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

Christopher Paciorek UC Berkeley Statistics

Joint work with:

Perry de Valpine (PI) UC Berkeley Environmental Science, Policy and Management

Daniel Turek Williams College

Nick Michaud UC Berkeley Statistics and ESPM

Duncan Temple Lang UC Davis Statistics

http://r-nimble.org

Imperial College seminar July 2018



What do we want to do with hierarchical models?

1. Core algorithms

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

What do we want to do with hierarchical models?

1. Core algorithms

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

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)
- 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 can a practitioner do with hierarchical models?

Two basic software designs:

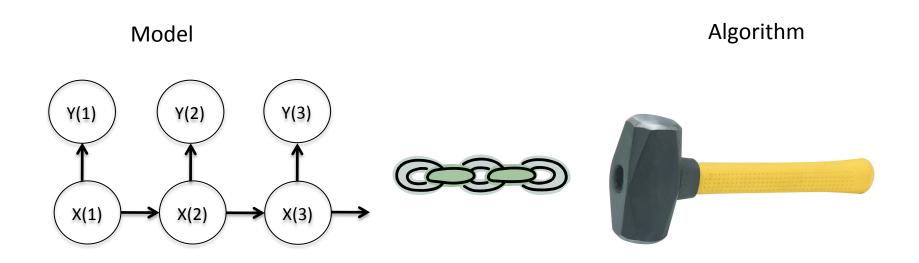
- 1. Typical R package = Model family + 1 or more algorithms
 - GLMMs: Ime4, MCMCglmm
 - GAMMs: mgcv
 - spatial models: spBayes, INLA

What can a practitioner do with hierarchical models?

Two basic software designs:

- 1. Typical R package = Model family + 1 or more algorithms
 - GLMMs: Ime4, MCMCglmm
 - GAMMs: mgcv
 - spatial models: spBayes, INLA
- 2. Flexible model + black box algorithm
 - BUGS: WinBUGS, OpenBUGS, JAGS
 - PyMC
 - INLA
 - Stan

Existing software

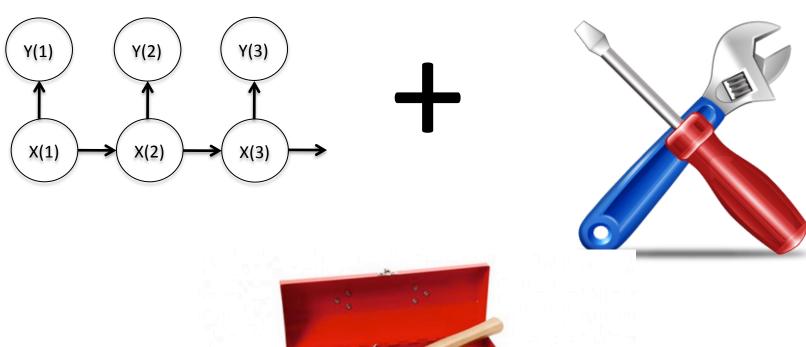


e.g., BUGS (WinBUGS, OpenBUGS, JAGS), INLA, Stan, various R packages

NIMBLE: The Goal

Model

Algorithm language

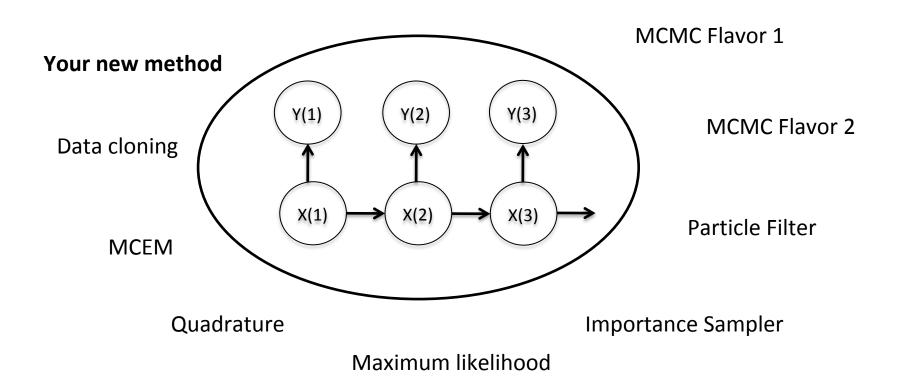






NIMBLE: extensible software for hierarchical models (r-nimble.org)

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,
- ♦ provide interface object.

