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

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Daniel Turek	Williams College
Nick Michaud	UC Berkeley Statistics and ESPM
Duncan Temple Lang	UC Davis Statistics

http://r-nimble.org

USC Biostatistics seminar

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What do we want to do with hierarchical models?

1. Core algorithms

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

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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
- Variational Bayes

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
- Many flavors of MCMC
- Gaussian quadrature
- Monte Carlo expectation maximization (MCEM)
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- Auxiliary particle filter
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- Posterior re-weighting
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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

What can a practitioner do with hierarchical models?

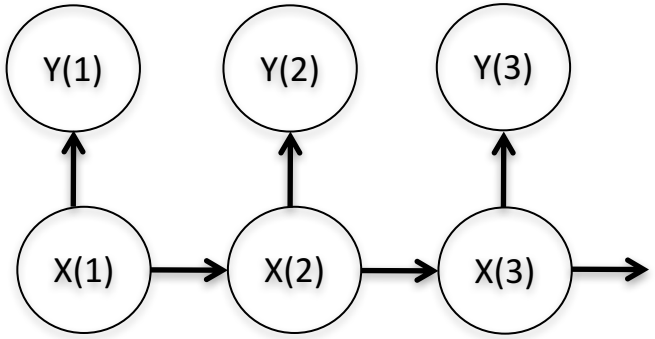
Two basic software designs:

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

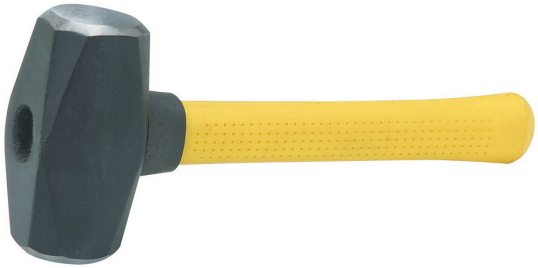
2. Flexible model + black box algorithm
   - BUGS: WinBUGS, OpenBUGS, JAGS
   - PyMC
   - INLA
   - Stan

Existing software

Model



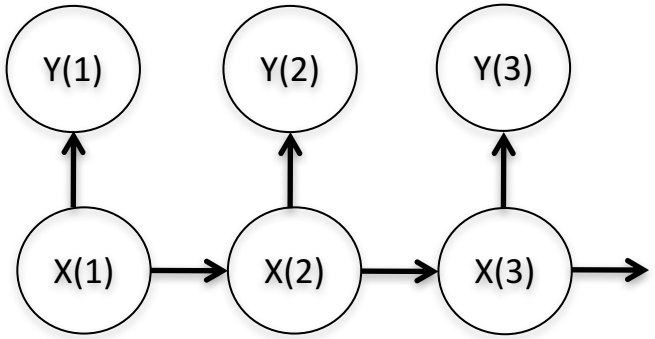
Algorithm



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

NIMBLE: The Goal

Model

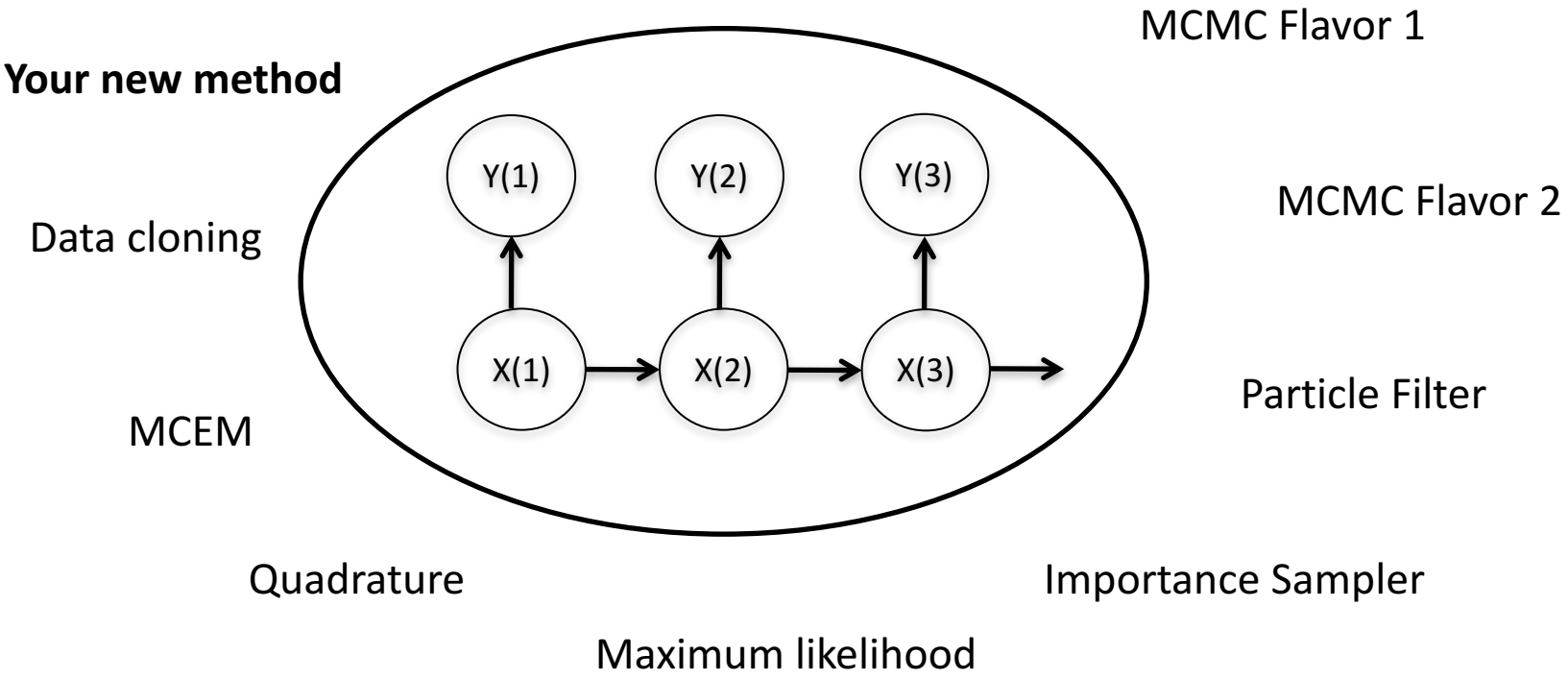


+

Algorithm language

=

Divorcing Model Specification from Algorithm

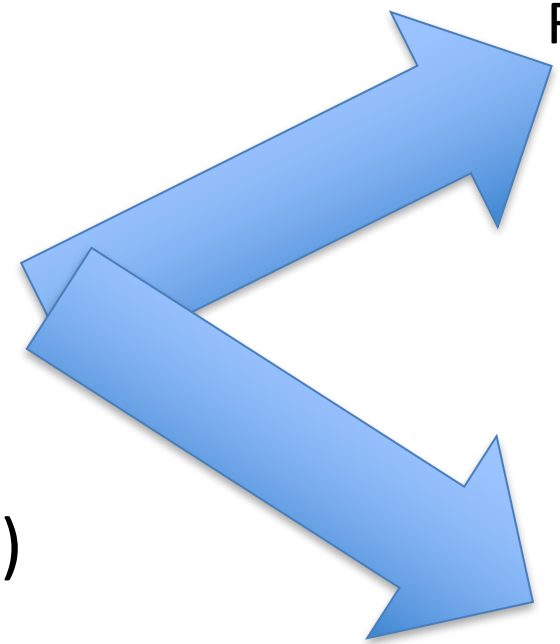


Goals

- Retaining BUGS compatibility
- Providing a variety of standard algorithms
- Allowing users to easily modify those 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

