Flexible Programming of Hierarchical Modeling Algorithms and Compilation of R Using NIMBLE

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http://r-nimble.org

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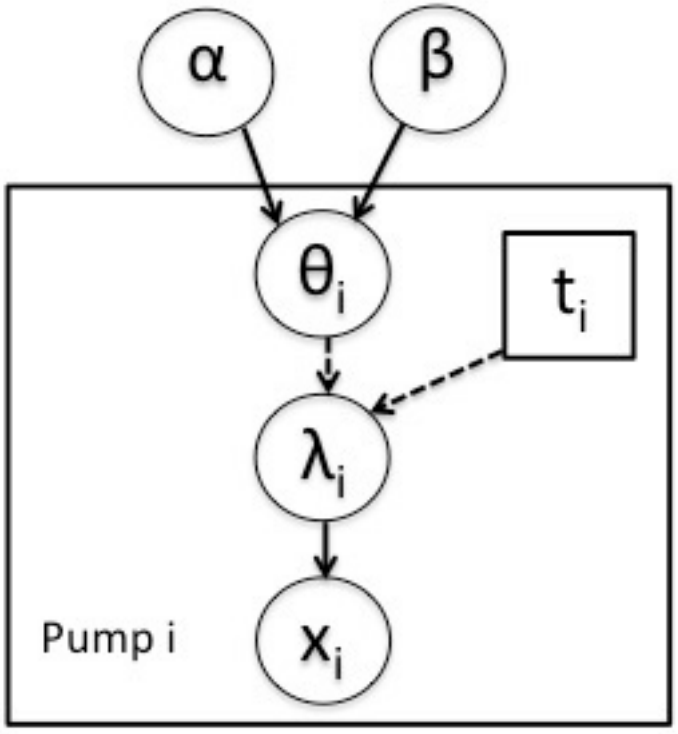
Hierarchical statistical models

A basic random effects / Bayesian hierarchical model



Probabilistic model

$$
\begin{aligned}
\alpha &\sim \text{Exp}(1) \\
\beta &\sim \text{Gamma}(0.1, 1.0) \\
\theta_i &\sim \text{Gamma}(\alpha, \beta) \\
\lambda_i &<- \theta_i t_i \\
x_i &\sim \text{Poisson}(\lambda_i)
\end{aligned}
$$

Hierarchical statistical models

A basic random effects / Bayesian hierarchical model

BUGS DSL code

```
# priors on hyperparameters
alpha ~ dexp(1.0)
beta ~ dgamma(0.1,1.0)
for (i in 1:N){
    # latent process (random effects)
    # random effects distribution
    theta[i] ~ dgamma(alpha,beta)
    # linear predictor
    lambda[i] <- theta[i]*t[i]
    # likelihood (data model)
    x[i] ~ dpois(lambda[i])
}
```

Probabilistic model

$$
\begin{aligned}
\alpha &\sim \text{Exp}(1) \\
\beta &\sim \text{Gamma}(0.1, 1.0) \\
\theta_i &\sim \text{Gamma}(\alpha, \beta) \\
\lambda_i &<- \theta_i t_i \\
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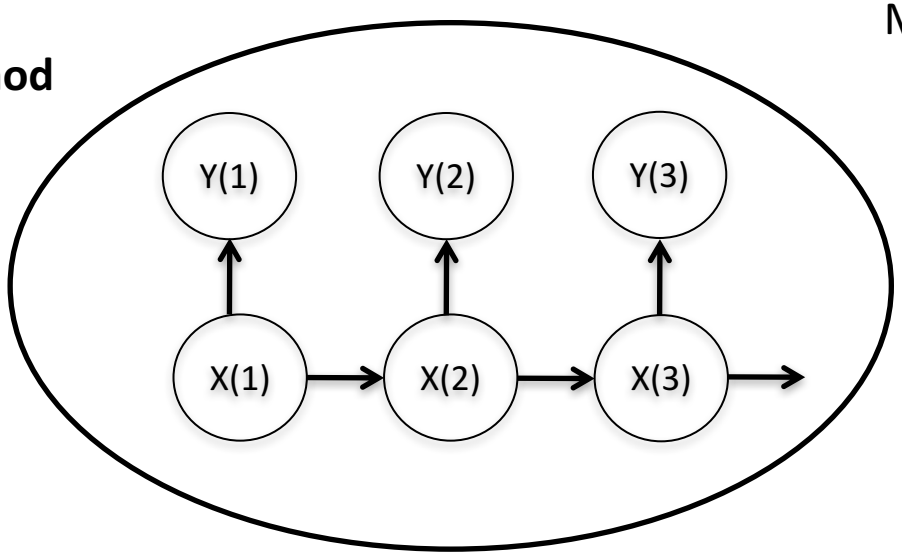
\end{aligned}
$$