NIMBLE

1. Model specification

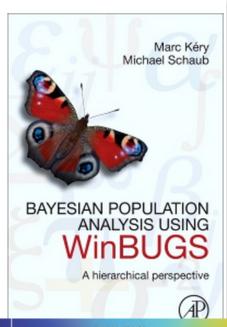
BUGS language → R/C++ model object

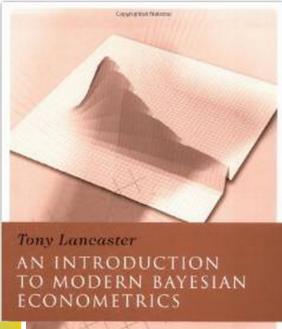
2. Algorithm library

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

3. Algorithm specification

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





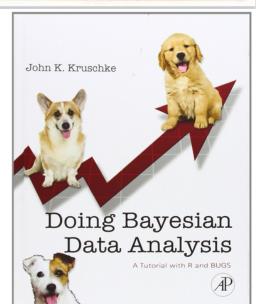
Springer Texts in Statistics

Brani Vidakovic

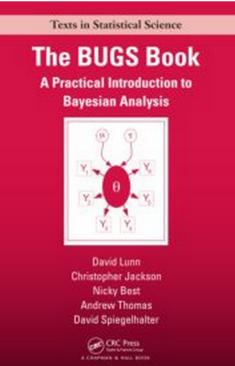
Statistics for Bioengineering Sciences

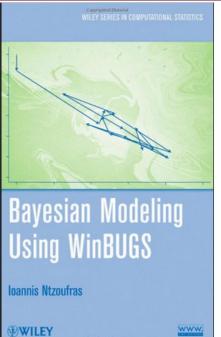
With MATLAB and WinBUGS Support





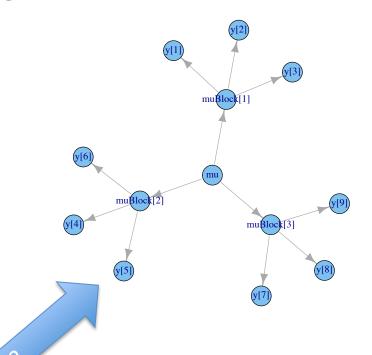
(Blockant





User Experience: Creating a Model from BUGS

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





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

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)

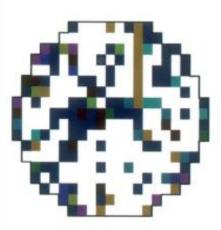


Provides variables and functions (calculate, simulate) for algorithms to use.

The Success of R

Copyrighted Material John M. Chambers Programming WITH DATA A Guide to the S Language





Programming with Models

```
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);
}</pre>
```

You give NIMBLE:

```
> 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')
```

You get this:

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(l 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);
})</pre>
```

```
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....]
...</pre>
```

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);
}</pre>
```

```
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
....</pre>
```

```
> 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

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

NIMBLE's algorithm library

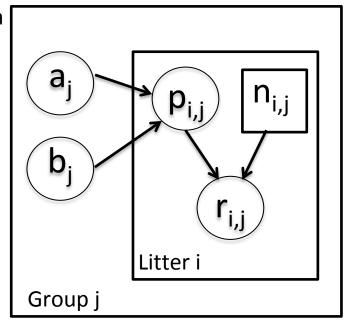
– MCMC samplers:

- 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(l 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);
}</pre>
```

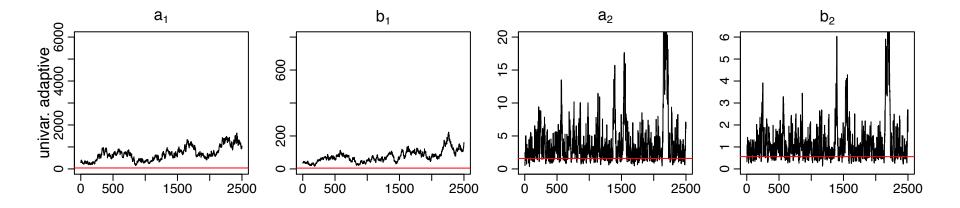


Challenges of the toy example:

- 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_i , whereas direct sampling of mu_i and theta $_i$ would be strongly preferable."
- But that's not all that's going on. Consider the dependence between the p's and their a_i, b_i hyperparameters.
- And perhaps we want to do something other than MCMC.