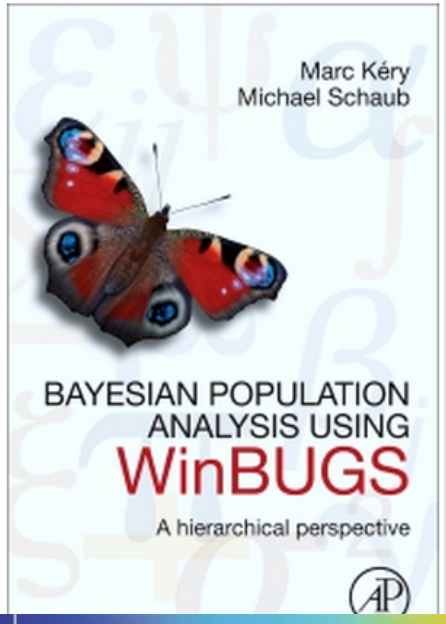
   BUGS language ➔ R/C++ model object

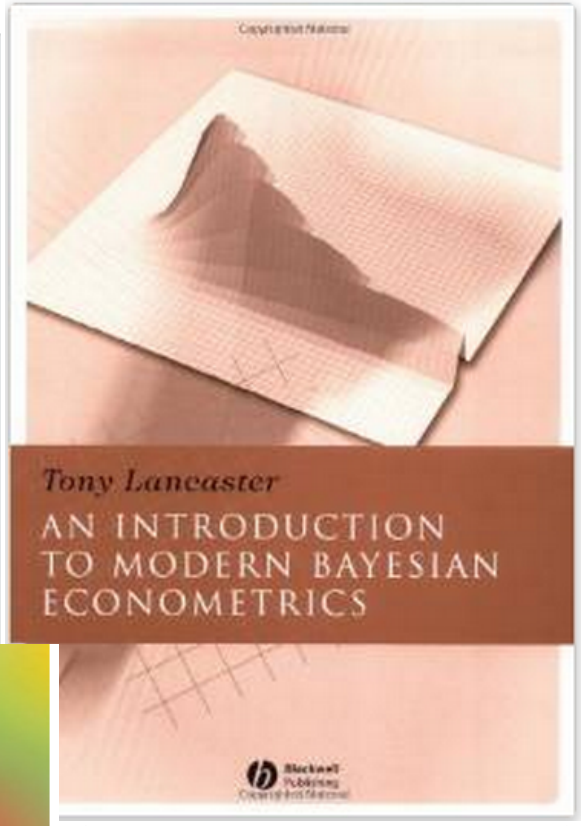
2. Algorithm library

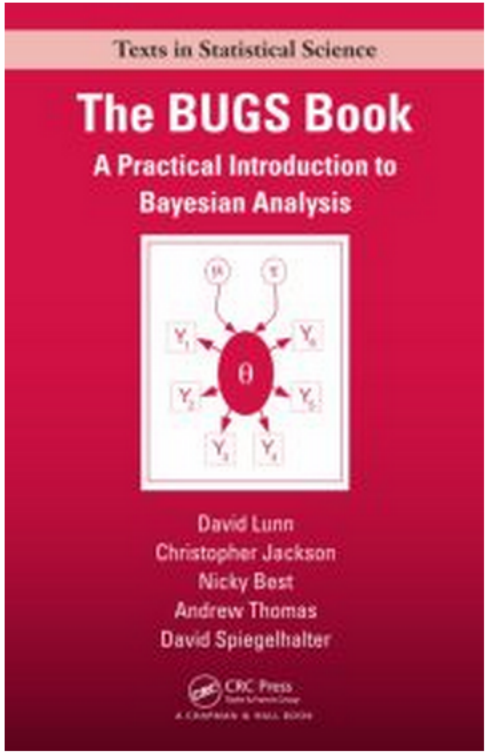
   MCMC, Particle Filter/Sequential MC, MCEM, etc.

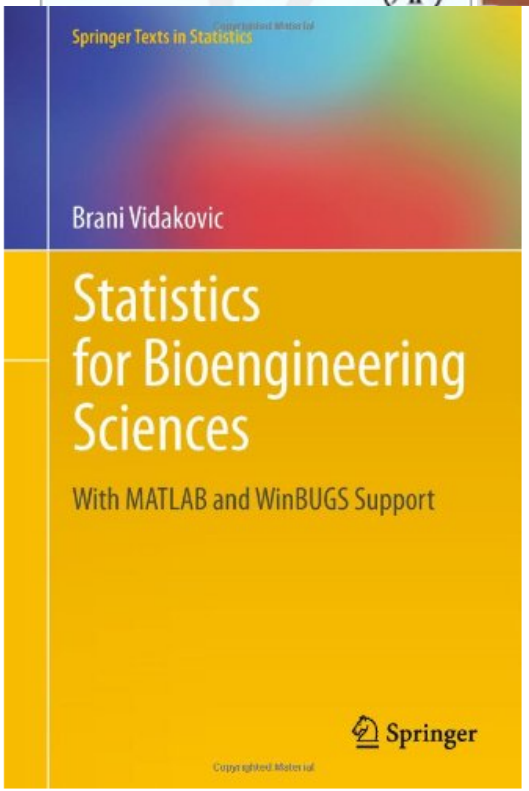
3. Algorithm specification

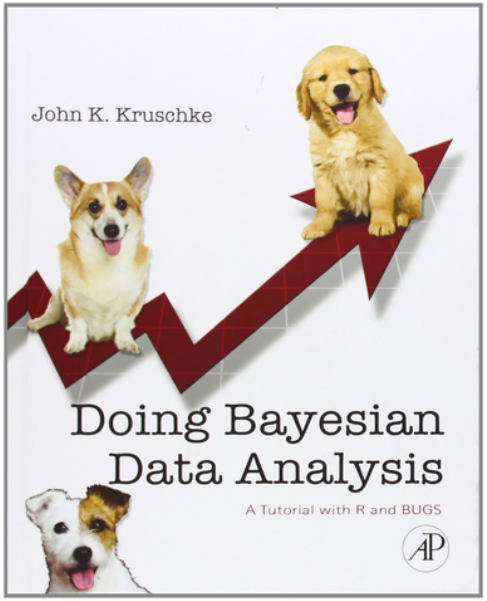
   NIMBLE programming language within R ➔ R/C++ algorithm object

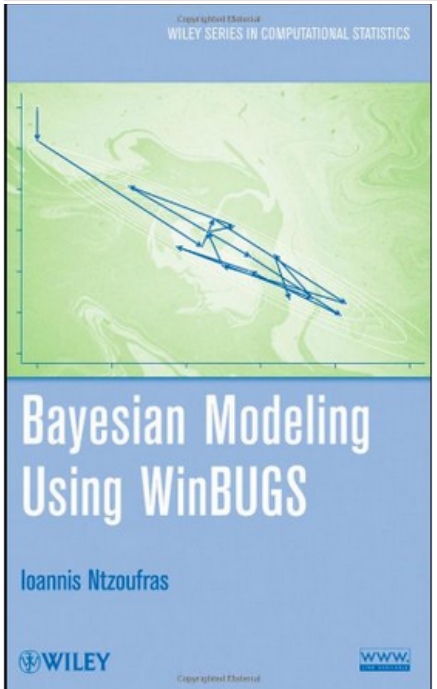

Marc Kéry
Michael Schaub
BAYESIAN POPULATION ANALYSIS USING
WinBUGS
A hierarchical perspective