Divorcing model specification from algorithm



Your new method

MCMC Flavor 1

MCMC Flavor 2

Particle Filter

Importance Sampler

Maximum likelihood

Quadrature

MCEM

Variational Bayes

What can a practitioner do with hierarchical models?

Two basic software designs:

1. Typical R/Python 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:

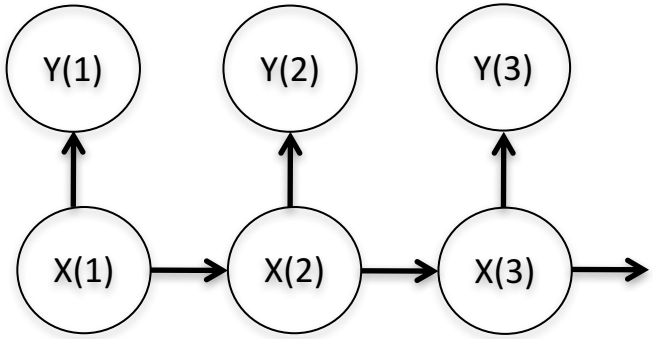
1. Typical R/Python package = Model family + 1 or more algorithms
   - GLMMs: lme4, MCMCglmm
   - GAMMs: mgcv
   - spatial models: spBayes, INLA

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

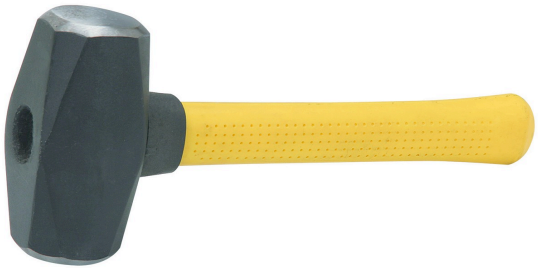
Existing software

Examples: BUGS (WinBUGS, OpenBUGS, JAGS), INLA, Stan

Model



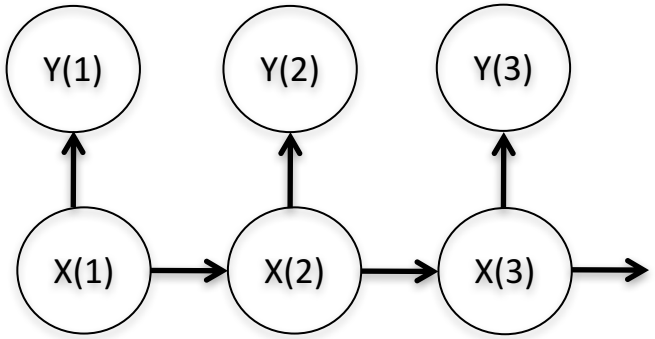
Algorithm



Widely used in various disciplines: environmental sciences, social sciences, biomedical/health sciences, statistics

NIMBLE: The Goal

Model



+

Algorithm language

=

NIMBLE philosophy

- Combine flexible model specification with flexible algorithm programming, while
  - Retaining BUGS DSL 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 components

