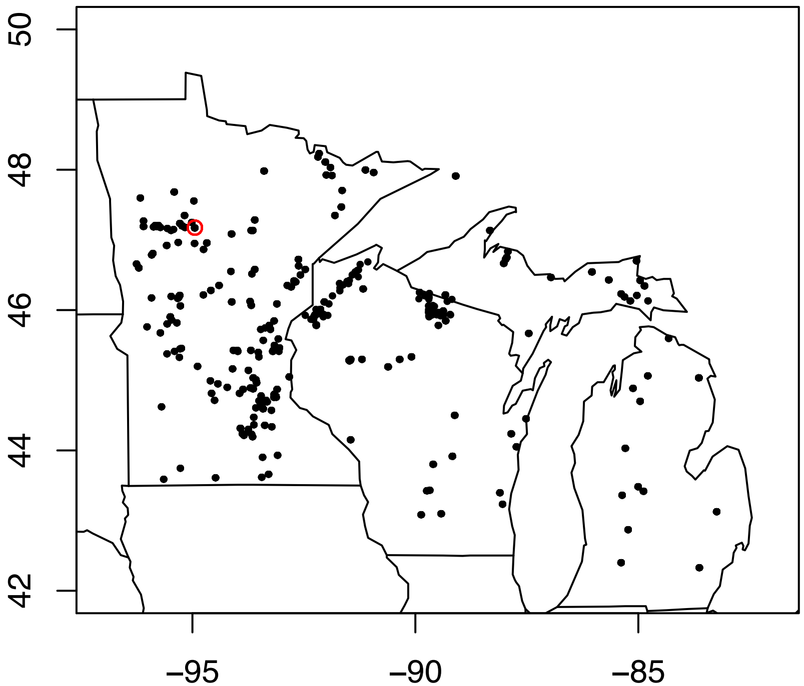
latent predictor

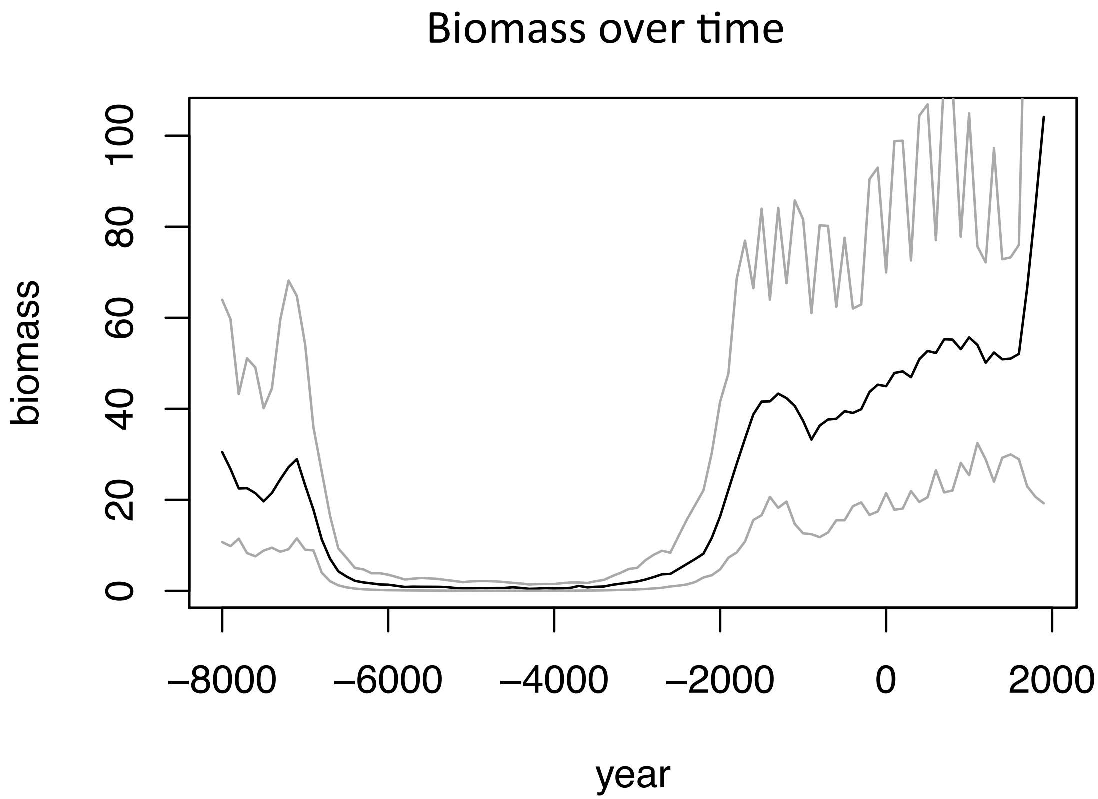
biomass evolution

hyperpriors

Results at one site

Calibration sites and prediction site (red)





How Can NIMBLE Help?

- More flexible model specification
  - Dirichlet-multinomial
  - b-spline construction
- User control over MCMC specification
- Alternative algorithms, such as particle filter, particle MCMC
- Provide algorithms for model comparison and model criticism
- Transparency when an algorithm fails

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