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

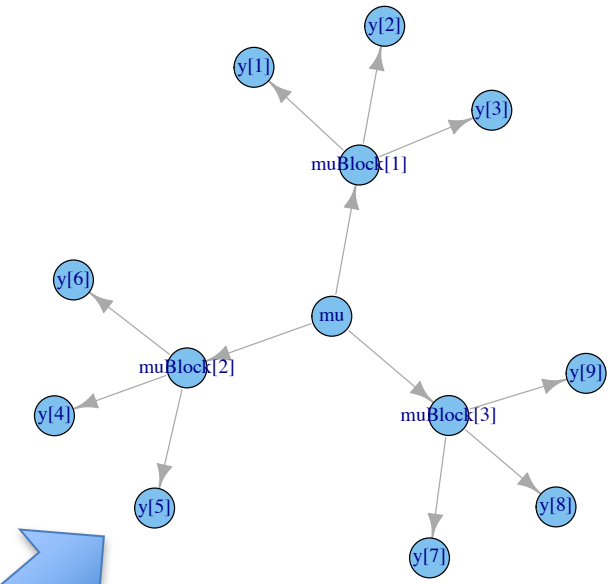

Springer Texts in Statistics
Brani Vidakovic
Statistics for Bioengineering Sciences
With MATLAB and WinBUGS Support
Springer


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

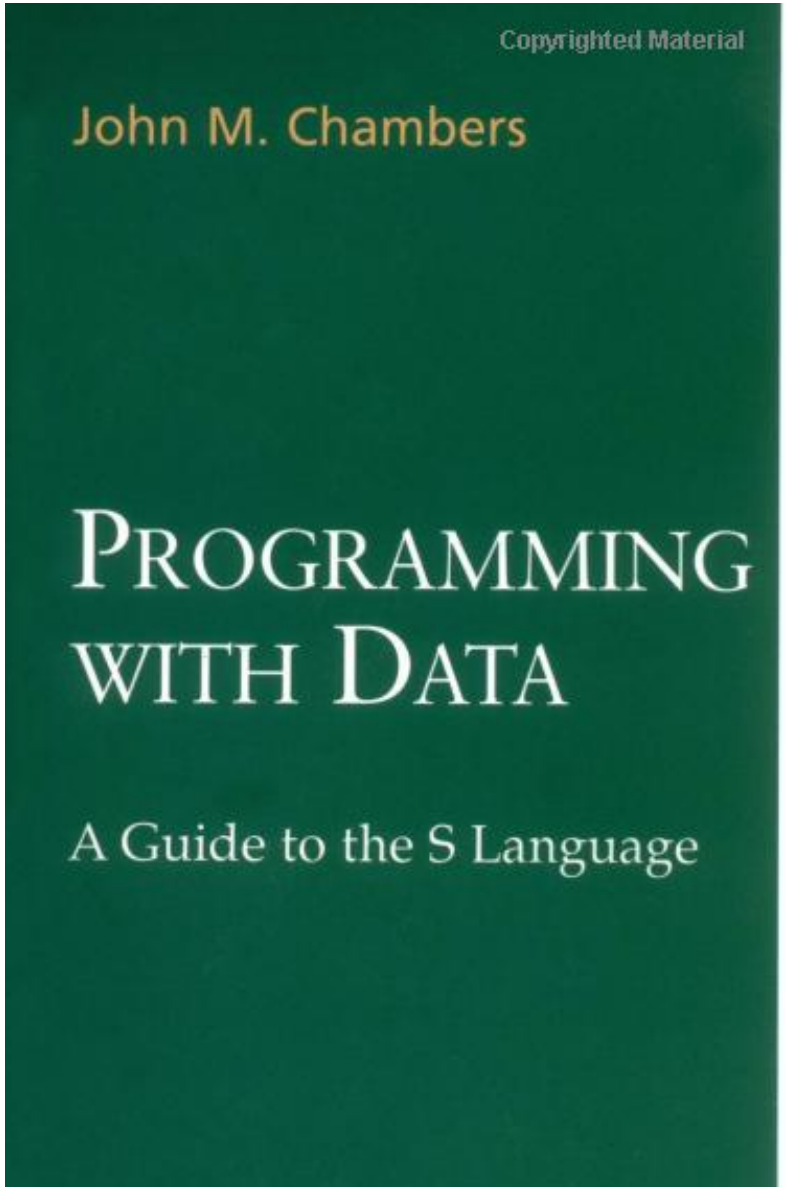
Use igraph plot method (we also use this to determine dependencies).

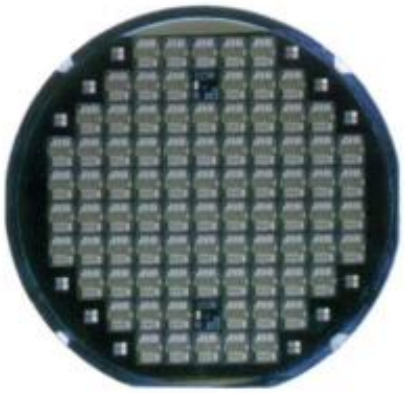
```
> littersModel <- nimbleModel(littersCode, constants = list(N = 16, G = 2), data = list(r = input$r))
> littersModel_cpp <- compileNimble(littersModel)
```

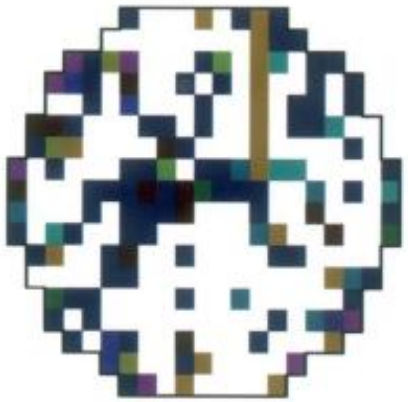
3

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$a[1] <- 5              # set values in model
> simulate(littersModel, 'p')         # simulate from prior
> p_deps <- littersModel$getDependencies('p')    # model structure
> calculate(littersModel, p_deps)  # calculate probability density
> 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….]
…
```

```
> littersMCMCconf <- configureMCMC(littersModel)
> littersMCMCconf$printSamplers()
[…snip…]
[3] RW sampler;   targetNode: b[1],  adaptive: TRUE,  adaptInterval: 200,  scale: 1
[4] RW sampler;   targetNode: b[2],  adaptive: TRUE,  adaptInterval: 200,  scale: 1
[5] conjugate_beta sampler;   targetNode: p[1, 1],  dependents_dbin: r[1, 1]
[6] conjugate_beta sampler;   targetNode: p[1, 2],  dependents_dbin: r[1, 2]
 [...snip...]
> littersMCMCconf$addSampler('a[1]', 'slice', list(adaptInterval = 100))
> littersMCMCconf$addSampler('a[2]', 'slice', list(adaptInterval = 100))
> littersMCMCconf$addMonitors('theta')
> littersMCMC <- buildMCMC(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.

NIMBLE

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NIMBLE's algorithm library

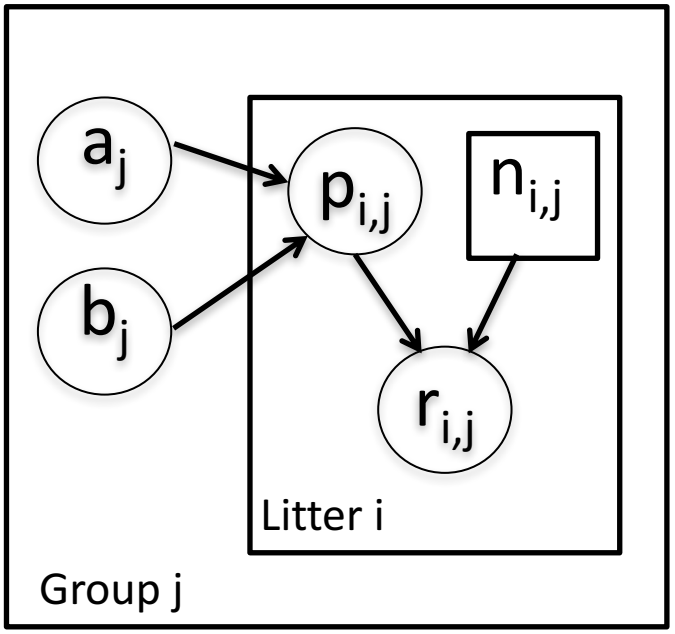
- MCMC samplers:
  - Conjugate, adaptive Metropolis, adaptive blocked Metropolis, slice, elliptical slice sampler, particle MCMC, specialized samplers for particular distributions (Dirichlet, CAR)
  - Flexible choice of sampler for each parameter
  - User-specified blocks of parameters
  - Cross-validation, WAIC
- Sequential Monte Carlo (particle filters)
  - Various flavors
- MCEM
- Write your own