1. Hierarchical model specification

   BUGS language ➔ R/C++ model object

2. Algorithm library

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

3. Algorithm programming via nimbleFunctions

   NIMBLE programming language (DSL) within R ➔ R/C++ algorithm object

NIMBLE: programming with models

You give NIMBLE BUGS DSL code:

```
pumpCode <- nimbleCode( {
  # priors on hyperparameters
  alpha ~ dexp(1.0)
  beta ~ dgamma(0.1,1.0)
  for (i in 1:N){
    theta[i] ~ dgamma(alpha,beta)
    lambda[i] <- theta[i]*t[i]
    x[i] ~ dpois(lambda[i])
  }
} )
```

You get a programmable model object:

```
> pumpModel$theta[1] <- 5              # set values in model
> simulate(pumpModel, 'theta')         # simulate from prior
> beta_deps <- pumpModel$getDependencies('beta')    # model
structure
> calculate(pumpModel, beta_deps)  # calculate probability density
> getLogProb(pumpModel, 'theta')
```

User experience: specializing an algorithm to a model

```
pumpCode <- nimbleCode( {
  alpha ~ dexp(1.0)
  beta ~ dgamma(0.1,1.0)
  for (i in 1:N){
    theta[i] ~ dgamma(alpha,beta)
    lambda[i] <- theta[i]*t[i]
    x[i] ~ dpois(lambda[i])
  }
} )
```

```
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….]
…
```

```
> pumpMCMCconf <- configureMCMC(pumpModel)
> pumpMCMCconf$printSamplers()
[1]  RW sampler: alpha
[2]  conjugate_dgamma_dgamma sampler: beta
[3]  conjugate_dgamma_dpois sampler: theta[1]
 [...snip...]
> pumpMCMCconf$addSampler('alpha', 'slice', list(adaptInterval = 100))
> pumpMCMCconf$removeSamplers('beta')
> pumpMCMCconf$addSampler('beta', 'slice', list(adaptInterval = 100))
> pumpMCMCconf$addMonitors('theta')
> pumpMCMC <- buildMCMC(pumpMCMCspec)
> pumpMCMC_Cpp <- compileNimble(pumpMCMC, project = pumpModel)
> pumpMCMC_Cpp$run(20000)
```

NIMBLE system components

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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
- Sequential Monte Carlo (particle filters)
  - Various flavors
- MCEM
- Write your own

NIMBLE system components

1. Hierarchical model specification

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Using nimbleFunctions for algorithms

Users can write nimbleFunctions for use with statistical models to:

- Code their own algorithms
- Create user-defined MCMC samplers for use in NIMBLE's MCMC engine
- Write distributions and functions for use in BUGS code

nimbleFunctions that work with models have two components:

- setup function that is written in R and provides information to specialize an algorithm to a model
- run function that encodes generic execution of algorithm on arbitrary model

NIMBLE: programming with models

```
sampler_myMetropolis_RandomWalk <- 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) {
   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 … #    })
```

query model structure ONCE (R code)

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 (NIMBLE DSL)

Using nimbleFunctions to compile R

R code for a Markov chain

```
mc <- function(n, rho1, rho2) {
   path <- rep(0, n)              # initialize
   path[1:2] <- rnorm(2)
   for(i in 3:n)                  # propagate forward in time
      path[i] <- rho1*path[i-1] + rho2*path[i-2] + rnorm(1)
   return(path)
}
```

NIMBLE code

```
nim_mc <- nimbleFunction(
  run = function(n = double(0), rho1 = double(0), rho2 = double(0)) {
     returnType(double(1))
     path <- numeric(n, init = FALSE)
     path[1:2] <- rnorm(2)
     for(i in 3:n)
          path[i] <- rho1*path[i-1] + rho2*path[i-2] + rnorm(1)
     return(path)
})
```

NIMBLE DSL

Compile to C++ (and then to executable)

```
cnim_mc <- compileNimble(nim_mc)
```

