Beyond the black box: Flexible algorithm programming for ecological models in NIMBLE

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Joint work with:

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https://r-nimble.org

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What do we want to do with hierarchical models?

1. More and better MCMC
- Many different samplers
- Better adaptive algorithms

2. Numerical integration
- Laplace approximation
- Adaptive Gaussian quadrature
- Hidden Markov models

3. Maximum likelihood estimation
- Monte Carlo EM
- Data cloning
- Monte Carlo Newton-Raphson

4. Sequential Monte Carlo
- Auxiliary Particle Filter
- Ensemble Kalman Filter
- Unscented Kalman Filter

5. Normalizing constants (AIC or Bayes Factors)
- Importance sampling
- Bridge sampling
- Others

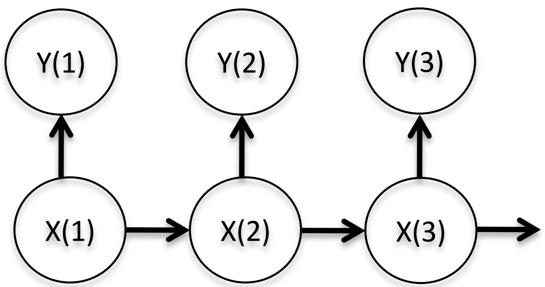
6. Model assessment
- Bootstrapping
- Calibrated posterior predictive checks
- Cross-validation
- Posterior re-weighting

7. Idea cominbations
- PF + MCMC
- Resample-move
- MCMC + Laplace/quadrature

These are just some ideas from a vast literature.

NIMBLE

Model language (BUGS/JAGS)



Algorithm Language

NIMBLE makes BUGS extensible from R:

- Add new functions
- Add new distributions
- Call external code

Goals

– Retaining BUGS compatibility
– Making BUGS more flexible
– 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

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, Chinese Restaurant Process)
  - Flexible choice of sampler for each parameter
  - User-specified blocks of parameters
  - Cross-validation, WAIC
- Sequential Monte Carlo (particle filters)
  - Various flavors
- Write your own / easily modify ours

NIMBLE in Ecology

- User-defined distributions for integrating over high-dimensional discrete latent states
  - E.g., capture-recapture, occupancy models
- Flexibility in coding numerical tricks within a BUGS model for faster computation
- User choice of samplers and blocking
- Users can modify and add custom samplers for use in combination with NIMBLE's samplers
- Useful model selection/assessment tools:
  - WAIC
  - calibrated posterior predictive p-values
  - reversible jump

Multi-state capture-recapture: geese

- N=11,200 Canada geese
- 3 locations of 'capture' (i.e., sighting)
- 4 years of data
- 153 unique sighting histories

(survival) $\phi_r \sim \text{Uniform}(0,1)$ $\quad r = 1,2,3$

(movement) $\{\psi_{1st}, \psi_{2st}, \psi_{3st}\} \sim \text{Dirichlet}(\alpha = \{1,1,1\})$ $\quad s = 1,2,3, \quad t = 2,3,4$

(detection) $p_{rt} \sim \text{Uniform}(0,1)$ $\quad r = 1,2,3, \quad t = 1,2,3,4$

$$X_{i1} = y_{i1}$$

(site location, dead) $X_{it} \mid X_{i,t-1} \sim \text{Categorical}(p = T_t \, x_{i,t-1})$ $\quad t = 2,\ldots,k$

(site observed, not seen) $Y_{it} \mid X_{it} \sim \text{Categorical}(p = Z_t \, x_{it})$ $\quad t = 1,\ldots,k$

- Data: Armstrup et al. (2010) Handbook of Capture-Recapture Analysis
- Methods: Turek et al (2016), Env. Ecol. Stat.

Multi-state capture-recapture: filtering

- 14,437 latent variables + 21 parameters
- Discrete filtering to numerically integrate (i.e., sum) over latent variables

Filtering equations

$$P_t(x) = \Pr(X_t = x \mid y_{1:t-1})$$
$$= \sum_{x_{t-1} \in \mathcal{X}} \Pr(X_t = x \mid X_{t-1} = x_{t-1}) \Pr(X_{t-1} = x_{t-1} \mid y_{1:t-1})$$

$$Q_t(x) = \Pr(X_t = x \mid y_{1:t})$$
$$= \Pr(X_t = x \mid y_{1:t-1}) \Pr(Y_t = y_t \mid X_t = x) / \Pr(Y_t = y_t \mid y_{1:t-1})$$

$$L_t = \Pr(Y_t = y_t \mid y_{1:t-1})$$
$$= \sum_{x_t \in \mathcal{X}} \Pr(Y_t = y_t \mid X_t = x_t) \Pr(X_t = x_t \mid y_{1:t-1})$$