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);
 })
```

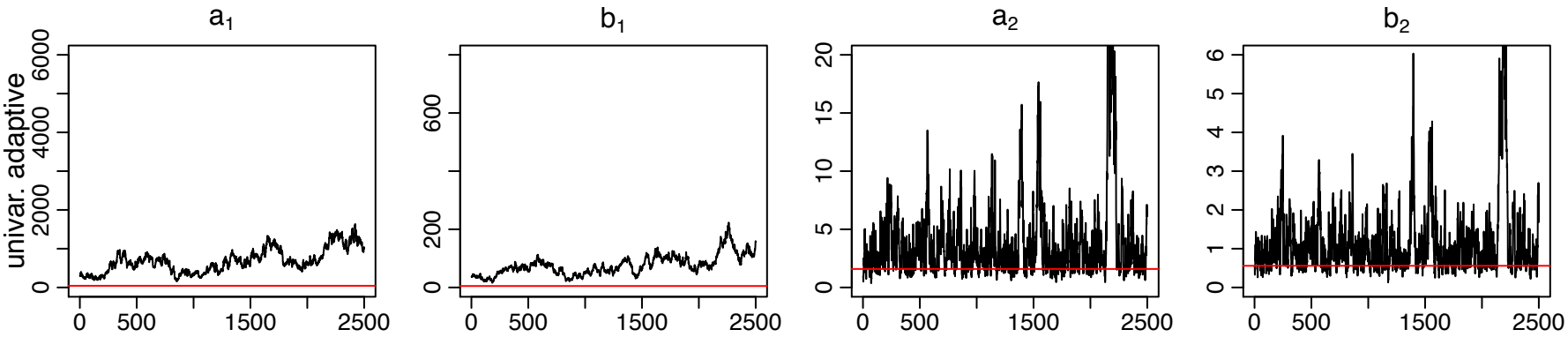


Challenges of the toy example:

- 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

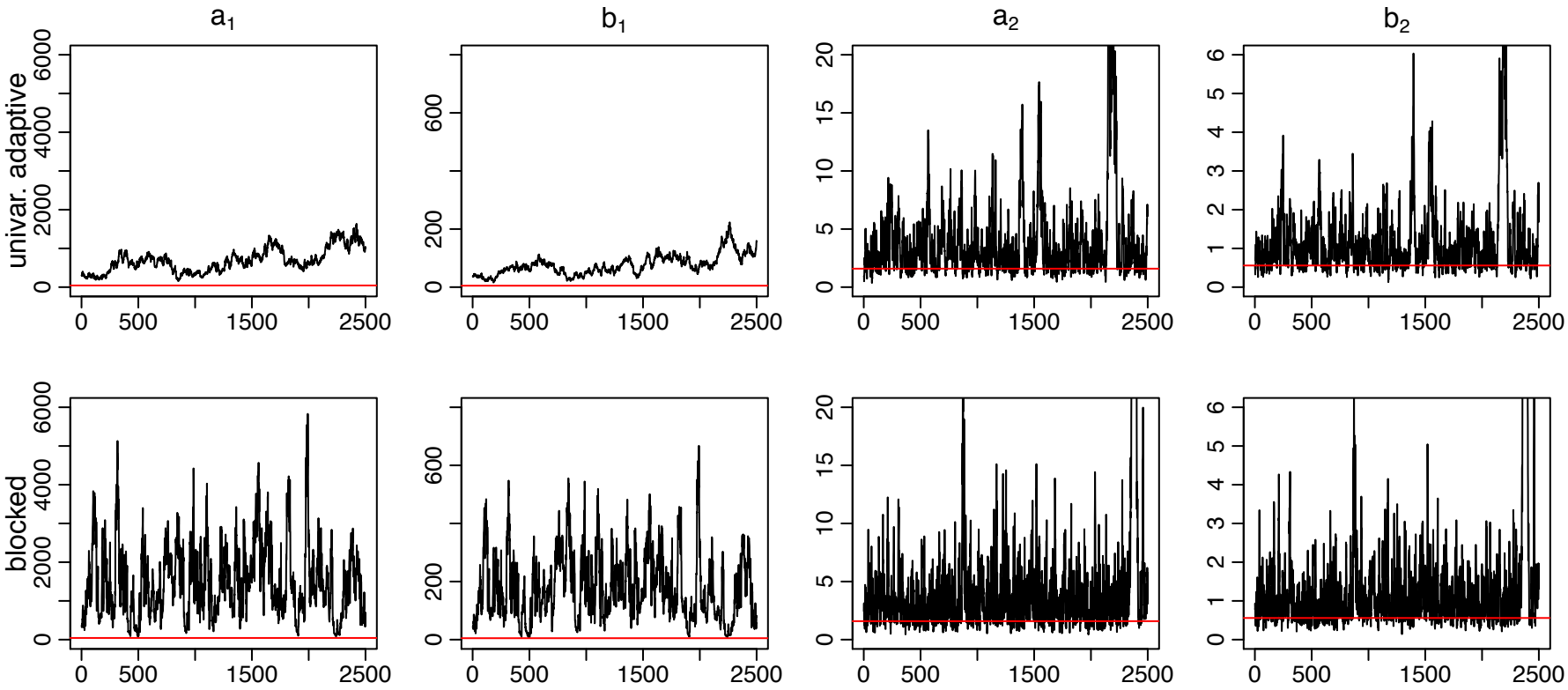
```
> littersMCMCspec <- configureMCMC(littersModel, list(adaptInterval = 100))
> littersMCMC <- buildMCMC(littersMCMCspec)
> littersMCMC_cpp <- compileNIMBLE(littersModel, project = littersModel)
> littersMCMC_cpp$run(10000)
```



Red line is MLE

Blocked MCMC: Gibbs + Blocked Metropolis

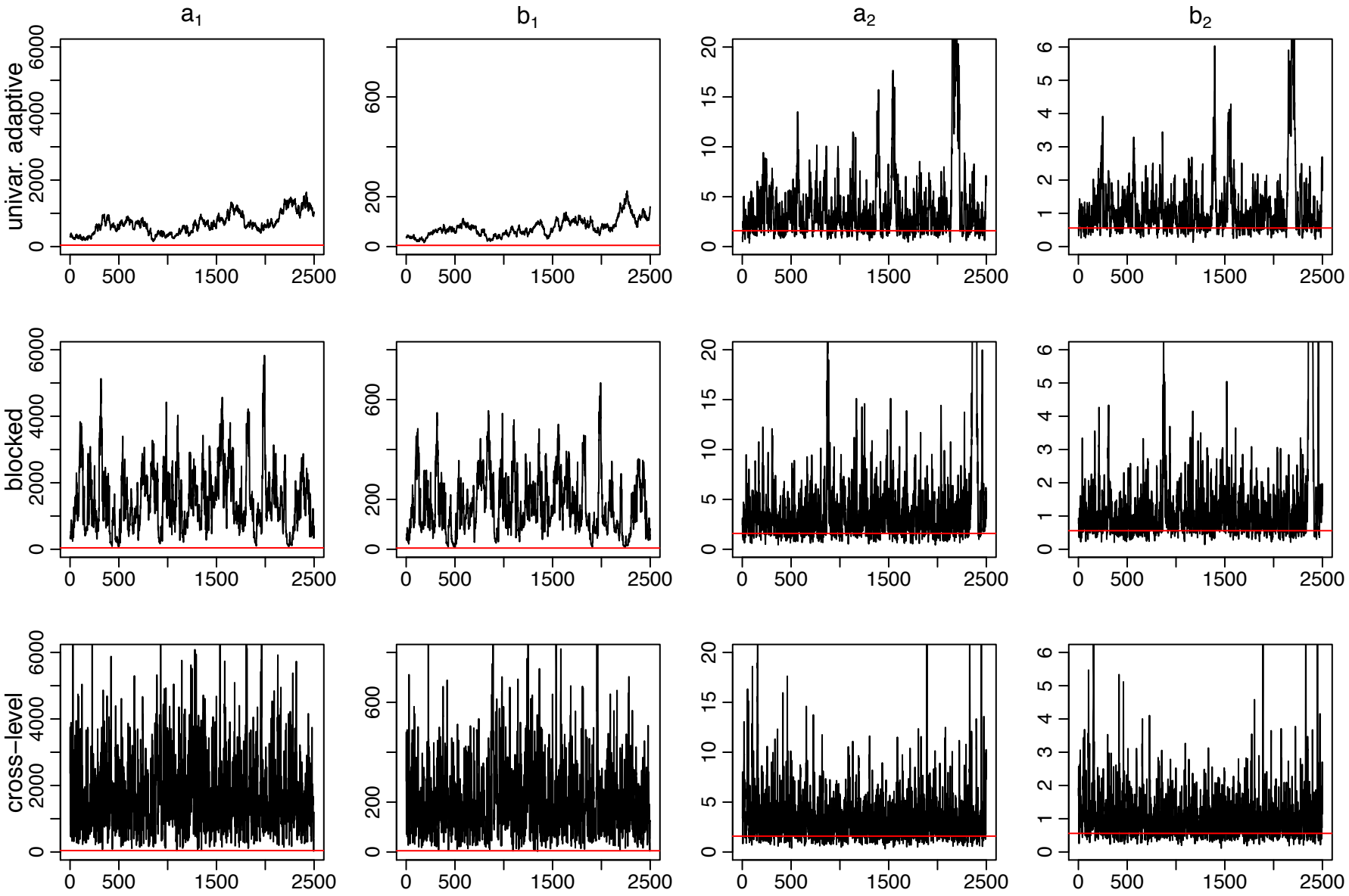
```
> littersMCMCspec2 <- configureMCMC(littersModel, list(adaptInterval = 100))
> littersMCMCspec2$addSampler(c('a[1]', 'b[1]'), 'RW_block', list(adaptInterval = 100)
> littersMCMCspec2$addSampler(c('a[2]', 'b[2]'), 'RW_block', list(adaptInterval = 100)
> littersMCMC2 <- buildMCMC(littersMCMCspec2)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