Using nimbleFunctions to compile R

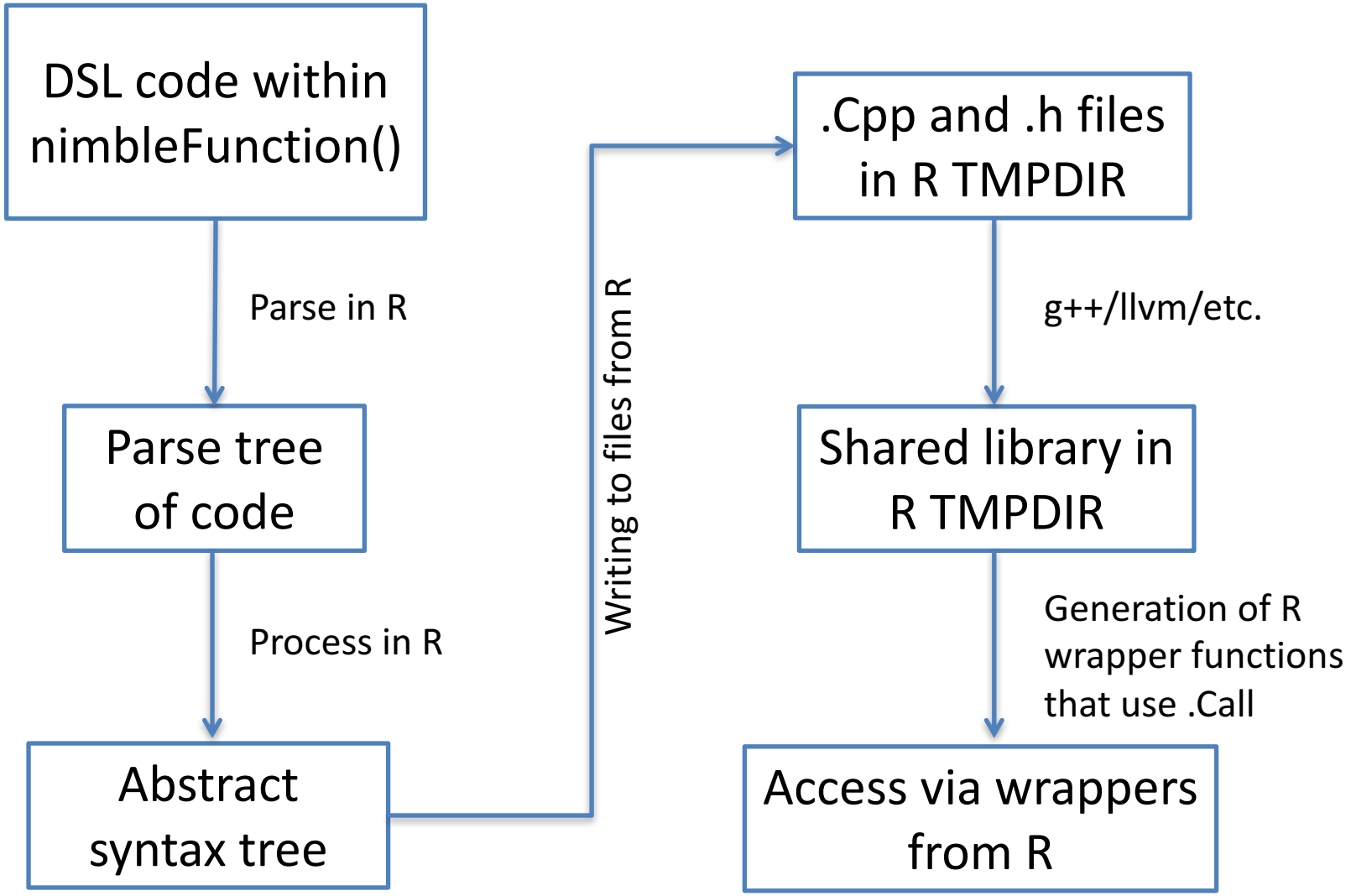
```
cnim_mc<- compileNimble(nim_mc)
#g++ -I/usr/share/R/include -DNDEBUG -DEIGEN_MPL2_ONLY=1 -
I"/home/paciorek/R/x86_64/3.2/nimble/include"     -fpic  -g -O2 -fstack-protector --
param=ssp-buffer-size=4 -Wformat -Werror=format-security -D_FORTIFY_SOURCE=2 -g  -c
P_1_rcFun_4.cpp -o P_1_rcFun_4.o
#g++ -shared -L/usr/lib/R/lib -Wl,-Bsymbolic-functions -Wl,-z,relro -o
P_1_rcFun_09_02_02.so P_1_rcFun_4.o -L/home/paciorek/R/x86_64/3.2/nimble/CppCode -
Wl,-rpath=/home/paciorek/R/x86_64/3.2/nimble/CppCode -lnimble -L/usr/lib/R/lib -lR

n <- 1e6
rho1 <- .8; rho2 <- .1
set.seed(0)
system.time( path1 <- mc(n, rho1, rho2) )    # original R version
#   user  system elapsed
#  3.883   0.001   3.883
set.seed(0)
system.time( path2 <- cnim_mc(n, rho1, rho2) )   # compiled version
#   user  system elapsed
#  0.070   0.004   0.074
> identical(path1, path2)
[1] TRUE
```