Matrix formulation

$$P_t = T_t \, Q_{t-1}, \qquad t \geq 2$$

$$Q_t = Z_t(y_t)' * P_t \,/\, L_t, \qquad t \geq 1$$

$$L_t = Z_t(y_t) \, P_t, \qquad t \geq 1$$

Marginalized likelihood:

$$L(\theta \mid y) = L_1 L_2 \cdots L_k$$

Multi-state capture-recapture: MCMC

– Embed filtering as a user-defined distribution in BUGS code

```
code <- nimbleCode({

   ### … priors for 'p', 'phi', 'psi' ###

   Z[1:4,1:4,1:4] <- calcZ(p[1:6])
   T[1:4,1:4,1:4] <- calcT(phi[1:3], psi[1:3,1:3,1:2])

   for (i in 1:nind) {
      y[i, first[i]:k] ~ dDHMM(length = k-first[i]+1, prior = prior[1:4], condition =
condition[1:4], Z = Z[1:k,1:k,first[i]:k], useZt = 1, T = T[1:k,1:k,first[i]:k], useTt = 1,
mult = mult[i])
   }
})
```

– 70-fold improvement in MCMC (including using weighted likelihood with unique sample histories)

Multi-state capture-recapture: MCMC (2)

Easily try out various samplers

```
conf <- configureMCMC(Rmodel)                    ## setup default MCMC samplers
conf$printSamplers()
# [1]   RW sampler: p[1]
# …
# [21] RW sampler: psi[2, 3, 2]
nodes <- Rmodel$getNodeNames(stochOnly = TRUE, includeData = FALSE)
conf$removeSamplers(nodes)                        ## remove default samplers
for(node in nodes) {
   conf$addSampler(node, type = 'slice')          ## add slice samplers
}
Rmcmc <- buildMCMC(conf)                          ## build MCMC algorithm
Cmcmc <- compileNimble(Rmcmc)                     ## compile MCMC algorithm
runMCMC(Cmcmc, 10000)                             ## run MCMC
```

Easily block parameters

```
nodes <- list(c('psi[1,1,1]','psi[2,1,1]'),       ## highly-correlated parameters (corr > 0.9)
          c('psi[1,2,1]','psi[2,2,1]'),
          c('psi[1,1,2]','psi[2,1,2]'))
for(i in seq_along(nodes)) {
   conf$removeSamplers(nodes[[i]])
   conf$addSampler(nodes[[i]], type = 'RW_block')   ## use block sampling for highly-correlated parameters
}
## build, compile and run as above
```

Multi-state capture-recapture: Results

MCMC performance aggregated across 21 parameters based on effective sample size with 10,000 iterations

Metric	Filtering (Metropolis)	Filtering + Slice	Filtering + Blocking
Minimum ESS	26	106	121
Mean ESS	294	1173	340

Multi-state capture-recapture: Results

MCMC performance aggregated across 21 parameters based on effective sample size with 10,000 iterations

Metric	Filtering (Metropolis)	Filtering + Slice	Filtering + Blocking
Minimum ESS	26	106	121
Mean ESS	294	1173	340
Minimum ESS/second	0.7	0.7	5.9
Mean ESS/second	7.8	7.6	16.7

Spatial capture-recapture: voles

- Field voles in a forest in northern England
- Data from summer 2000
- N=158 tagged voles
- Spatial grid of traps: 192 traps on 11x18 grid
- 20 observation periods
- Interest lies in understanding demographics, including survival and movement

- Model for each individual:
  - Latent state: alive or dead/emigrated at each time
  - Latent activity center at each time
  - Dispersal kernel to model movement from time to time
  - Detection and survival probabilities

Work by: Daniel Turek (NIMBLE), Torbjørn Ergon (University of Oslo)

Spatial capture-recapture: computation

Computational strategies enabled by NIMBLE:

1. Custom BUGS distribution: Integrate over latent alive/dead status via discrete filtering (see goose example).
2. Custom BUGS distribution: Move computation of dispersal into a second user-defined distribution to remove parameters and reduce model size.
3. Custom BUGS function: Carefully limit computations of "trap exposure" to avoid doing all pairwise computations of probabilities of each individual being caught in each trap.