Default MCMC: Gibbs + Metropolis

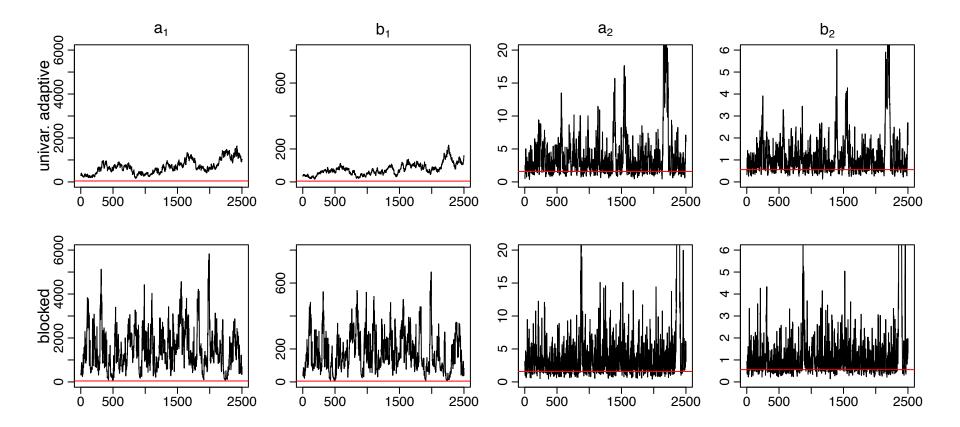
- > littersMCMCspec <- configureMCMC(littersModel, list(adaptInterval = 100))
- > littersMCMC <- buildMCMC(littersMCMCspec)
- > littersMCMC_cpp <- compileNIMBLE(littersModel, project = littersModel)
- > runMCMC(littersMCMC_cpp, niter = 10000)



Red line is MLE

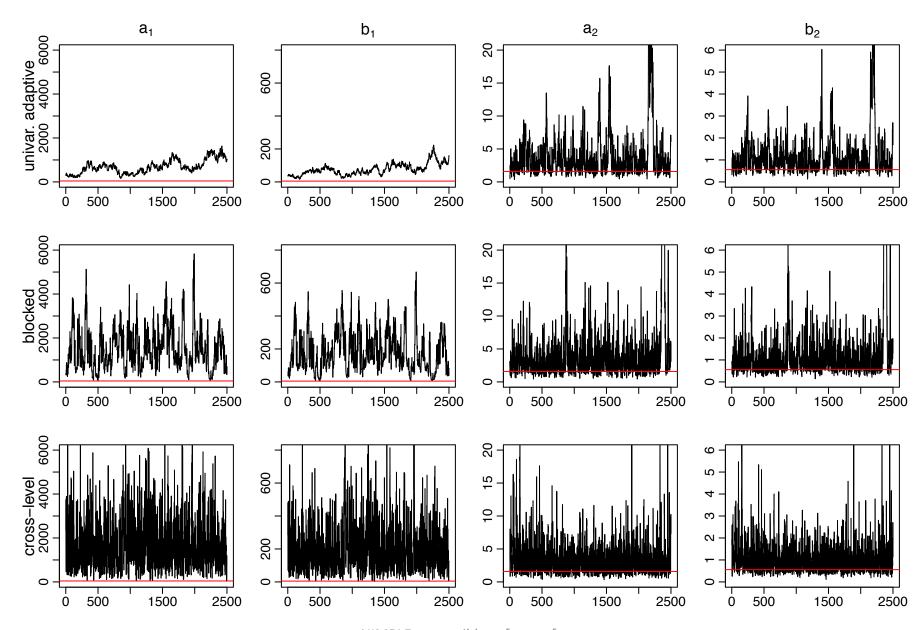
Blocked MCMC: Gibbs + Blocked Metropolis

- > 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)
- > runMCMC(littersMCMC2_cpp, niter = 10000)



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)
- > runMCMC(littersMCMC3_cpp, niter = 10000)



NIMBLE: extensible software for hierarchical models (r-nimble.org)

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.