The NIMBLE compiler (NIMBLE DSL 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 DSL code is compiled in NIMBLE



Key steps in compiling R -> C++

nf <- nimbleFunction(…)

Generate **custom class definition**

Evaluate setup code in R (possible for multiple cases)

Symbol table initiated from setup code results

Run function and other member functions converted to **Abstract Syntax Tree (AST)**.

Partial evaluation of some functions (mostly for generic model uses).

AST transformed and annotated:
- Types inferred
- Symbol table populated
- Sizes tracked as expressions
- Resizing and size-checking calls inserted
- Intermediate variables inserted
- Labeling for Eigen compatibility
- Insertion of Eigen matrix / map setup

Creation of object to **manage C++ function/class content**.
- Also creates AST for C function for .C()
- Includes generic void* system to access any member data easily from R.

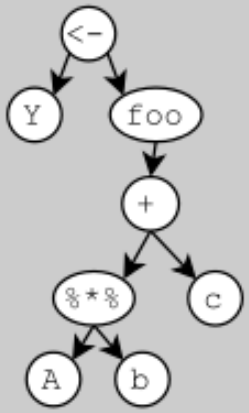
Write .cpp and .h files and compile them

Generate class definition to **access function or object(s) of compiled code**
- creates natural R calls
- allows natural access to C++ member data

Compilation steps

(a) Original NIMBLE code: `Y <- foo(A %*% b + c) ## %*% is matrix multiplication in R`

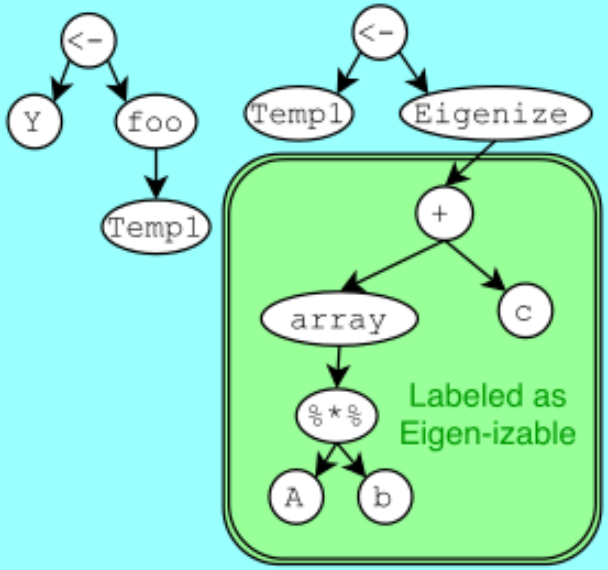
(b): Create Abstract Syntax Tree (AST)



(c): Label types at every AST vertex (not shown)

(d). Add Y to symbol table if needed

(e). Label for Eigen and transform as needed



(f). Add Temp1 and necessary Eigen variables to symbol table.