Spatial capture-recapture: computation

2. Custom BUGS distribution: Move computation of dispersal into a second user-defined distribution to remove parameters and reduce model size

Original BUGS code:

```
for(k in first[i]:(last[i]-1)) {
   theta[i, k] ~ dunif(-3.141593, 3.141593)              # dispersal direction
   d[i, k] ~ dexp(dlambda[gr[i]])                        # dispersal distance
   S[i, 1, k+1] <- S[i, 1, k] + d[i, k] * cos(theta[i, k])   # evolution of activity center
   S[i, 2, k+1] <- S[i, 2, k] + d[i, k] * sin(theta[i, k])
}
```

Revised BUGS code:

```
for(k in first[i]:(last[i]-1)) {
   S[i, 1:2, k+1] ~ dSS(S[i, 1:2, k], dlambda[gr[i]])     # direct distribution over center
}
```

Spatial capture-recapture: computation

3. Custom BUGS functions: Carefully limit computations of "trap exposure" to avoid doing all pairwise computations of probabilities of each individual being caught in each trap.

- Original BUGS code:

```
for(k in first[i]:last[i]) {
    D[i, k, 1:R] <- sqrt((S[i, 1, k] - X[1:R, 1])^2 + (S[i, 2, k] - X[1:R, 2])^2)
    g[i, k, 1:R] <- exp(-(D[i, k, 1:R]/sigma[gr[i]])^kappa[gr[i]])  # trap exposure
    G[i, k] <- sum(g[i, k, 1:R])                                   # total trap exposure
 }
```

- Revised BUGS code:
  - Replace middle line with calls to user-defined functions that implement efficient algorithms for computing only the probabilities of an individual being trapped near to the current activity center

    ```
    g[i, k, 1:R] <- calcLocalTrapExposure(localTrapIndices, …)
    ```

  - Cache determination of nearby traps as part of model graph to limit recalculation

    ```
    localTrapIndices[i, k, 1:MaxNumberLocalTraps] <- getLocalTrapIndices(…)
    ```

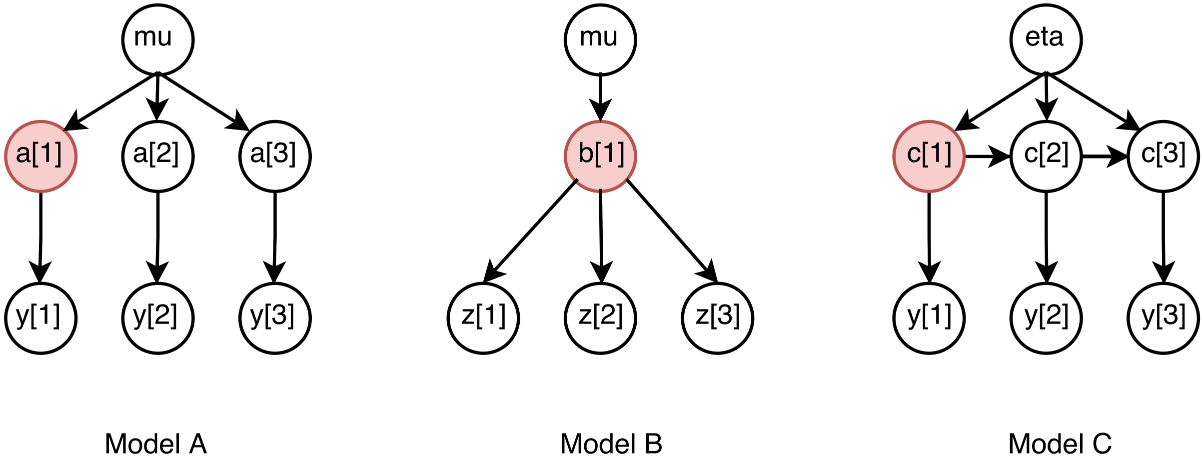
Spatial capture-recapture: computation

Time per single effectively independent sample

0. Default model (full latent state model)
   5 minutes / sample
1. Custom BUGS distribution: Integrate over latent alive/dead status via discrete filtering (see goose example).
   40 seconds / sample
2. Custom BUGS distribution: Move computation of dispersal into a second user-defined distribution to remove parameters and reduce model size.
   21 seconds / sample
3. Custom BUGS function: Carefully limit computations of “trap exposure” to avoid doing all pairwise computations of probabilities of each individual being caught in each trap.
   8 seconds per sample

Model-generic algorithm programming

Wanted: a Metropolis-Hastings sampler with normal random-walk proposals.



Challenge: It should work for any node of any model.

Solution: Two-stage evaluation.