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

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(</pre>
```

```
setup = function(model, mvSaved, targetNode, scale) {
  calcNodes <- model$getDependencies(targetNode)</pre>
},
run = function() {
  model | p initial <- calculate(model, calcNodes)
  proposal <- rnorm(1, model[[targetNode]], scale)</pre>
  model[[targetNode]] <<- proposal
  model | 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) { query model calcNodes <- model\$getDependencies(targetNode)</pre> structure run = function() { model | p initial <- calculate(model, calcNodes) proposal <- rnorm(1, model[[targetNode]], scale)</pre> model[[targetNode]] <<- proposal model | 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 ... # })

NIMBLE: Programming with Models

```
sampler myRW <- nimbleFunction(
setup = function(model, mvSaved, targetNode, scale) {
  calcNodes <- model$getDependencies(targetNode)
},
run = function() {
  model | p initial <- calculate(model, calcNodes)
  proposal <- rnorm(1, model[[targetNode]], scale)</pre>
  model[[targetNode]] <<- proposal
  model | p | proposed <- calculate(model, calcNodes)
  log_MH_ratio <- model_lp_proposed - model_lp initial</pre>
  if(decide(log_MH_ratio)) jump <- TRUE</pre>
    else
                  jump <- FALSE
  # .... Various bookkeeping operations ... #
```

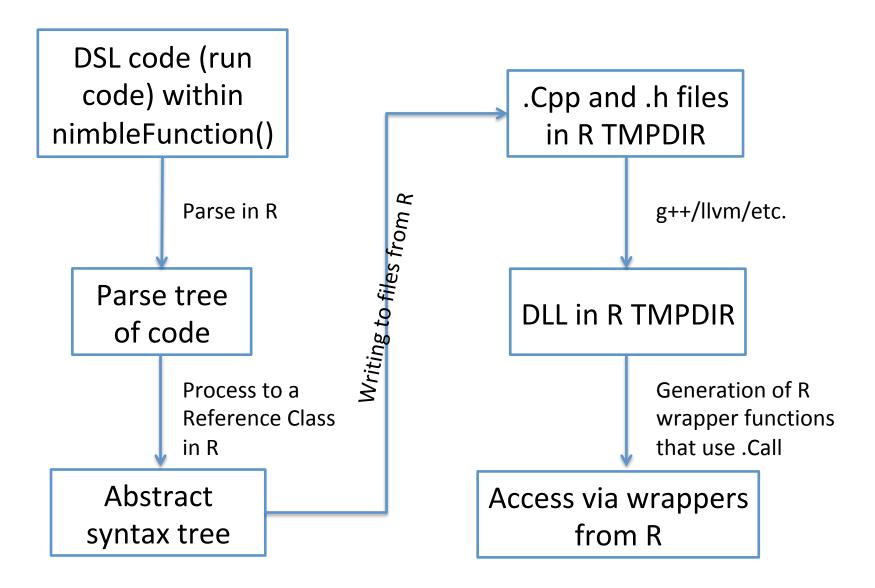
the actual (generic) algorithm

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: $p(x_t|y_{1:t}, heta)$

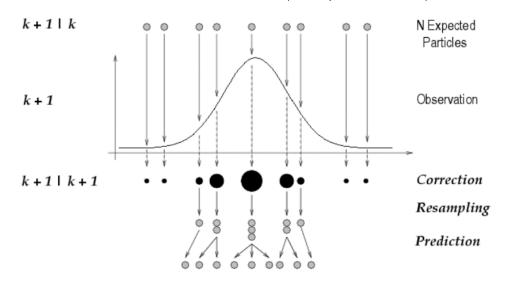


Figure 2: Particle filtering (from (Lehmann 2003))