a1
b1
a2
b2
univar. adaptive
blocked
0
500
1500
2500
2000
4000
6000
200
600
5
10
15
20
1
2
3
4
5
6

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)
```


a1
b1
a2
b2
univar. adaptive
blocked
cross−level
0
2000
4000
6000
200
600
5
10
15
20
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.

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2. Algorithm library

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

3. Algorithm specification

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

NIMBLE: Programming With Models

We want:

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

NIMBLE: Programming with Models

```
sampler_myRW <- nimbleFunction(

setup = function(model, mvSaved, targetNode, scale) {
   calcNodes <- model$getDependencies(targetNode)
},
run = function() {
   model_lp_initial <- calculate(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
    # …. Various bookkeeping operations … #    })
```

2 kinds of functions

NIMBLE: Programming with Models

```
sampler_myRW <- nimbleFunction(

setup = function(model, mvSaved, targetNode, scale) {
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    # …. Various bookkeeping operations … #    })
```

query model structure ONCE

NIMBLE: Programming with Models

```
sampler_myRW <- nimbleFunction(

setup = function(model, mvSaved, targetNode, scale) {
   calcNodes <- model$getDependencies(targetNode)
},
run = function() {
   model_lp_initial <- calculate(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
    # …. Various bookkeeping operations … #    })
```

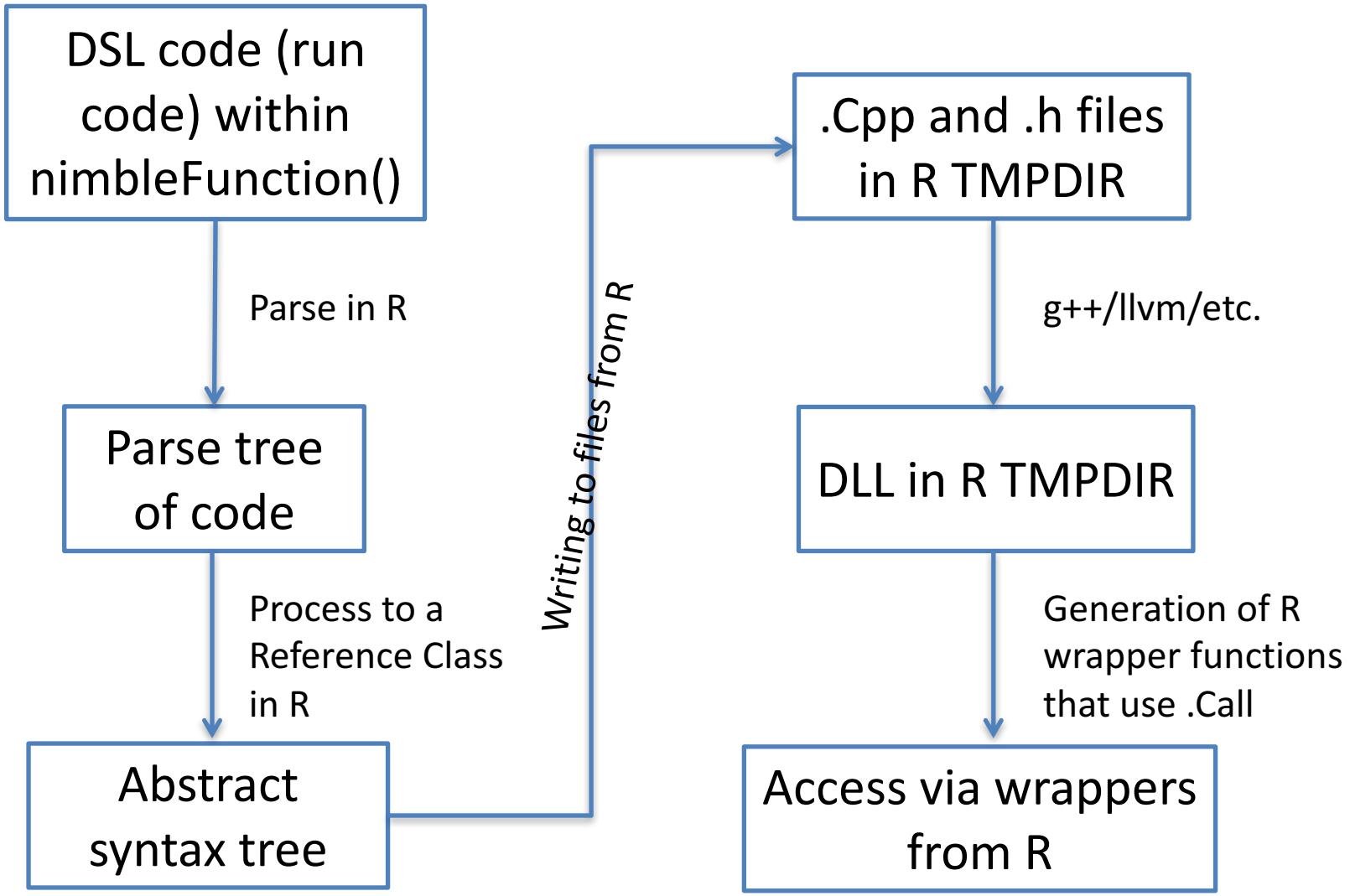
the actual (generic) algorithm

The NIMBLE compiler (run code)

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
- Access to much of Rmath.h (e.g. distributions)
- Automatic R interface / wrapper
- Call out to your own C/C++ or back to R
- Many improvements / extensions planned

How an Algorithm is Processed in NIMBLE



Modular algorithms: particle MCMC

- Particle filter (SMC) approximates a posterior for latent states using a sample
- Traditionally used in state space models where the sample particles are propagated in time to approximate: $p(x_t|y_{1:t},\theta)$

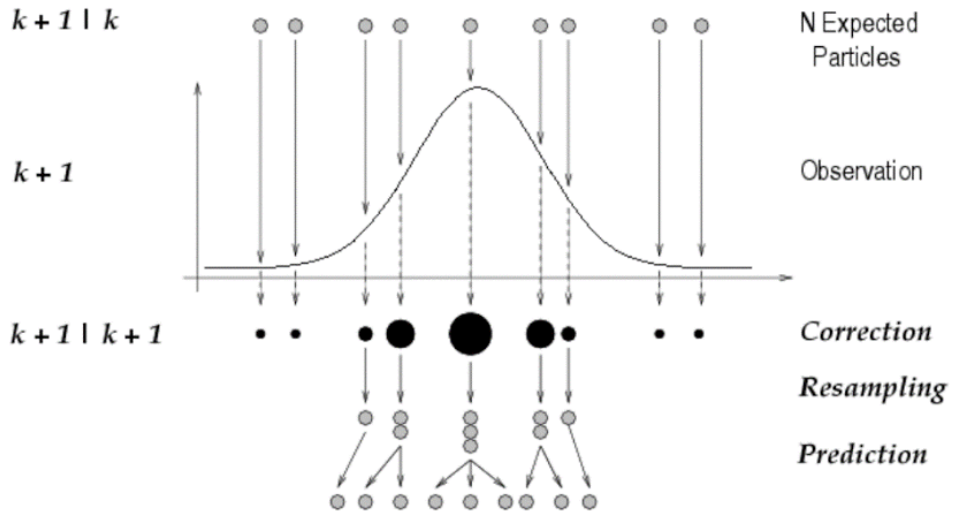


Figure 2: Particle filtering (from (Lehmann 2003))

- Weights from 'correction' step can be used to estimate $p(y_{1:t}|\theta)$
- Embed in MCMC to do approximate marginalization over $x_{1:t}$

Particle MCMC in NIMBLE