NIMBLE: Model-generic programming

```
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: Model-generic programming

```
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   log_MH_ratio <- model_lp_proposed - model_lp_initial

    if(decide(log_MH_ratio)) jump <- TRUE
      else jump <- FALSE
    # …. Various bookkeeping operations … #    })
```

query model structure ONCE

NIMBLE: Model-generic programming

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   log_MH_ratio <- model_lp_proposed - model_lp_initial

    if(decide(log_MH_ratio)) jump <- TRUE
      else jump <- FALSE
    # .... Various bookkeeping operations ... #    })
```

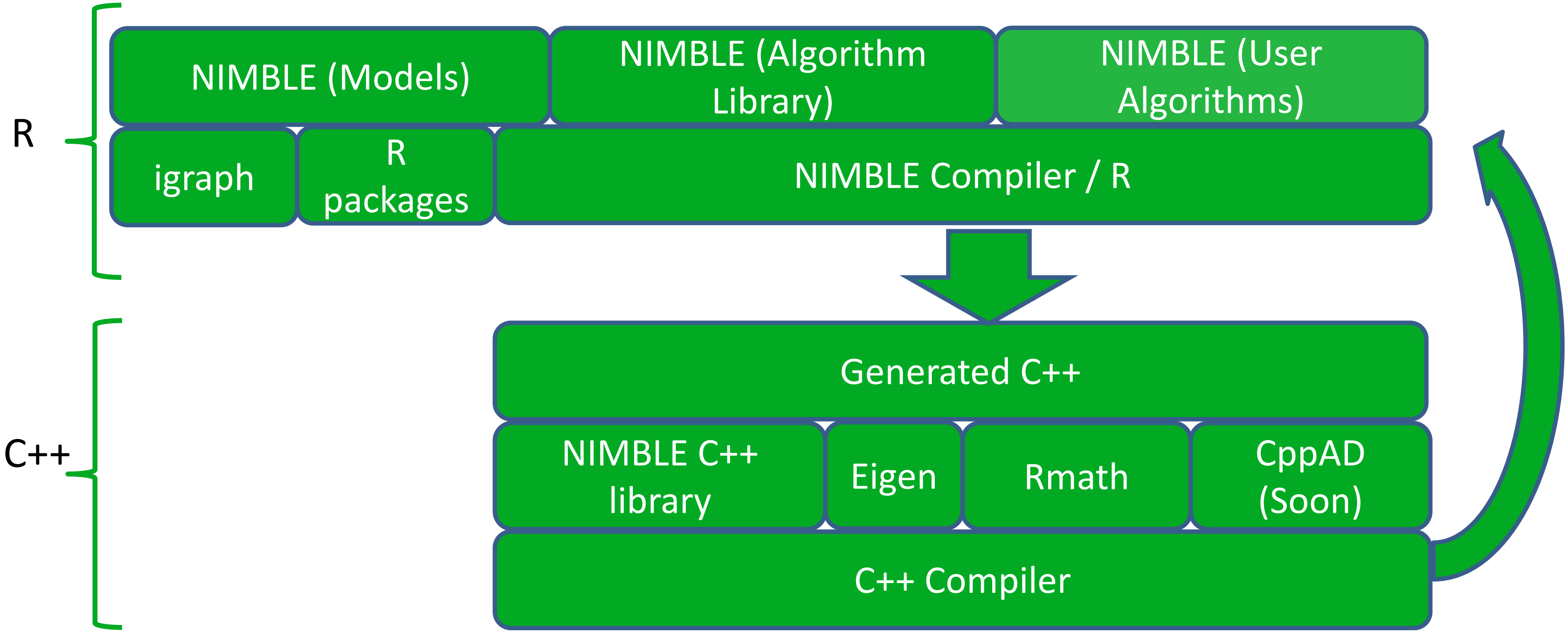
the actual (generic) algorithm

The NIMBLE compiler (run code)

<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
- Access to much of Rmath.h (e.g. distributions)
- Call out to your own C/C++ or back to R
- Many improvements / extensions planned
    - Derivatives (coming soon)

NIMBLE software stack



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)

NIMBLE in Ecology

- User-defined distributions for integrating over high-dimensional discrete latent states
  - To be provided in forthcoming nimbleEcology R package
- Flexibility in coding numerical tricks within a BUGS model for faster computation
- User choice of samplers and blocking
- Users can modify and add custom samplers for use in combination with NIMBLE's samplers
- Useful model selection/assessment tools: WAIC (in NIMBLE), calibrated posterior predictive p-values (nearing release), reversible jump (see r-nimble.org example)

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)
  - Ongoing Bayesian nonparametrics with Claudia Wehrhahn & Abel Rodriguez
  - 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, Hamiltonian MC

- Interested?
  - **We have funding for a postdoc or programmer**
  - **We have funding to bring selected users to Berkeley for intensive collaboration**
  - 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