Future

Annotate and transform AST for

- distributed processing
- automatic differentiation

(g) Final C++

```
double Y;
NimbleArray<2, double> Temp1;
EigenMap Eig_Temp1, Eig_A, Eig_b, Eig_c;
// pointer and resizing details omitted
Temp1 = (Eig_A * Eig_b).array() + Eig_c;
Y = foo(Temp1);
```

Basic example: calls from R

```
> nim_mc
function (n, rho1, rho2)
{
   path <- nimNumeric(n, init = FALSE)
   path[1] <- rnorm(1)
   path[2] <- rnorm(1)
   for (i in 3:n) path[i] <- rho1 * path[i - 1] + rho2 * path[i - 2] + rnorm(1)
   return(path)
}

> cnim_mc
function (n, rho1, rho2)
{
   if (is.null(CnativeSymbolInfo_)) {
      warning("Trying to call compiled nimbleFunction that does not exist (may have been cleared).")
      return(NULL)
   }
   ans <- .Call(CnativeSymbolInfo_, n, rho1, rho2)
   ans <- ans[[4]]
   ans
}
```

Basic example: generated C++ code

```
NimArr<1, double>  rcFun_2 ( double ARG1_n_, double ARG2_rho1_, double ARG3_rho2_ )  {
  NimArr<1, double> path;
  double i;
  path.initialize(0, false, true, true, ARG1_n_);
  path[0] = rnorm(0, 1);
  path[1] = rnorm(0, 1);
  for(i=3; i<= static_cast<int>(ARG1_n_); ++i) {
    path[(i) - 1] = (ARG2_rho1_ * path[(i - 1) - 1] + ARG3_rho2_ * path[(i - 2) - 1]) + rnorm(0, 1);
  }
  return(path);
}

SEXP  CALL_rcFun_4 ( SEXP S_ARG1_n_, SEXP S_ARG2_rho1_, SEXP S_ARG3_rho2_ ) {
  // ...
}
```

Basic example using Eigen for vectorization

Uncompiled nimbleFunction (DSL) code

```
example_vec <- nimbleFunction(
    run = function(x = double(1)) {
        returnType(double(1))
        out <- acos(tanh(x))
        return(out)
})
```

Compiled C++ code

```
NimArr<1, double>  rcFun_5 ( NimArr<1, double> & ARG1_x_ ) {
        NimArr<1, double> out;
        Map<MatrixXd> Eig_out(0,0,0);
        EigenMapStr Eig_ARG1_x_Interm_1(0,0,0, EigStrDyn(0, 0));
        out.setSize(ARG1_x_.dim()[0]);
        new (&Eig_out) Map< MatrixXd >(out.getPtr(),ARG1_x_.dim()[0],1);
        new (&Eig_ARG1_x_Interm_1) EigenMapStr(ARG1_x_.getPtr() +
        static_cast<int>(ARG1_x_.getOffset() + static_cast<int>(0)),ARG1_x_.dim()[0],1,EigStrDyn(0,
        ARG1_x_.strides()[0]));
        Eig_out = (((Eig_ARG1_x_Interm_1).array()).unaryExpr(std::ptr_fun<double, double>(tanh))).acos();
return(out);
}
```

Compiler extensibility

- Compiler is written in R with extensibility in mind.
- Adding new functions requires/allows:
  - Possible syntax modification
  - A function to annotate AST with appropriate sizes and types (can be an existing function or a new one)
  - Determination of C++ output format
  - Other details
- Adding new types is more involved.
- Goal is to automate /isolate some extensibility steps.

Goals for extending NIMBLE

- Advanced math
  - Automatic differentiation (generate code to use existing C++ CppAD library): well underway
  - More linear algebra (sparsity and more)
- Advanced computing
  - Parallelization via compilation to Tensorflow (in place of Eigen): initial steps done
  - More modular compilation units
  - More native use of R objects in C++ (less copying)
- Scalability
  - Faster R processing of model and algorithm code
  - Vectorization of algorithms for replicated model nodes
- More algorithms

Interested?

- Version 0.6-6 on R package repository (CRAN)
- Lots of information (manual, examples, etc.) on r-nimble.org
- Development: github.com/nimble-dev/nimble
- Announcements: nimble-announce Google site
- User support/discussion: nimble-users Google site