```
sampler_PMCMC <- nimbleFunction(

setup = function(model, mvSaved, target, control) {
    ….
    my_particleFilter <- buildAuxiliaryFilter(model, control$latents, control =
list(saveAll = TRUE, smoothing = TRUE, lookahead = lookahead))
    ….
},
run = function() {
    ….
    modelLP0 <- modelLL0 + calculate(model, target)
    propValue <- rnorm(1, mean = model[[target]], sd = scale)
    model[[target]] <<- propValue
    modelLL1 <- my_particleFilter$run(m)
    modelLP1 <- modelLL1 + calculate(model, target)
    jump <- my_decideAndJump$run(modelLP1, modelLP0, 0, 0)
    ….
})
```

Status of NIMBLE and Next Steps

- First release was June 2014 with regular releases since. Lots to do:
  - Improve the user interface and speed up compilation (in progress)
  - Scalability for large models (in progress)
  - Bayesian nonparametrics with Claudia Wehrhahn & Abel Rodriguez (UCSC) (in progress)
  - Refinement/extension of the DSL for algorithms (in progress)
    - e.g., automatic differentiation, parallelization
  - Additional algorithms written in NIMBLE DSL
    - e.g., normalizing constant calculation, Laplace approximations

- 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

NIMBLE: What can I program?

- Your own distribution for use in a model
- Your own function for use in a model
- Your own MCMC sampler for a variable in a model
- A new MCMC sampling algorithm for general use
- A new algorithm for hierarchical models
- An algorithm that composes other existing algorithms (e.g., MCMC-SMC combinations)

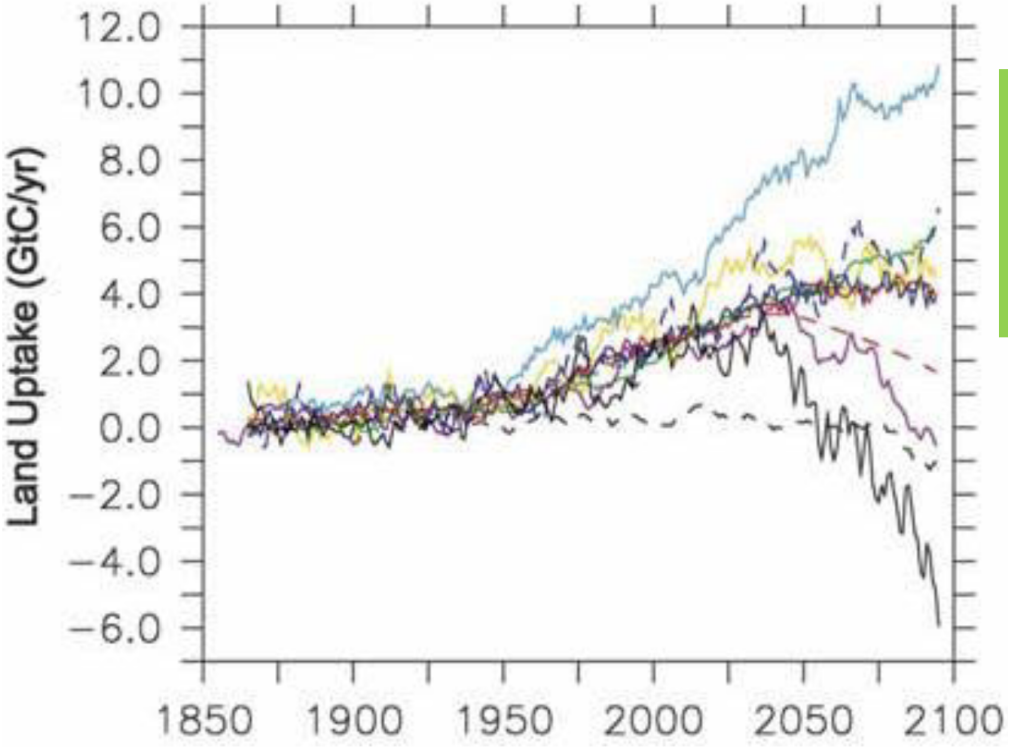
PalEON Project

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

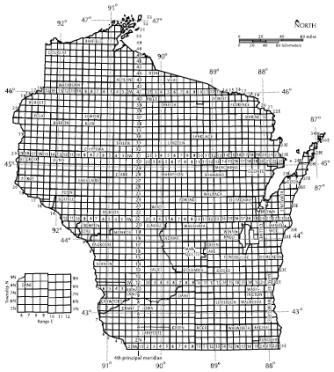
