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

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Nick Michaud         UC Berkeley Statistics and ESPM

https://r-nimble.org
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 combinations
   • PF + MCMC
   • Resample-move
   • MCMC + Laplace/quadrature

These are just some ideas from a vast literature.

NIMBLE: extensible software for hierarchical models (r-nimble.org)
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 $\rightarrow$ R/C++ model object

2. Algorithm library
   
   MCMC, Particle Filter/Sequential MC, MCEM, etc.

3. Algorithm specification
   
   NIMBLE programming language within R $\rightarrow$ 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) \( \phi_r \sim \text{Uniform}(0, 1) \) \( r = 1, 2, 3 \)

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

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

\( X_{i1} = y_{i1} \)

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

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

- Data: Armstrup et al. (2010) Handbook of Capture-Recapture Analysis
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

\[ P_t = T_t Q_{t-1}, \quad t \geq 2 \]

\[ Q_t = Z_t(y_t)' P_t / L_t, \quad t \geq 1 \]

\[ L_t = Z_t(y_t) P_t, \quad t \geq 1 \]

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

```r
code <- nimbleCode({

    ### ... priors for ‘p’, ‘phi’, ‘psi’ ###


    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

```r
conf <- configureMCMC(Rmodel)          ## setup default MCMC samplers
conf$printSamplers()

# ...
# [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

```r
nodes <- list(c('psi[1,1,1]','psi[2,1,1]'),
    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

<table>
<thead>
<tr>
<th>Metric</th>
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<td>Minimum ESS/second</td>
<td>0.7</td>
<td>0.7</td>
<td>5.9</td>
</tr>
<tr>
<td>Mean ESS/second</td>
<td>7.8</td>
<td>7.6</td>
<td>16.7</td>
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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:

```r
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:

```r
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$dependencies(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 ...
})
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 ...
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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 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)
• Call out to your own C/C++ or back to R
• Many improvements / extensions planned
  • Derivatives (coming soon)
NIMBLE: extensible software for hierarchical models (r-nimble.org)
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