- Weights from 'correction' step can be used to estimate $p(y_{1:t}| heta)$
- 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$latents, control =
list(saveAll = TRUE, smoothing = TRUE, lookahead = lookahead))
},
run = function() {
    modelLP0 <- modelLL0 + calculate(model, target)
    propValue <- rnorm(1, mean = model[[target]], sd = scale)</pre>
    model[[target]] <<- propValue
    modelLL1 <- my particleFilter$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) (first release a few weeks ago and more work 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?
 - We have funding for a postdoc/programmer!
 - We have funding to bring users/developers to Berkeley.
 - Announcements: <u>nimble-announce</u> Google site
 - User support/discussion: <u>nimble-users</u> Google site
 - Write an algorithm using NIMBLE!
 - Help with development of NIMBLE: email <u>nimble.stats@gmail.com</u> 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

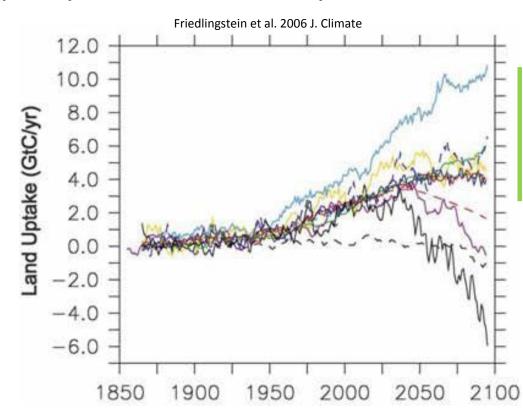
www3.nd.edu/~paleolab/paleonproject

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



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

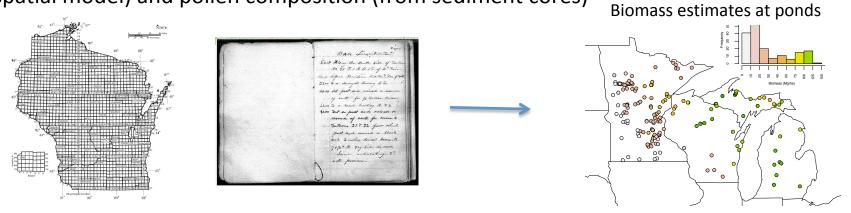
- Estimate spatially-varying composition and biomass of tree species from count and zeroinflated size data in year 1850
- Estimate temporal variations in temperature and precipitation over 2000 years from tree rings and lake/bog records
- Estimate tree composition spatially over 2000 years from fossil 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)
 - $\alpha_k = \exp(Z(b_t)\beta_k)$

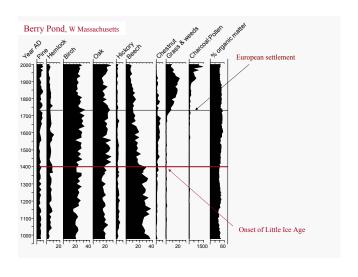
Predicting biomass from compositional data