- Estimate spatially-varying composition and biomass of tree species from count and zero-inflated size data in year 1850
- Estimate temporal variations in temperature and precipitation over 2000 years from tree rings and lake/bog records
- Estimate tree composition spatially over 2000 years from fossil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

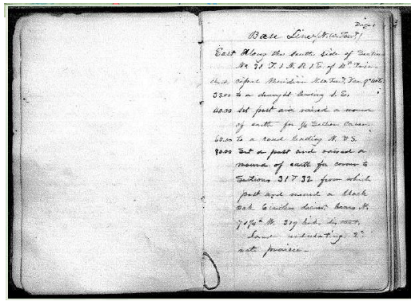
Inferring Biomass from Pollen

- 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 parameters of Beta distributions:
    - $\alpha_k = \exp(Z(b)\beta_k)$
  - 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)
    - $\alpha_k = \exp(Z(b_t)\beta_k)$

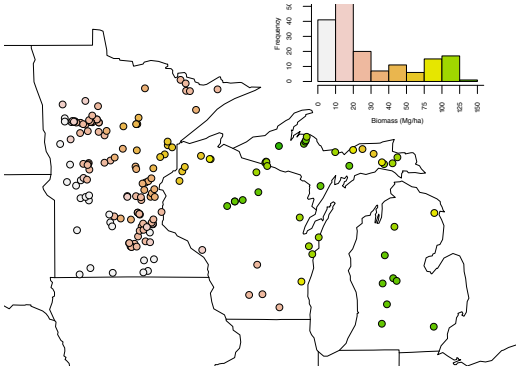
Predicting biomass from compositional data

Calibration: at settlement time we have biomass estimates (based on survey data and a spatial model) and pollen composition (from sediment cores)

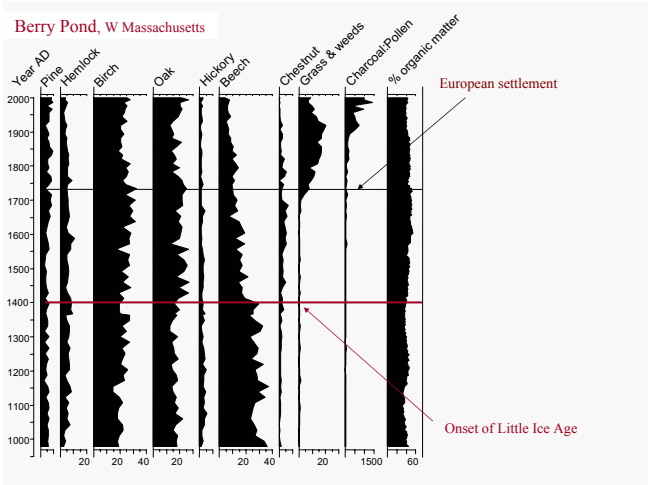




Biomass estimates at ponds



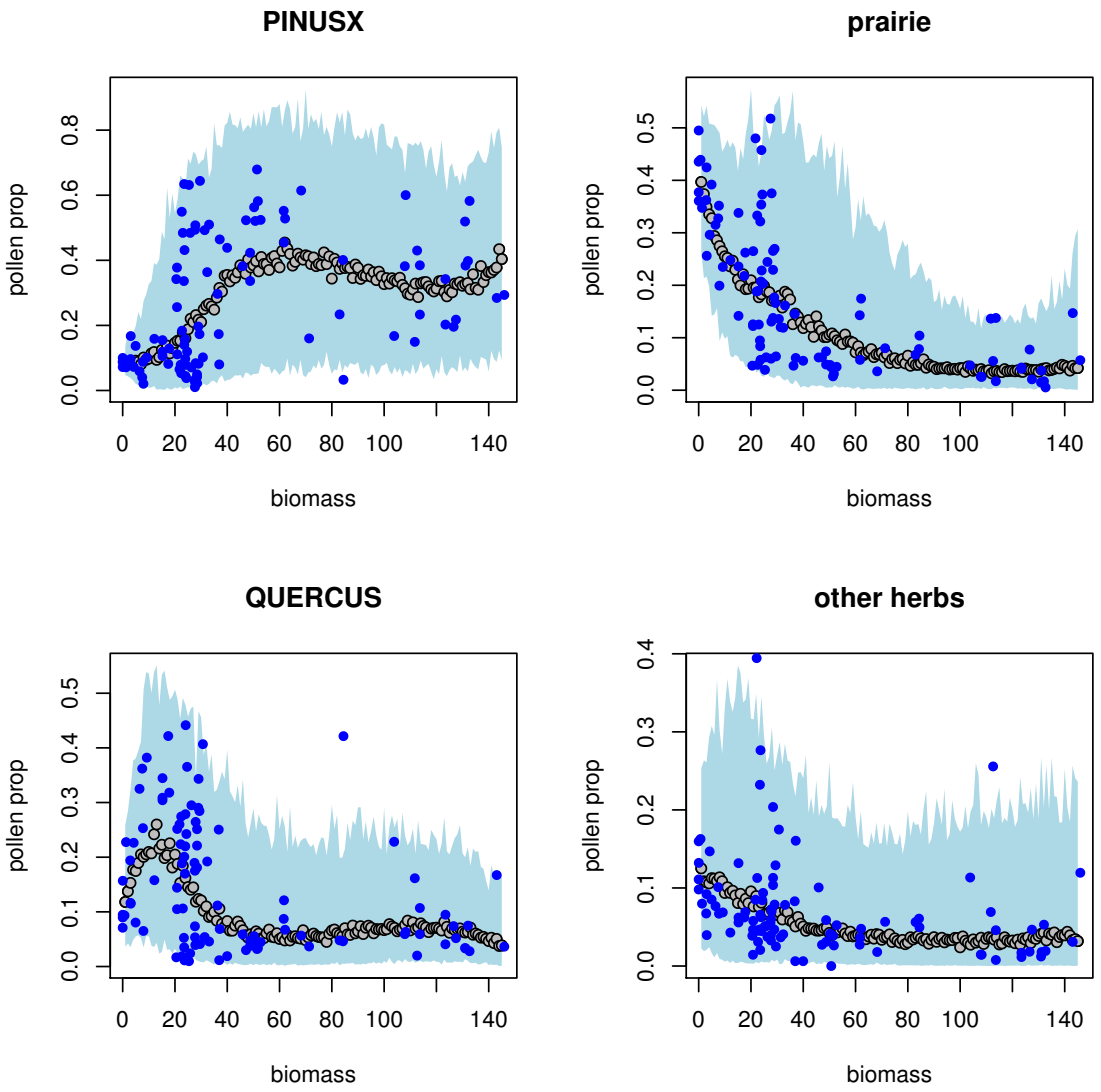
Prediction: based on calibration model and pollen composition over time, predict biomass



Calibration model

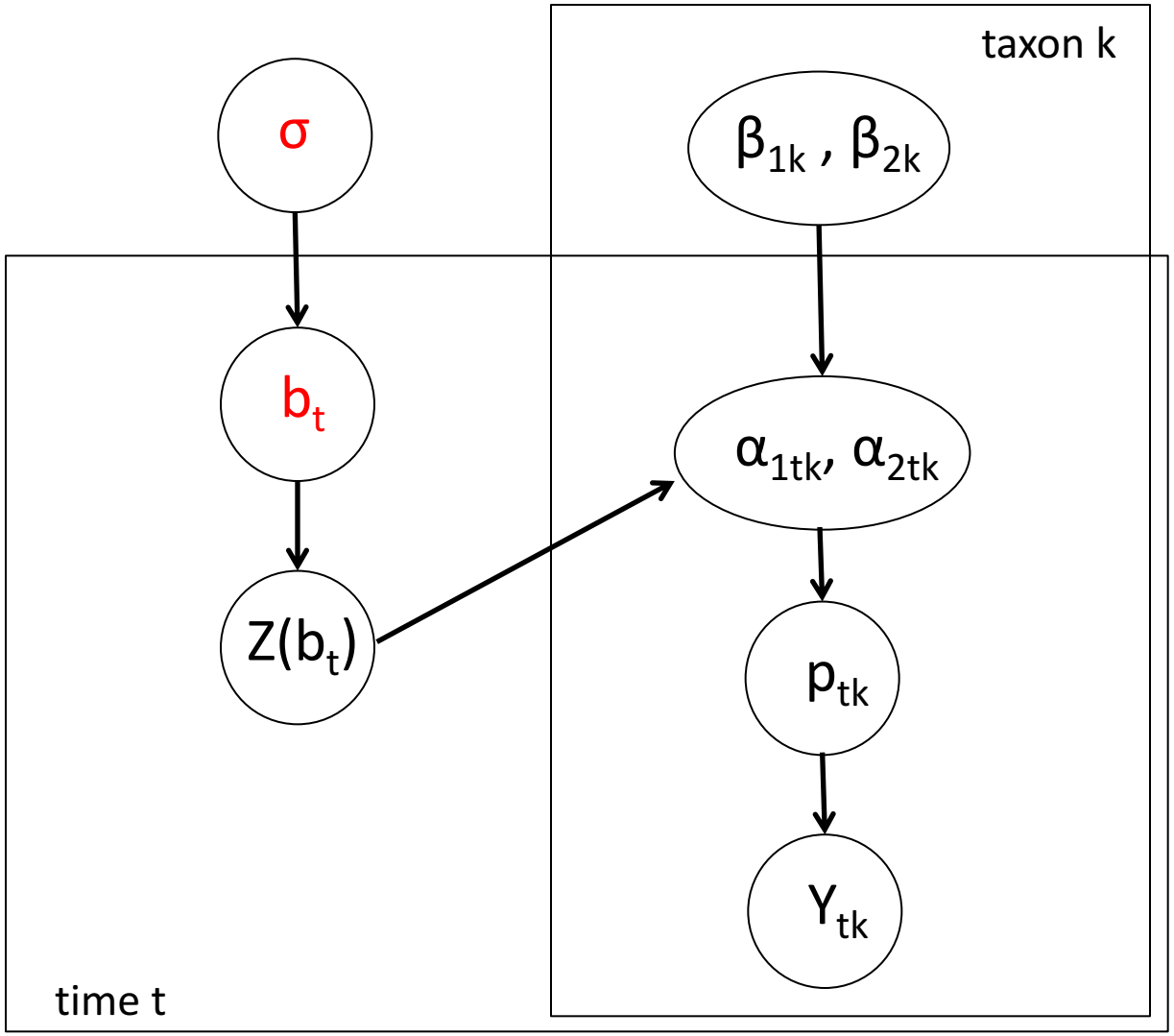
- Pollen proportion for each taxon determined by transformation of a flexible (spline) function of biomass
  - shape1 and shape2 parameters of beta distribution (stick-breaking prior for multinomial) are splines of biomass
  - Primary calibration parameters are spline coefficients
- Overdispersed multinomial likelihood for pollen counts given modeled proportions
- Fit in NIMBLE (could be fit in various other packages)

Calibration model fit



Mean and variability of modeled pollen proportions across ponds vary with biomass

Prediction Model



Prediction Model

```
for(t in 1:nTimes)
        Y[t, 1] ~ dbetabin(shape1[t, 1], shape2[t, 1], n[t])
        for(k in 2:(nTaxa-1)) {
                Y[t, k] ~  dbetabin(shape1[t, k], shape2[t, k], n[t]-sum(Y[t, 1:(k-1)])

for (k in 1:nTaxa)
   for(t in 1:nTimes) {
        shape1[t, k] <- exp(Zb[t, 1:nKnots] %*% beta1[1:nKnots, k])
        shape2[t, k] <- exp(Zb[t, 1:nKnots] %*% beta2[1:nKnots, k])
        }
for( t in 1:nTimes)
        Zb[t, 1:nKnots] <- bspline(b[t], knots[1:nKnots])

for(t in 2:nTimes)
        b[t] ~ dGenPareto (3b[t-1]-3b[t-2]+b[t-3], sigma)

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

pollen likelihood

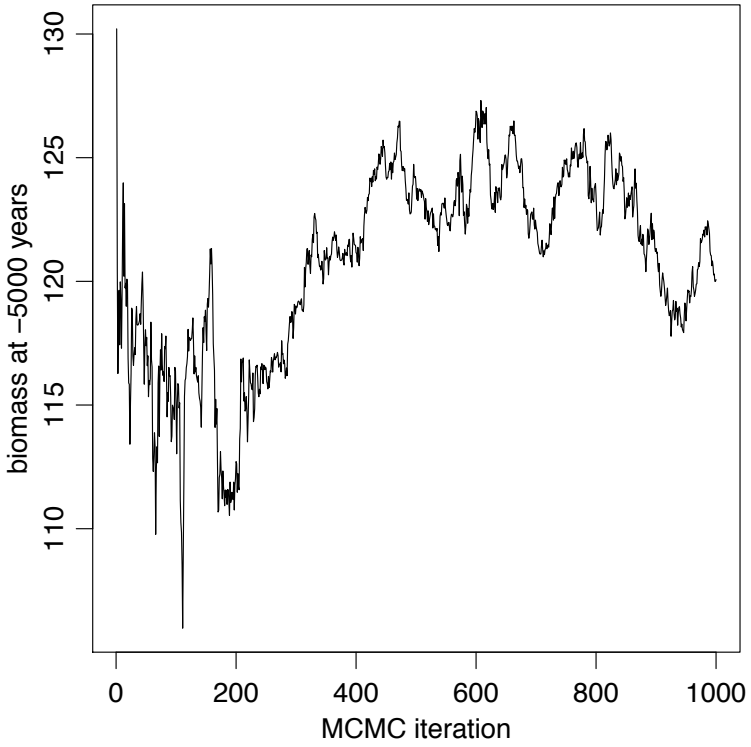
latent predictor

(nonstationary) biomass evolution

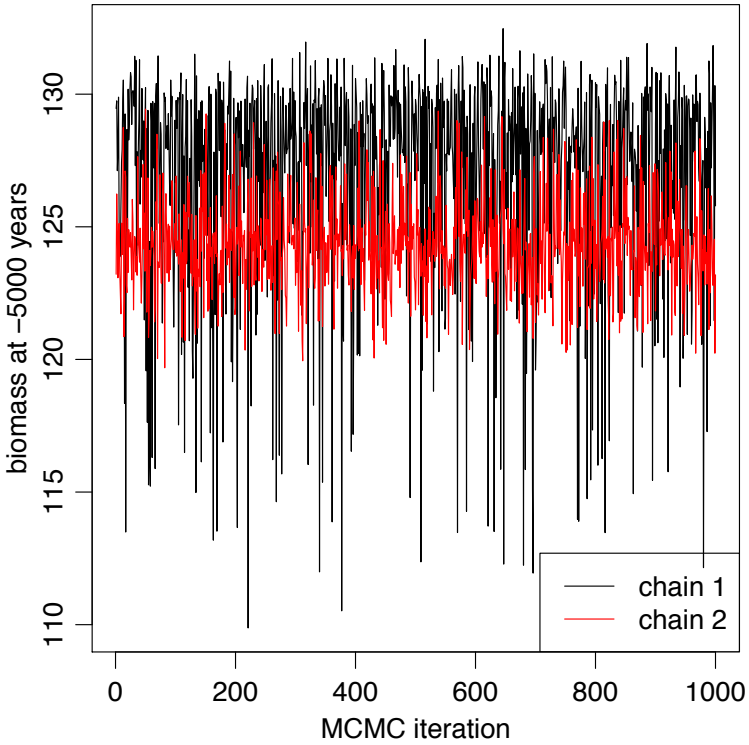
hyperpriors

MCMC performance

Mixing with data augmentation using default NIMBLE MCMC



Mixing in marginalized model using HMC in Stan



(recall non-differentiable spike at zero from generalized Pareto)

NIMBLE solution: customized MCMC sampler for {b[t-3], b[t-2], b[t-1], b[t], b[t+1], b[t+2], b[t+3]}, with a normal approximation to likelihood to generate good (quasi-conjugate) proposals.

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