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



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

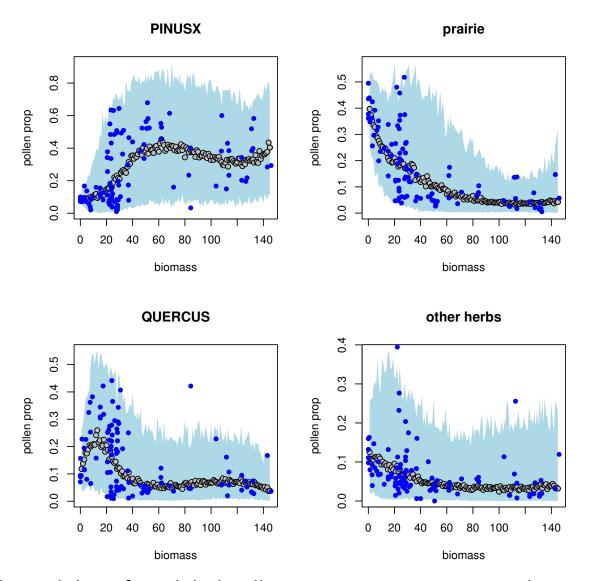




Calibration model

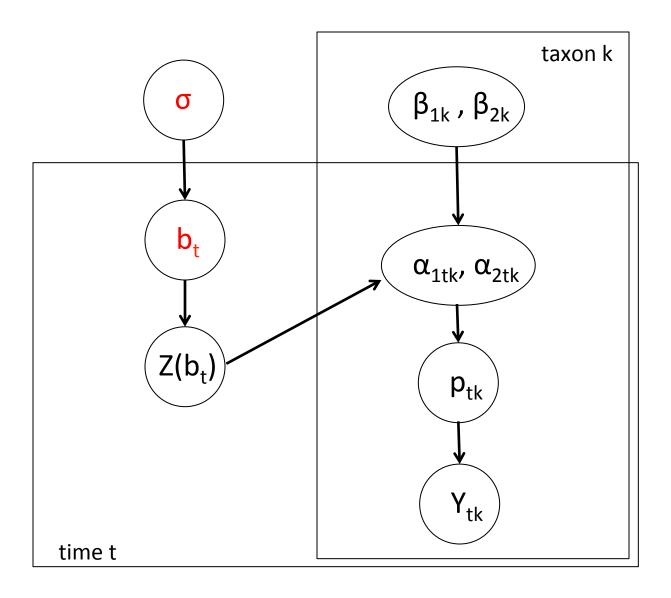
- Pollen proportion for each taxon determined by transformation of a flexible (spline) function of biomass
 - shape1 and shape2 parameters of beta distribution (stickbreaking prior for multinomial) are splines of biomass
 - Primary calibration parameters are spline coefficients
- Overdispersed multinomial 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

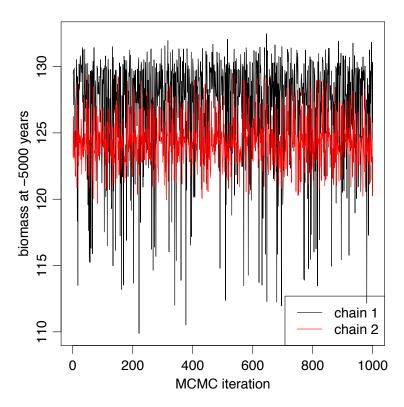
```
pollen likelihood
for(t in 1:nTimes)
    Y[t, 1] ~ dbetabin(shape1[t, 1], shape2[t, 1], n[t])
    for(k in 2:(nTaxa-1)) {
        Y[t, k] ~ dbetabin(shape1[t, k], shape2[t, k], n[t]-sum(Y[t, 1:(k-1)])
shape1[ , ] <- exp(Zb[ , ] %*% beta1[ ,])
shape2[,] <- exp(Zb[,] %*% beta2[,])
for(t in 1:nTimes)
    Zb[t, 1:nKnots] <- bspline(b[t], knots[1:nKnots])</pre>
for(t in 2:nTimes)
                                                            (nonstationary)
    b[t] \sim dGenPareto (3b[t-1]-3b[t-2]+b[t-3], sigma)
                                                            biomass evolution
sigma ~ dunif(0, 10) # Gelman (2006)
b[1] ~ dunif(0, 400)
```

MCMC performance

Mixing with data augmentation using default NIMBLF MCMC

130 125 biomass at -5000 years 120 200 400 600 800 1000 0 MCMC iteration

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+1], b[t+2], b[t+3]}, with a normal approximation to likelihood to generate good (quasi-conjugate) proposals.

PalEON Acknowledgements

- Pollen-biomass Collaborators: Ann Raiho, Jason McLachlan (Notre Dame Biology)
- PalEON investigators: Jason McLachlan (Notre Dame, PI), Mike Dietze (BU), Andrew Finley (Michigan State), Amy Hessl (West Virginia), Phil Higuera (Idaho), Mevin Hooten (USGS/ Colorado State), Steve Jackson (USGS/ Arizona), Dave Moore (Arizona), Neil Pederson (Harvard Forest), Jack Williams (Wisconsin), Jun Zhu (Wisconsin)
- NSF Macrosystems Program